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Heat and solute diffusion with a moving interface: a boundary element approach

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Abstract—A boundary element model to deal with heat and solute diffusion involving a moving interface is presented. The problem requires the solution of two parabolic partial differential equations in variable domains separated by a moving interface, whose temperature and velocity, as well as the concentration jump across it, are not know *a priori* but have to be determined as part of the solution. Moreover, the temperature of the interface is concentration-dependent while its velocity depends on both temperature and concentration gradients. To validate the scheme a test problem, which has an explicit similarity solution (analytical), is considered. Numerical results show that the boundary element method is very accurate, especially in regard to the concentration jump across the interface. © 1998 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

Many engineering processes are modelled as moving boundary problems, where a set of partial differential equations are to be solved for a domain whose boundaries are moving as a consequence of the dynamics of the internal process. Such problems are widely, but no exclusively, encountered in the metal, glass, plastic and oil industries. However, moving boundary, or Stefan, problems have been, for many decades, synonymous with phase change and diffusion problems. Due to their complexity, analytical solutions are impossible to obtain, with the exception of relatively simple cases, and therefore, recourse is often made to numerical techniques, such as Finite Differences (FDM), Control Volume (CVM), Finite Elements (FEM) and Boundary Elements (BEM) Methods [1].

Unlike the classical Stefan problem alloy phase change involves coupled partial differential equations for both heat and solute transfer. This is a moving boundary problem in which the equations of heat and mass transfer are coupled through the conditions at the phase boundary. This situation is more complicated than the classical Stefan problem, or phase change in pure substances, in which the temperature at the moving boundary is known. Phase-change in alloy systems can be efficiently computed, in an average sense at the macroscopic scale, using 'fixed domain methods' [2]. However, when a more accurate evolution of the interface is required, the so-called 'front tracking methods' are more appropriate [2]. Furthermore, not all Stefan-type problems can be reformulated in a rigorously justified 'weak form', let alone the convergence of a fixed domain numerical solution associated with it [3].

In recent years, the boundary element method has emerged as a powerful technique for many problems particularly those with variable and extended domains, since only discretization of the boundary is necessary [4]. In this paper a boundary element based technique to deal with such superposed Stefan problems is presented. In order to validate the scheme a problem which has an analytical solution is considered [5]. The numerical results are in good agreement with the analytical solution and that obtained with other numerical methods. This gave some confidence in the applicability of the method to more general situations where analytical solutions are impossible to obtain.

2. BOUNDARY INTEGRAL FORMULATION

Consider the following diffusion equation, defined over a time-dependent domain $\Omega(t)$:

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = \alpha \nabla^2 u(\mathbf{x}, t) \quad \text{for } \mathbf{x} \in \Omega(t) \tag{1}$$

with certain conditions, of Dirichlet, Neumann or mixed types, on the boundary $\Gamma = \partial\Omega$. An integral

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NOMENCLATURE

c	heat capacity per unit volume
C	concentration
d	chemical diffusivity
K	thermal conductivity
s	position of the moving interface
t	time
T	temperature
u	field variable, which can be concentration or temperature
v	velocity of the moving interface
x	space coordinate.

Greek symbols

α	thermal/chemical diffusivity
λ	latent heat of phase change
ξ	source/collation point
ω	a relaxation parameter.

Subscripts/superscripts

0	initial condition ($t = 0$)
$j = 1, 2$	homogenous region/domain index
k	iteration index
n	time step index.

equation corresponding to (1) over the entire space-time domain can be obtained from the general weighted residual statement:

$$\int_{t_0}^{\tau} \mathrm{d}t \int_{\Omega(t)} u^* \left(\alpha \nabla^2 u - \frac{\partial u}{\partial t}\right) \mathrm{d}\Omega = 0 \tag{2}$$

where u^* is the free-space Green's function, or fundamental solution, given by:

$$u^*(\xi, \mathbf{x}, \tau, t) = \frac{1}{[4\pi\alpha(\tau - t)]^{D/2}} \exp\left\{-\frac{r^2}{4\alpha(\tau - t)}\right\} \tag{3}$$

which is the solution of:

$$\frac{\partial u^*}{\partial t} + \alpha \nabla^2 u^* = -\delta(\xi - \mathbf{x})\delta(\tau - t) \tag{4}$$

where δ denotes the Dirac delta function, D is the dimension of the problem, and $r = \|\xi - \mathbf{x}\|$ is the Euclidian distance between the field point $\mathbf{x}$ and the source point ξ. Using Green's second identity and making use of the Reynolds transport theorem, the integral representation of (1) is obtained in the form [6–13]:

$$\beta(\xi)\, u(\xi, \tau) = \alpha \int_{t_0}^{\tau} \mathrm{d}t \int_{\Gamma(t)} \left[u^* \frac{\partial u}{\partial n} - u \frac{\partial u^*}{\partial n} + \frac{1}{\alpha} u u^* \mathbf{\dot{v}} \cdot \mathbf{\dot{n}}\right] \mathrm{d}\Gamma + \int_{\Omega(t_0)} u^* u \, \mathrm{d}\Omega \tag{5}$$

where $\mathbf{\dot{v}}$ is the rate of boundary motion in the outward normal direction $\mathbf{\dot{n}}$, and $\beta(\xi)$ is a constant which depends on the position of the source point ξ, the smoothness and shape of the boundary [14].

3. APPLICATION TO SUPERPOSED STEFAN PROBLEMS

Consider a problem in which two substances diffuse simultaneously into a domain $\Omega = \Omega_1 \bigcup \Omega_2$, where Ω_1 and Ω_2 are two homogeneous adjacent domains separated by a moving interface $s(t)$. This self-similar, superposed, Stefan problem occurs in many fields of science and engineering, for instance in precipitant–protein systems, where the crystal protein is grown with a precipitating agent such as salt [15]. It can also be seen as a model for binary-phase change [3]. However, the numerical aspects in both cases remain the same, consisting of solving two diffusion partial differential equations in each region and insuring mass and energy balance across the interface. Without further probe into the merits and application of such formulation, and since this paper focus on the problem from the numerical point of view, let us consider the same system of equations considered by previous authors [5, 16–18]. It consists of heat and concentration diffusion through two different regions separated by a moving interface; the problem is governed by:

$$c_j \frac{\partial T_j}{\partial t} = K_j \frac{\partial^2 T_j}{\partial x^2}; \quad \frac{\partial C_j}{\partial t} = d_j \frac{\partial^2 C_j}{\partial x^2}, \quad \text{for } (x, t) \in \Omega_j(t), \quad j = 1, 2 \tag{6}$$

where $T_j(x, t)$ and $C_j(x, t)$ refer to temperature and concentration at position x at time t, respectively; $\Omega_1(t) = \{(x, t) : 0 \leqslant x \leqslant s(t), t > 0\}$ and $\Omega_2(t) = \{(x, t) : s(t) \leqslant x \leqslant a, t > 0\}$; K, c and d refer to thermal conductivity, heat capacity/unit volume and chemical diffusivity, respectively. The initial and boundary conditions are:

$$T_2(x, t_0) = T_0, \quad C_2(x, t_0) = C_0, \quad s(t_0) = 0 \tag{7}$$

$$\begin{cases} p_1^T T_1 + f_1^T \partial T_1/\partial x = F_1^T(t) \\ p_1^c C_1 + f_1^c \partial C_1/\partial x = F_1^c(t) \end{cases} \quad \text{at } x = 0 \tag{8}$$

$$\begin{cases} p_2^T T_2 + f_2^T \partial T_2/\partial x = F_2^T(t) \\ p_2^c C_2 + f_2^c \partial C_2/\partial x = F_2^c(t) \end{cases} \quad \text{at } x = a \tag{9}$$

where F_1^T, F_1^c, F_2^T and F_2^c are known functions and

$p_1^T, f_1^T, p_1^c, f_1^c, p_2^T, f_2^T, p_2^c, f_2^c$ are real constants. At the interface, $x = s(t)$, we have

$$T_1(s(t),t) = T_2(s(t),t) = h_1[C_1(s(t),t)] = h_2[C_2(s(t),t)] \quad (10)$$

$$\lambda\frac{\mathrm{d}s}{\mathrm{d}t} = K_1\left.\frac{\partial T_1}{\partial x}\right|_{x=s(t)} - K_2\left.\frac{\partial T_2}{\partial x}\right|_{x=s(t)} \quad (11)$$

$$[C_1(s,t)-C_2(s,t)]\frac{\mathrm{d}s}{\mathrm{d}t} = -d_1\left.\frac{\partial C_1}{\partial x}\right|_{x=s(t)} + d_2\left.\frac{\partial C_2}{\partial x}\right|_{x=s(t)} \quad (12)$$

where h_1 and h_2 are two known functions (e.g., in the case of alloy phase change, these functions are derived from the phase diagram as the solidus and liquidus curves); λ is the latent heat of melting/solidification per unit volume.

Defining a new variable $u_j(x,t)$, which could represent either $T_j(x,t)$ or $C_j(x,t)$ and applying equation (5) to any region Ω_j, bounded by the boundaries X_j^1 and X_j^2, the following can be written:

$$\beta(\xi)u_j(\xi,t_n) = \alpha_j\int_{t_0}^{t_n}\left[u_j^*(\xi,x,t_n,t)\bar{u}_j(x,t) - u_j(x,t)\bar{u}_j^*(\xi,x,t_n,t) + \frac{1}{\alpha_j}u_j(x,t)u_j^*(\xi,x,t_n,t)\frac{\mathrm{d}x}{\mathrm{d}t}\right]_{X_j^1(t)}^{X_j^2(t)}\mathrm{d}t + \psi_j^u(\xi,t_n) \quad (13)$$

where $\alpha_j = K_j/c_j$ or $\alpha_j = d_j$ if u_j represents T_j or C_j, respectively; $\bar{u}_j := \partial u_j/\partial x$, $\bar{u}_j^* = \partial u_j^*/\partial x$,

$$u_j^*(\xi,x,t_n,t) = \frac{1}{\sqrt{4\pi\alpha_j(t_n-t)}}\exp\left\{-\frac{|\xi-x|^2}{4\alpha_j(t_n-t)}\right\} \quad (14)$$

and

$$\psi_2^u(\xi,t_n) = \int_0^a u_2(x,0)u_2^*(\xi,x,t_n\,0)\,\mathrm{d}x, \quad \psi_1^u(\xi,t_n) = 0. \quad (15)$$

Equation (13) is general and applies to the case where both X_j^1 and X_j^2 are moving. Applying (13) to the case in hand (i.e., $X_1^1 = 0$, $X_1^2 = X_2^1 = s(t)$ and $X_2^2 = a$) and taking ξ to the boundaries of each domain Ω_j and assuming a step-wise variation of the variable u and its derivatives, and a linear propagation of the moving boundary $s_n = s_{n-1} + v_n(t_n - t_{n-1})$, within each time step, the following system for the time step $t_n = t_{n-1} + \Delta t$ is obtained:

$$\frac{1}{2}u_\xi^n = \alpha_1\sum_{i=0}^{n} g_1(\xi,s_n,t_n,t_i)\left(\bar{u}_{s^-}^i + \frac{1}{\alpha_1}v_i u_{s^-}^i\right) - u_{s^-}^i h_1(\xi,s_n,t_n,t_i) - \alpha_1\sum_{i=0}^{n} g_1(\xi,0,t_n,t_i)\bar{u}_0^i - u_0^i h_1(\xi,0,t_n,t_i) + \psi_1^u(\xi,t_n); \quad \xi = 0, s^- \quad (16)$$

$$\frac{1}{2}u_\xi^n = -\alpha_2\sum_{i=0}^{n} g_2(\xi,s_n,t_n,t_i)\left(u_{s^+}^i + \frac{1}{\alpha_2}v_i u_{s^+}^i\right) - \bar{u}_{s^+}^i h_2(\xi,s_n,t_n,t_i) + \alpha_2\sum_{i=0}^{n} g_2(\xi,a,t_n,t_i)\bar{u}_a^i - u_a^i h_2(\xi,a,t_n,t_i) + \psi_2^u(\xi,t_n); \quad \xi = s^+, a \quad (17)$$

where Δt denotes the time step length, $u_0^k = u_1(0,t_k)$, $u_{s^-}^k = u_1(s,t_k)$, $u_{s^+}^k = u_2(s,t_k)$, $u_a^k = u_2(a,t_k)$, $\bar{u}_0^k = (\partial u_1/\partial x)(0,t_k)$, $\bar{u}_{s^-}^k = (\partial u_1/\partial x)(s,t_k)$, $\bar{u}_{s^-}^k = (\partial u_2/\partial x)(s,t_k)$, $\bar{u}_a^k = (\partial u_2/\partial x)(a,t_k)$, $s_n = s(t_n)$, $v_n = (\mathrm{d}s/\mathrm{d}t)(t_n)$ and

$$g_j(\xi,s,\tau,t_i) = \int_{t_{i-1}}^{t_i} u_j^*(\xi,s(t),\tau,t)\,\mathrm{d}t,$$

$$h_j(\xi,s,\tau,t_i) = \int_{t_{i-1}}^{t_i} \bar{u}_j^*(\xi,s(t),\tau,t)\,\mathrm{d}t. \quad (18)$$

The integrals in (18) can be calculated analytically (see appendix for details). After some manipulation of (16) and (17) and using a matrix form, for every time step n, a system of equations must be solved:

$$\begin{bmatrix}\mathbf{H}_{1u}^n & \mathbf{0}\\ \mathbf{0} & \mathbf{H}_{2u}^n\end{bmatrix}\mathbf{u}^n + \begin{bmatrix}\bar{\mathbf{H}}_{1u}^n & \mathbf{0}\\ \mathbf{0} & \bar{\mathbf{H}}_{2u}^n\end{bmatrix}\bar{\mathbf{u}}^n = \begin{bmatrix}\mathbf{H}_{1u}^n & \mathbf{0} & \bar{\mathbf{H}}_{1u}^n & \mathbf{0}\\ \mathbf{0} & \mathbf{H}_{2u}^n & \mathbf{0} & \bar{\mathbf{H}}_{2u}^2\end{bmatrix}\begin{bmatrix}\mathbf{u}^n\\ \bar{\mathbf{u}}^n\end{bmatrix} = \mathbf{M}_u^n \quad (19)$$

where $\mathbf{H}_{1u}^n$, $\mathbf{H}_{2u}^n$, $\bar{\mathbf{H}}_{1u}^n$ and $\bar{\mathbf{H}}_{2u}^n$ are matrices of 2×2 elements, and $\mathbf{M}_u^n$ is a vector of 4 elements (see appendix for details), $\mathbf{u}^n = [u_0^n \;\; u_{s^-}^n \;\; u_{s^+}^n \;\; u_a^n]^T$ and $\bar{\mathbf{u}}^n = [\bar{u}_0^n \;\; \bar{u}_{s^-}^n \;\; \bar{u}_{s^+}^n \;\; \bar{u}_a^n]^T$, where $[..]^T$ denotes the matrix transpose.

It can be seen that to solve the system (19), v_n and s_n must be known. Since the velocity and the position of the moving boundary are not known in advance, an iterative procedure is employed. Assuming a velocity v_n, hence a position $s_n = s_{n-1} + v_n(t_n - t_{n-1})$, of the moving interface, using an extrapolation from the two previous time steps, the temperature field is solved from the following system:

$$\begin{bmatrix}\mathbf{H}_{1T}^n & \mathbf{0} & \bar{\mathbf{H}}_{1T}^n & \mathbf{0}\\ \mathbf{0} & \mathbf{H}_{2T}^n & \mathbf{0} & \bar{\mathbf{H}}_{2T}^n\\ \mathbf{U}_1 & \mathbf{U}_2 & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{K}_1 & \mathbf{K}_2\end{bmatrix}\begin{bmatrix}\mathbf{T}^n\\ \bar{\mathbf{T}}^n\end{bmatrix} = \begin{bmatrix}\mathbf{M}_i^n\\ \mathbf{M}_T^e\end{bmatrix} \quad (20)$$

where $\mathbf{U}_1 = [0 \;\; -1]$, $\mathbf{U}_2 = [1 \;\; 0]$, $\mathbf{K}_1 = [0 \;\; K_1]$, $\mathbf{K}_2 = [-K_2 \;\; 0]$, and $\mathbf{M}_T^e = [0 \;\; \lambda v_n]^T$. The system (20) is obtained by writing (19) for T and incorporating the interface conditions (10) and (11).

Similarly, the concentration field is obtained by solving the following system:

$$\begin{bmatrix} \mathbf{H}_{1C}^n & \mathbf{0} & \bar{\mathbf{H}}_{1C}^n & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{2C}^n & \mathbf{0} & \bar{\mathbf{H}}_{2C}^n \\ \mathbf{V}_1 & \mathbf{V}_2 & \mathbf{D}_1 & \mathbf{D}_2 \\ \mathbf{F}_1 & \mathbf{F}_2 & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{C}^n \\ \bar{\mathbf{C}}^n \end{bmatrix} = \begin{bmatrix} \mathbf{M}_C^n \\ \mathbf{M}_C^e \end{bmatrix} \quad (21)$$

where $\mathbf{V}_1 = [0 \quad v_n]$, $\mathbf{V}_2 = [-v_n \quad 0]$, $\mathbf{D}_1 = [0 \quad -d_1]$, $\mathbf{D} = [d_2 \quad 0]$, $\mathbf{F}_1 = [0 \quad \gamma_1]$, $\mathbf{F}_2 = [-\gamma_2 \quad 0]$ and $\mathbf{M}_C^e = [0 \quad \eta_2 - \eta_1]^T$. It must be emphasized that the system (21) is written for the case where h_1 and h_2 are linear functions, given as $h_1(x) = \gamma_1 x + \eta_1$ and $h_2(x) = \gamma_2 x + \eta_2$.

If the Stefan conditions (11) and (12) are re-written as:

$$v = \frac{\mathrm{d}s}{\mathrm{d}t} = \varphi_T(\bar{T}_{s^-}, \bar{T}_{s^+}, K_1, K_2, \lambda)$$

$$= \varphi_c(C_{s^-}, C_{2^+}, \bar{C}_{s^-}, \bar{C}_{s^+}, d_1, d_2) \quad (22)$$

then, once the system (20) and (21) are solved, thus giving, as part of their solutions, the values of $\bar{T}_{s^-}^n$, $\bar{T}_{s^+}^n$, $T_{s^-}^n$, $T_{s^+}^n$, $\bar{C}_{s^-}^n$ and $\bar{C}_{s^+}^n$, which altogether with v_n are used to calculate the velocity for the next iteration; the velocity v_n^k at the k-ith iteration is given by:

$$v_n^k = (1-\omega)v_n^{k-1} + \omega(\varphi_c^n)^{k-1} \quad (23)$$

where ω is a relaxation factor ($0 < \omega \leqslant 1$) and

$$(\varphi_c^n)^k = \varphi_c(h_1^{-1}(T_{s^-}^n), h_2^{-1}(T_{s^+}^n), \bar{C}_{s^-}^n, \bar{C}_{s^+}^n, d_1, d_2)^k \quad (24)$$

where h^{-1} refers to the inverse of h. The iterative process is stopped when:

$$\left| 100 \times \frac{v_n^k - v_n^{k-1}}{v_n^{k-1}} \right| \leqslant \varepsilon \quad (25)$$

where ε is a small prescribed relative error.

For the general case where h_1 and h_2 are any functions, the above procedure can be changed slightly where after the solution of (20), the concentrations left and right of the interface can be calculated separately from

$$C_{s^-}^n = h_1^{-1}(T_{s^-}^n) \quad \text{and} \quad C_{s^+}^n = h_2^{-1}(T_{s^+}^n) \quad (26)$$

and the concentration field is obtained from

$$\begin{bmatrix} \mathbf{H}_{1C}^n & \mathbf{0} & \bar{\mathbf{H}}_{1C}^n & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{2C}^n & \mathbf{0} & \bar{\mathbf{H}}_{2C}^n \end{bmatrix} \begin{bmatrix} \mathbf{C}^n \\ \bar{\mathbf{C}}^n \end{bmatrix} = [\mathbf{M}_C^n]. \quad (27)$$

The rest of the procedure remains the same. It is worth mentioning that, for simplicity, the systems (20), (21) and (27) are left in their general form (i.e., not square); however, the systems become square when the known values (fixed and moving boundary conditions) are transferred to the right-hand side; a standard algorithm such as Gaussian elimination can then be used for their solutions.

The extension of the present scheme to higher dimension is straightforward from the theoretical point of view. It consists of the implementation of two superposed moving boundary problems. For detailed numerical aspects of boundary element implementation for moving boundary problems in higher dimension, see DeLima-Silva and Wrobel [19, 20]. However, the evaluation of the convolution integral describing the time-history of the boundary solution become the dominant and a costly task from the cpu-time point of view, especially for large number of time steps. However, much progress has been made recently in this general topic of efficient computation in relation to the inherent time-history dependence in the integral representation of transient problems [21–25]. For instance Demirel and Wang [21] divided the whole integral into near-history and far-history integrals, where the near-history is evaluated in the normal procedure while the far-history one is computed using a truncation approximation. Davey and Hinduja [22] approximate the integral from one time step to another, using some weights deduced from the known solution at the previous steps. Greengard and Strain [23] instead of using the free-space Green's function, as a weighting function, they used a complimentary representation of the fundamental solution obtained by Fourier series and the method of images. Davey and Bounds [24] used an approach whereby the fundamental solution at any time step is approximated by a linear combination of solutions evaluated at previous time steps. Zerroukat [25] eliminates the time-history dependence, by replacing the time-history integral with a domain integral which is evaluated using radial basis functions approximation and the solution at the previous step. These general ideas, which can be the basis of a fast and efficient boundary element algorithm for transient problems, can be easily incorporated into the present scheme.

4. RESULTS AND DISCUSSION

In order to validate the scheme, let us consider the problem treated in [5], which is defined by (6)–(12), where

$$h_1(C) = \gamma_1 C + \eta_1, \quad h_2(C) = \gamma_2 C + \eta_2, \quad a = \infty$$

$$p_1^T = f_1^c = p_2^T = p_2^c = 1, \quad f_1^T = p_1^c = f_2^T = f_2^c = 0$$

$$F_1^T = T_0, \quad F_1^c = 0, \quad F_2^T = T_\infty, \quad F_2^c = C_\infty. \quad (28)$$

If the initial conditions are $s(0) = 0$, $C_2(x,0) = C_\infty$ and $T_2(x,0) = T_\infty$, the problem has the following analytical solution:

$$\left.\begin{aligned} C_1(x,t) &= C_{r1} \\ T_1(x,t) &= T_0 + (T_{cr} - T_0)\,\mathrm{erf}(x/2\sqrt{\alpha_1 t})/\,\mathrm{erf}\,\kappa \end{aligned}\right\} \quad \text{for } 0 \leqslant x \leqslant s(t).$$

$$\left.\begin{aligned} C_2(x,t) &= C_\infty + (C_{r2} - C_\infty)\,\mathrm{erfc}(x/2\sqrt{d_2 t})/\,\mathrm{erfc}(\kappa\sqrt{\alpha_1/d_2}) \\ T_2(x,t) &= T_\infty + (T_{cr} - T_\infty)\,\mathrm{erfc}(x/2\sqrt{\alpha_2 t})/\,\mathrm{erfc}(\kappa\sqrt{\alpha_1/\alpha_2}) \end{aligned}\right\} \quad \text{for } x > s(t) \quad (29)$$

where $s(t) = 2\kappa\sqrt{\alpha_1 t}$ and $\alpha_i = K_i/c_i$; erf(x) and erfc(x) = 1 − erf(x) are the error and its complementary functions, respectively. T_{cr}, C_{r1}, C_{r2} and κ are four unknowns to be determined from the following system:

$$\begin{aligned} T_{cr} &= (\lambda + T_0\psi_1(\kappa) + T_\infty\psi_2(\kappa))/(\psi_1(\kappa) + \psi_2(\kappa)) \\ (C_\infty - C_{r2})/(C_{r1} - C_{r2}) &= \psi_3(\kappa\sqrt{\alpha_1/d_2}) \\ T_{cr} &= h_1(C_{r1}) \\ T_{cr} &= h_2(C_{r2}) \end{aligned} \tag{30}$$

where the functions ψ_i ($i = 1, 4$) are given as:

$$\psi_i(z) = \begin{cases} K_1/(\alpha_1\psi_4(z)), & i = 1 \\ K_2/[\alpha_2\psi_3(z\sqrt{\alpha_1/\alpha_2})], & i = 2 \\ \sqrt{\pi}z\exp(z^2)\,\mathrm{erf}(z), & i = 3 \\ \sqrt{\pi}z\exp(z^2)\,\mathrm{erfc}(z), & i = 4 \end{cases} \tag{31}$$

For simplicity, the material properties are considered as non-dimensional quantities.

Problem 1

$$\begin{aligned} &d_1 = d_2 = 1,\ c_1 = 0.1,\ c_2 = 0.5,\ K_1 = 1 \\ &K_2 = 1,\ T_0 = 50,\ T_\infty = 115,\ C_\infty = 0.1 \\ &\gamma_1 = 20,\ \gamma_2 = 40,\ \eta_1 = \eta_2 = 83. \end{aligned} \tag{32}$$

Table 1 shows a comparison between the FDM, analytical and BEM solutions for Problem 1. Although the results of all the methods are in agreement, BEM certainly outperforms the FDM when it comes to accuracy per time-step length. For instance, Table 1 shows that the BEM gives a similar or more accurate solution with a time step 1000 times larger than that required by the FDM for similar accuracy.

In order to see more details about the vicinity of the interface, Table 2 shows the temperature and concentration distributions around the moving interface for Problem 1. Although, in principle the two regions across the interface could be any homogeneous states, they are assumed to be solid and liquid in order to give the results physical meaning and to show some drawbacks of the inability of handling the discontinuity at the interface. It can be seen that the FDM smooths the transition across the interface, whereas the BEM preserves the sharp jump in the concentration. This is due to the inherent Dirac-delta like nature of the fundamental solution in BEM. As a consequence of the smoothing of that transition, the FDM gives rise to an artificial (i.e., numerical) mushy zone, a zone where the material is in an intermediate meta-stable state, which is neither totally solid nor totally liquid, but a combination of the two. This may confuse the scale of a real mushy-zone which may arise due to the physics of the problem, such as in Problem 2. However, in agreement with the analytical solution, the BEM does not show this behaviour because, unlike Problem 2, a physical mushy zone in this case should not arise.

For a mushy zone to occur in the above problem, the following condition must be satisfied [26]:

$$\zeta = \frac{\partial}{\partial x}[T_2(s(t), t) - h_2(C_2(s(t), t))] < 0. \tag{33}$$

Since for the analytical solution, the quantity ζ in (33)

Table 1. Temperature $T(x, t)$ and concentration $C(x, t)$ distributions at $t = 0.4$ for Problem 1

	Temperature				Concentration			
x	FDM [5] $\Delta t = 0.000025$	Analytic	BEM $\Delta t = 0.025$	BEM $\Delta t = 0.01$	FDM [5] $\Delta t = 0.000025$	Analytic	BEM $\Delta t = 0.025$	BEM $\Delta t = 0.01$
0.00	50.000	50.000	50.000	50.000	0.132	0.132	0.132	0.132
0.05	53.10	53.136	53.131	53.137	0.132	0.132	0.132	0.132
0.10	56.20	56.272	56.258	56.271	0.132	0.132	0.132	0.132
0.15	59.30	59.405	59.381	59.401	0.132	0.132	0.132	0.132
0.20	62.40	62.536	62.500	62.527	0.132	0.132	0.132	0.132
0.25	65.50	65.663	65.613	65.649	0.132	0.132	0.132	0.132
0.30	69.59	68.785	68.721	68.766	0.132	0.132	0.132	0.132
0.35	71.69	71.901	71.824	71.877	0.132	0.132	0.132	0.132
0.40	74.79	75.010	74.920	74.981	0.132	0.132	0.132	0.132
0.45	77.89	78.111	78.010	78.079	0.132	0.132	0.132	0.132
0.50	80.99	81.204	81.094	81.169	0.132	0.132	0.132	0.132
0.55	84.08	84.287	84.170	84.251	0.132	0.132	0.132	0.132
0.60	86.20	86.355	86.298	86.343	0.067	0.068	0.068	0.068
0.65	87.35	87.614	87.544	87.596	0.069	0.070	0.070	0.070
0.70	88.49	88.847	88.763	88.822	0.071	0.072	0.072	0.072
0.75	89.61	90.054	89.954	90.022	0.073	0.074	0.074	0.074
0.80	90.71	91.233	91.117	91.194	0.075	0.076	0.076	0.076
0.85	91.78	92.382	92.251	92.338	0.077	0.078	0.078	0.078
0.90	92.82	93.502	93.355	93.452	0.079	0.080	0.080	0.080
0.95	93.83	94.590	94.429	94.535	0.081	0.082	0.082	0.082
1.00	94.80	95.647	95.472	95.587	0.083	0.083	0.083	0.083

Table 2. Temperature $T(x, t)$ and concentration $C(x, t)$ distributions around the interface at $t = 0.4$ for Problem 1

	Analytic			Finite difference [5]			BEM		
x	$T(x,t)$	$C(x,t)$	State	$T(x,t)$	$C(x,t)$	State	$T(x,t)$	$C(x,t)$	State
0.500	81.204	0.1320	Solid	80.99	0.132	Solid	81.170	0.1318	Solid
0.525	82.746	0.1320	Solid	82.53	0.132	Solid	82.713	0.1319	Solid
0.550	84.287	0.1320	Solid	84.08	0.132	Solid	84.254	0.1320	Solid
0.575	85.717	0.0667	Liquid	85.63	0.109	Mushy	85.704	0.0662	Liquid
0.600	86.355	0.0679	Liquid	86.20	0.067	Liquid	86.342	0.0674	Liquid
0.625	86.988	0.0690	Liquid	86.77	0.068	Liquid	86.968	0.0686	Liquid
0.650	87.614	0.0701	Liquid	87.35	0.069	Liquid	87.591	0.0689	Liquid
0.675	88.234	0.0712	Liquid	87.92	0.070	Liquid	88.208	0.0709	Liquid
0.700	88.847	0.0723	Liquid	88.49	0.071	Liquid	88.816	0.0710	Liquid

Table 3. Temperature $T(x, t)$ and concentration $C(x, t)$ distributions at $t = 0.8$ with $\Delta t = 0.01$ for Problem 2

	Concentration		Temperature		
x	Analytic	BEM	Analytic	BEM	State
0.55000	0.10200	0.10168	1.01722	1.01984	Solid
0.55750	0.10200	0.10168	1.03023	1.03288	Solid
0.56500	0.10200	0.10168	1.04319	1.04599	Solid
0.57250	0.10200	0.10168	1.05613	1.05885	Solid
0.58000	0.10200	0.10168	1.06903	1.07177	Solid
0.58750	0.10200	0.10168	1.08189	1.08470	Solid
0.59500	0.10200	0.10168	1.09472	1.09752	Solid
0.60250	0.06089	0.05978	1.10629	1.10851	Mushy
0.61000	0.07067	0.07015	1.11623	1.11855	Mushy
0.61750	0.07800	0.07798	1.12614	1.12857	Mushy
0.62500	0.08411	0.08377	1.13603	1.13858	Mushy
0.63250	0.08778	0.08811	1.14588	1.14851	Mushy
0.64000	0.09144	0.09130	1.15570	1.15844	Mushy
0.64750	0.09389	0.09366	1.16550	1.16835	Mushy
0.65500	0.09511	0.09540	1.17526	1.17820	Mushy
0.66250	0.09633	0.09666	1.18500	1.18805	Mushy
0.67000	0.09756	0.09760	1.19470	1.19786	Liquid
0.67750	0.09878	0.09827	1.20438	1.20761	Liquid
0.68500	0.09878	0.09876	1.21402	1.21737	Liquid
0.69250	0.09878	0.09912	1.22363	1.22706	Liquid
0.70000	0.09878	0.09937	1.23321	1.23674	Liquid

is a constant divided by $\sqrt{t}$, the sign of ζ cannot change in time. However, one can obtain the same effect of (33) by taking d_2 relatively small. To this end, the following data are considered:

Problem 2

$$d_1 = c_1 = c_2 = K_1 = K_2 = 1$$

$$d_2 = 0.01,\ T_0 = 0,\ T_\infty = 2.6,\ C_\infty = 0.1$$

$$\gamma_1 = 1,\ \gamma_2 = 2,\ \eta_1 = \eta_2 = 1. \tag{34}$$

Table 3 shows a comparison between the analytical and BEM solutions for Problem 2 where a physical mushy zone occurs [26]. In addition to the good agreement between the analytical and BEM solutions, Table 3 clearly shows a finite region which is neither completely liquid nor completely solid, and whose temperatures lies in between the two curves, solidus and liquidus, given by $T = 1 + C$ and $T = 1 + 2C$, respectively. This situation occurs very often in binary and in general alloy phase change. Since in most materials the chemical diffusivity is generally much smaller than the thermal diffusivity, this mushy zone occurrence would be expected in most realistic problems.

5. CONCLUSIONS

The numerical results show that the boundary element method is very suitable for this kind of problems, especially when the interface presents a discontinuity. When computations are to be performed for extended time, the use of large time steps is very desirable to reduce the computational cost. The results clearly show that, to obtain a certain accuracy, the time step in FDM ought to be many times smaller than that required for BEM for a similar accuracy.

The high accurate convolution time-integration of the BEM has been well established for boundary-value problems and it seems that the same conclusions can be extrapolated to moving boundary problems. This makes the BEM a more attractive alternative when the use of large time steps is required.

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APPENDIX

The integrals of the Green's function and its derivative with respect to space when the field point x is stationary are given by:

$$\int_{t_1}^{t_2} u_j^*(\xi, x, t_n, t)\,\mathrm{d}t = \frac{-r}{2\alpha_j\sqrt{\pi}}\left\{\left[\frac{1}{a}\exp(-a^2)+\sqrt{\pi}\,\mathrm{erf}(a)\right]_{a_1}^{a_2}\right\} \tag{A1}$$

where

$$a_i = \frac{r}{\sqrt{4\alpha_j(t_n-t_i)}} \quad i = 1, 2$$

and

$$\int_{t_1}^{t_2} q_j^*(\xi, x, t_n, t)\,\mathrm{d}t = \frac{\mathrm{sign}(\xi-x)}{2\alpha_j}(\mathrm{erf}(a_2)-\mathrm{erf}(a_1)) \tag{A2}$$

where sign $(x) = |x|/x$ and erf(x) is the error function.

When the field point is moving with time, i.e. $x = s(t)$; instead of (A1) and (A2), the following are used:

$$\int_{t_1}^{t_2} u_j^*(\xi, s(t), t_n, t)\,\mathrm{d}t = -\frac{1}{2v}\left\{\exp\left(-\frac{bv}{\alpha_j}\right)\left[\mathrm{erf}\left(-\frac{v(t_n-t)-b}{\sqrt{4\alpha_j(t_n-t)}}\right)\right]_{t_1}^{t_2} + \left[\mathrm{erf}\left(-\frac{v(t_n-t)+b}{\sqrt{4\alpha_j(t_n-t)}}\right)\right]_{t_1}^{t_2}\right\} \tag{A3}$$

for any $s(t) = x+v(t-t')$ and $b(t) = \xi - s(t) = \xi - x - v(t-t')$.

$$\int_{t_1}^{t_2} \bar{u}_j^*(\xi, s(t), t_n, t)\,\mathrm{d}t$$

$$= -\frac{1}{2\alpha_j}\exp\left(-\frac{bv}{\alpha_j}\right)\left[\operatorname{erf}\left(-\frac{v(t_n-t)-b}{\sqrt{4\alpha_j(t_n-t)}}\right)\right]_{t_1}^{t_2}. \quad \text{(A4)}$$

It is worth mentioning that expressions (A1)–(A4) are singular for $r = |\xi - x| = 0$ and $t_n = t_2$. For these cases, the limit of the right-hand side of (A1)–(A4) are taken as the value of the integrals. The coefficients of matrices $\mathbf{H}_{ju}^n$ and $\bar{\mathbf{H}}_{ju}^n$ and vector $\mathbf{M}_u^n$ in (19) can be deduced from (16) and (17) as:

$$\mathbf{H}_{1u}^n = \begin{bmatrix} \frac{1}{2} - \alpha_1 h_1(0,0,t_n,t_n) & \alpha_1 h_1(0,s_n,t_n,t_n) - v_n g_1(0,s_n,t_n,t_n) \\ -\alpha_1 h_1(s_n,0,t_n,t_n) & \frac{1}{2} + \alpha_1 h_1(s_n,s_n,t_n,t_n) - v_n g_1(s_n,s_n,t_n,t_n) \end{bmatrix} \quad \text{(A5)}$$

$$\mathbf{H}_{2u}^n = \begin{bmatrix} \frac{1}{2} - \alpha_2 h_2(s_n,s_n,t_n,t_n) + v_n g_2(s_n,s_n,t_n,t_n) & \alpha_2 h_2(s_n,a,t_n,t_n) \\ -\alpha_2 h_2(a,s_n,t_n,t_n) + v_n g_2(a,s_n,t_n,t_n) & \frac{1}{2} + \alpha_2 h_2(a,a,t_n,t_n) \end{bmatrix} \quad \text{(A6)}$$

$$\bar{\mathbf{H}}_{1u}^n = \alpha_1 \begin{bmatrix} g_1(0,0,t_n,t_n) & -g_1(0,s_n,t_n,t_n) \\ g_1(s_n,0,t_n,t_n) & -g_1(s_n,s_n,t_n,t_n) \end{bmatrix} \quad \text{(A7)}$$

$$\bar{\mathbf{H}}_{2u}^n = \alpha_2 \begin{bmatrix} g_2(s_n,s_n,t_n,t_n) & -g_2(s_n,a,t_n,t_n) \\ g_2(a,s_n,t_n,t_n) & -g_2(a,a,t_n,t_n) \end{bmatrix} \quad \text{(A8)}$$

$$\mathbf{M}_u^n = \begin{bmatrix} \alpha_1 \Psi_{1u}^n(0) + \psi_1^u(0,t_n) \\ \alpha_1 \Psi_{1u}^n(s_n) + \psi_1^u(s_n,t_n) \\ \alpha_2 \Psi_{2u}^n(s_n) + \psi_2^u(s_n,t_n) \\ \alpha_2 \Psi_{2u}^n(a) + \psi_2^u(a,t_n) \end{bmatrix} \quad \text{(A9)}$$

where

$$\Psi_{1u}^n(\xi) = \sum_{i=0}^{n-1} \times \begin{Bmatrix} g_1(\xi,s_n,t_n,t_i)\left(\bar{u}_{s^-}^i + \frac{1}{\alpha_1} v_i u_{s^-}^i\right) - h_1(\xi,s_n,t_n,t_i)u_{s^-}^i \\ -g_1(\xi,0,t_n,t_i)\bar{u}_0^i + h_1(\xi,0,t_n,t_i)u_0^i \end{Bmatrix} \quad \text{(A10)}$$

$$\Psi_{2u}^n(\xi) = -\sum_{i=0}^{n-1} \times \begin{Bmatrix} g_2(\xi,s_n,t_n,t_i)\left(\bar{u}_{s^+}^i + \frac{1}{\alpha_2} v_i u_{s^+}^i\right) - h_2(\xi,s_n,t_n,t_i)u_{s^+}^i \\ -g_2(\xi,a,t_n,t_i)\bar{u}_a^i + h_2(\xi,a,t_n,t_i)u_a^i \end{Bmatrix}. \quad \text{(A11)}$$