Boundary integral formulation and mushy zone model for phase change problem

S.G. Ahmed
Department of Engineering, Mathematics & Physics, Faculty of Engineering, Zagazig University, Zagazig, Egypt

Received April 2000
Revised February 2001
Accepted February 2001

Keywords *Boundary integral equation, Phase change*

Abstract *In the present paper, a simple mushy zone model and the boundary integral technique are applied to solve a phase change moving boundary problem. Owing to the use of the mushy zone model, some mathematical considerations are taken when applying the integral equation at the extreme points of the domain. A numerical algorithm is developed to track the moving boundaries that appear throughout the process. Good accuracy is obtained using the developed algorithm and the results give good agreement with previous solutions.*

Nomenclature

a_ℓ = Thermal diffusivity for liquid
a_s = Thermal diffusivity for solid
D = A cooling temperature applied at $x = 0$
ε = Fraction of latent heat in the mushy zone $0 < \varepsilon < 1$
K_ℓ = Conductivity for liquid
K_s = Conductivity for solid
L = Latent heat
u_ℓ = Temperature for liquid phase
u_s = Temperature for solid phase
U_F = Phase change temperature applied at $x = s(t)$
U_i = Initial temperature

1. Introduction

Conduction heat transfer involving melting or solidification plays an important role in a wide variety of materials processing applications, from foundry operations to growth of high purity semi-conductor crystals. All of these problems have the characteristic of an interface boundary, which moves into the solid or into the liquid in accordance with the relative magnitude of the latent heat on either side of it.

Heat transfer problems with phase change have been studied because of their wide scientific and technological applications, e.g. Alexiades and Solomon (1993), Lunardini (1991) and Rubinstein (1971). A review of a long bibliography is presented in Tarzia (1981).

Boundary integral methods are very convenient to use for solution of Stefan problems. In these methods, nodal points are located only on the boundaries and move together with the phase change interface. This means that there is no need for any mesh adjustment (Ahmed and Wrobel, 1995). For multidimensional problems, mesh adjustment is necessary but much easier to perform than in standard domain methods. The solution of Stefan problems based on boundary integral methods started in early 1970 with papers by Chuang and Szekely (1972). Other applications include those of Shaw (1982), Wrobel (1983), Heinlein

International Journal of Numerical Methods for Heat & Fluid Flow, Vol. 11 No. 4, 2001, pp. 371-379.

et al. (1986), Zabaras *et al.* (1988), Hsieh *et al.* (1992), Delima-Silva and Wrobel (1993) and others.

In the present paper, a boundary integral method and the mushy zone model with a developed algorithm are applied to solve the phase change problem with moving boundaries. The results are compared with a previously available approximate solution introduced by Tarzia (1995) and give good agreement.

2. Problem description and formulation

A semi-infinite liquid material occupying the region $0 \leq x < \infty$ was initially at zero temperature. At time $t > 0$ the boundary $x = 0$ is subjected to a cooling temperature. Three different phases appear, i.e. solid, mushy and liquid, respectively. The problem configuration is shown in Figure 1.

In the mushy zone $s(t) \leq x \leq r(t)$ two assumptions are made on its structure (Tarzia, 1995); they are:

(1) The material in the mushy zone contains a fixed fraction εL, where L is the total latent heat and $0 < \varepsilon < 1$.

(2) The width of the mushy zone is inversely proportional to the temperature gradient at the moving boundary $s(t)$.

The governing equations for solid phase:

$$a_s \frac{\partial^2 u_s}{\partial x^2} = \frac{\partial u_s}{\partial t} \quad 0 \leq x \leq s(t) \tag{1}$$

with

$$u_s(x = 0, t) = D \tag{2}$$

$$u_s(x = s(t), t) = U_F \tag{3}$$

For solid-mushy-liquid zone $s(t) \leq x \leq r(t)$

$$K_s \frac{\partial u_s(x = s(t), t)}{\partial x} - K_\ell \frac{\partial u_\ell(x = r(t), t)}{\partial x} = \rho L \left(\varepsilon \frac{ds}{dt} + (1 - \varepsilon) \frac{dr}{dt} \right) \tag{4}$$

$$\frac{\partial u_s}{\partial x} \times [r(t) - s(t)] = \gamma \tag{5}$$

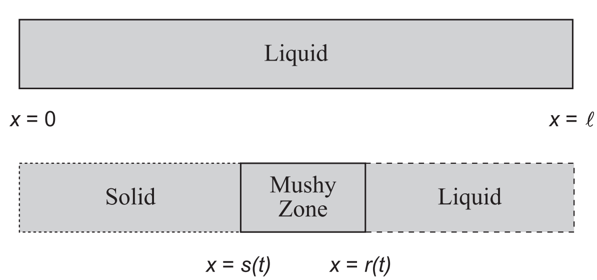

Figure 1.
Problem configuration

Liquid phase $x > r(t)$

$$a_\ell \frac{\partial^2 u_\ell}{\partial x^2} = \frac{\partial u_\ell}{\partial t} \quad x \geq s(t) \tag{6}$$

$$u_\ell(x = r(t), t) = U_F \tag{7}$$

$$u_\ell(x \rightarrow \infty) = U_i \tag{8}$$

$$s(0) = r(0) = 0 \tag{9}$$

3. Boundary integral formulation

According to Chuang and Szekely (1972), Zabaras *et al.* (1988), Ahmed and Wrobel (1995) the integral equation corresponding to the diffusion equation in the solid phase $0 \leq x \leq s(t)$ can take the following form:

$$C(\xi)u(\xi, t_F) = a_s \int_{to}^{t_F} \left[u^*(\xi, x, t_F, t) \frac{\partial u(x,t)}{\partial x} - u(x,t) \frac{\partial u^*(\xi, x, t_F, t)}{\partial_x} + \frac{1}{a_s} u(x,t) u^*(\xi, x, t_F, t) \frac{ds(t)}{dt} \right]_0^{s(t)} dt \tag{10}$$

And for the liquid phase $r(t) \leq x \leq \ell$:

$$C(\xi)u(\xi, t_F) = a_\ell \int_{t_o}^{t_F} \left[u^*(\xi, x, t_F, t) \frac{\partial u(x,t)}{\partial x} - u(x,t) \frac{\partial u^*(\xi, x, t_F, t)}{\partial x} + \frac{1}{a_\ell} u(x,t) u^*(\xi, x, t_F, t) \frac{ds(t)}{dt} \right]_{r(t)}^{\ell} dt \tag{11}$$

In these equations ξ is defined as the source point and $u^*(\xi, x; t_F, t)$ is Green's function defined by:

$$u^*(\xi, x, t_F, t) = \frac{1}{\sqrt{4\pi a(t_F - t)}} \exp\left\{ \frac{r^2(\xi, x)}{4a(t_F - t)} \right\} \tag{12}$$

with r being the distance between the source point ξ and field point x.

4. The proposed numerical algorithm

The present algorithm is developed to solve the phase change problem with mushy zone appearing throughout the process. In this algorithm, the boundary integral method is used to find the unknowns at the boundaries for each phase separately such that the non-linear conditions at these boundaries should be satisfied.

The algorithm starts by guessing an initial velocity of the moving boundary and solves the problem at discrete values of the fraction parameter ε. The flow chart describing the iteration procedure is shown in Figure 2.

5. Results and discussion

A test problem was solved with the proposed algorithm. For simplicity, all thermophysical parameters were assigned a unit value except that the latent heat was chosen to have two.

The test problem considers a semi-infinite slab with initial temperature $u_0 = 2°C$ and the phase change temperature equals zero. The temperature at $x = 0$ dropped to $u = -10°C$ while the temperature at $x \rightarrow \infty$ remained at the initial state.

In the simple mushy zone model used in the present paper with the boundary integral formulation there are two basic parameters which affect the process. These parameters are ε which represent the fraction of the latent heat in the mushy zone, which is assumed to vary in the range $0 < \varepsilon < 1$. The second parameter is γ, which represents the constant of proportionality between the mushy zone thickness and the flux at the first moving boundary $s(t)$.

Figure 3 shows the relation between these parameters based on the present algorithm. It is clear that the present algorithm helps to determine a range for γ corresponding to ε. This describes the process very well, since ε represents the fraction of the latent heat in the mushy zone and by increasing ε the thickness of the mushy zone increases.

The fraction of the latent heat in the mushy zone, which is represented by the parameter ε, affects directly the movement of the second moving boundary $r(t)$ and is shown in Figure 4. It is clear from this Figure that by increasing the fraction of the latent heat the movement of $r(t)$ increases.

The thickness of the mushy zone is affected by two major factors, namely, time and latent heat fraction. Figure 5 shows the thickness of the mushy zone at different values of the latent heat fraction. It is clear that the thickness of the mushy zone increases by increasing the time and the latent heat fraction.

To check the validity and the accuracy of the proposed method, a comparison is made for the movement of the moving boundaries for fixed $\varepsilon = 0.1$ between the present method and a previous approximate solution developed by Tarzia (1995). Results of this comparison are shown in Figure 6, which shows good agreement.

The temperature distribution for both phases that appear throughout the process was evaluated based on the present algorithm. The solid phase temperature at two different times and for a fixed value of $\varepsilon = 0.5$ is shown in Figure 7. It is clear that the temperature at the two times starts from $u = -10°C$, which is the boundary condition at $x = 0$ and increases until it reaches the phase change temperature at the moving boundary $s(t)$.

As mentioned before, the fraction of the latent heat in the mushy zone controls the movement of the moving boundary in the liquid phase. Another effect of this amount of fraction appears in the liquid phase temperature, as

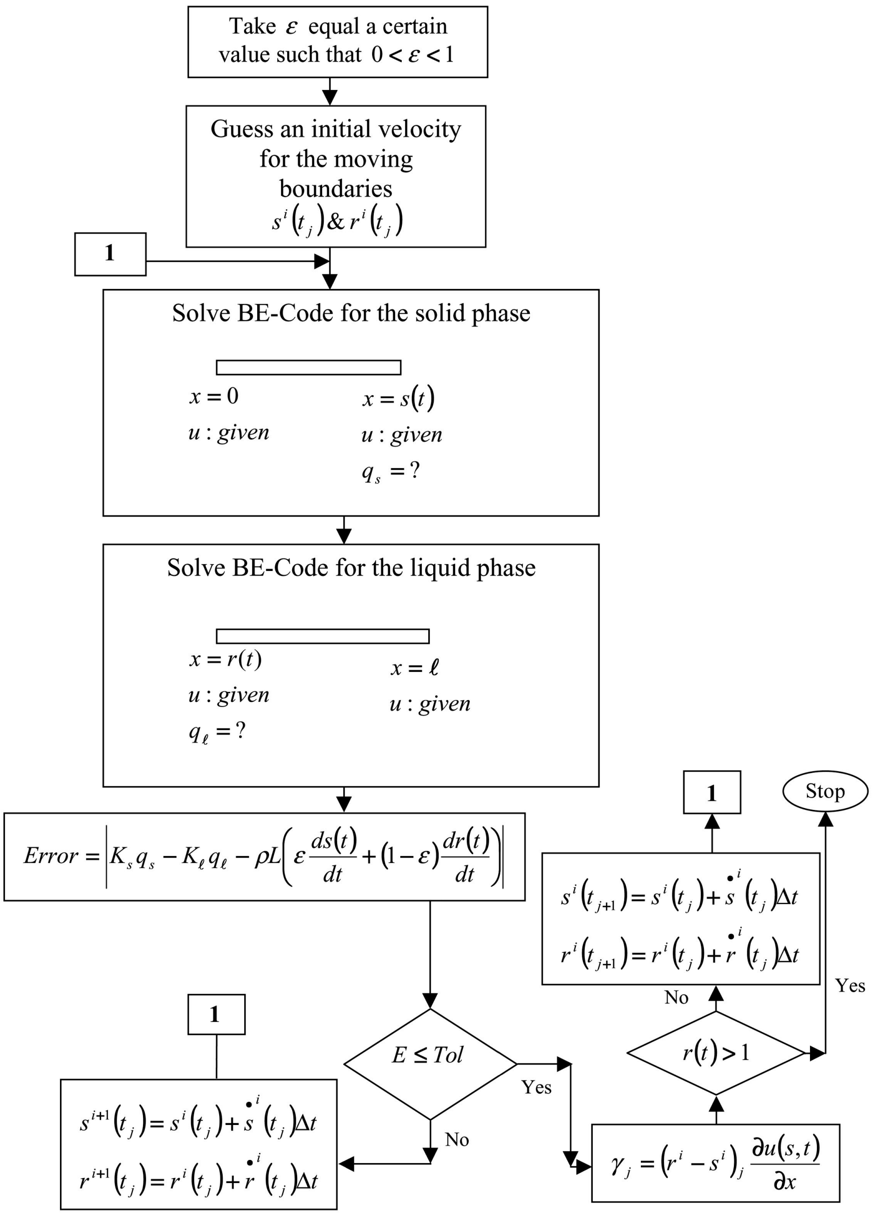

Figure 2.
Flow chart

shown in Figure 8. In this Figure the liquid phase temperature is evaluated for different values of ε.

It is clear that at the same time step the liquid phase temperature increases by increasing the amount of latent heat fraction. For example at $t = 0.01$, the temperature at $\varepsilon = 0.1$ is less than the temperature at $\varepsilon = 0.5$ and the latter is less than that at $\varepsilon = 0.9$.

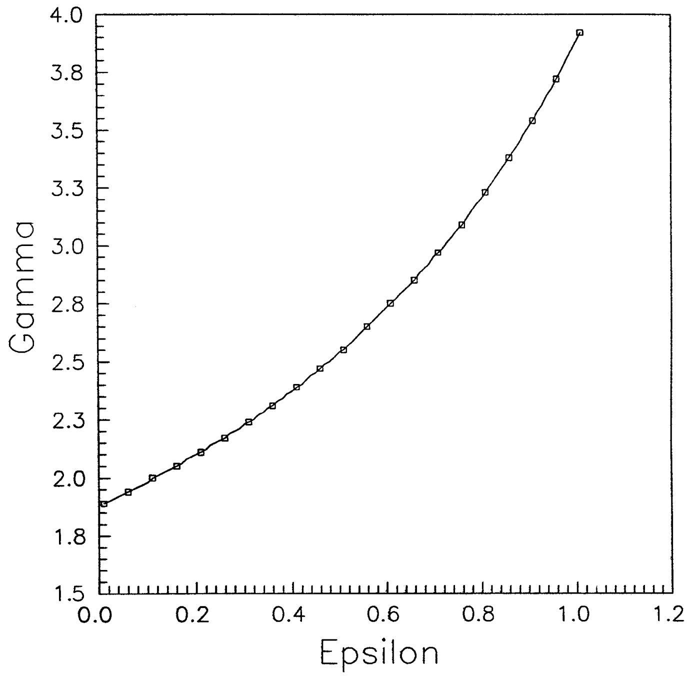

Figure 3.
Relation between ε and γ

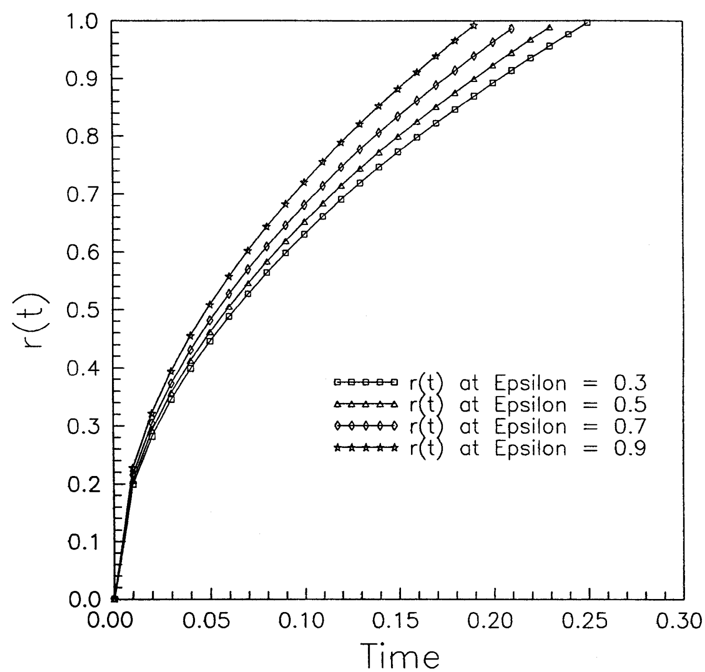

Figure 4.
Variation of $r(t)$ with time at different ε

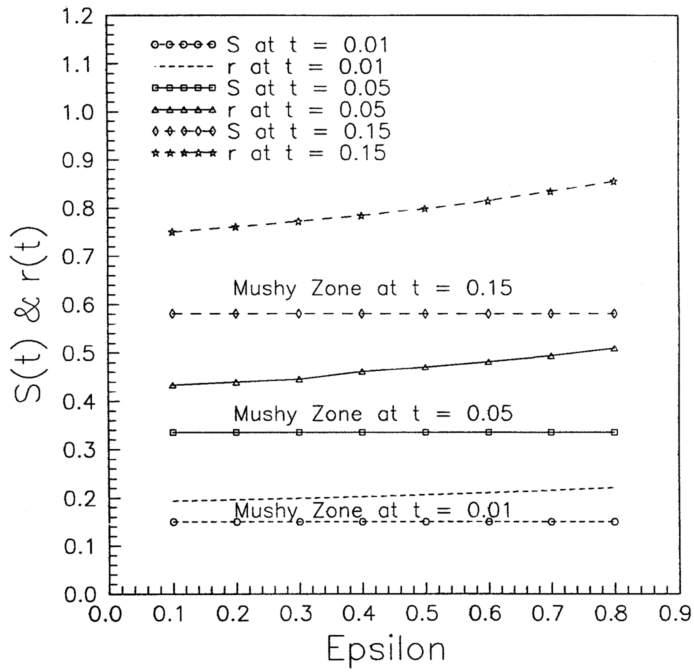

Figure 5.
Thickness of mushy zone at different times

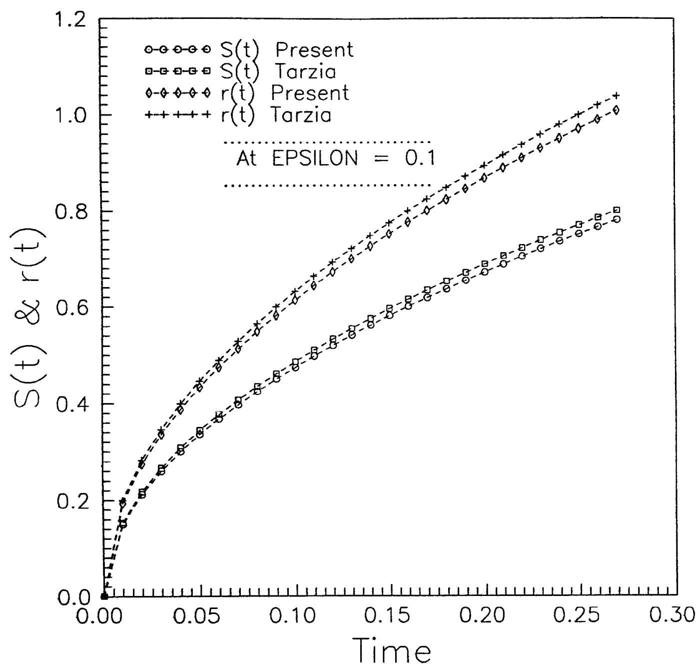

Figure 6.
Comparison for the moving boundaries

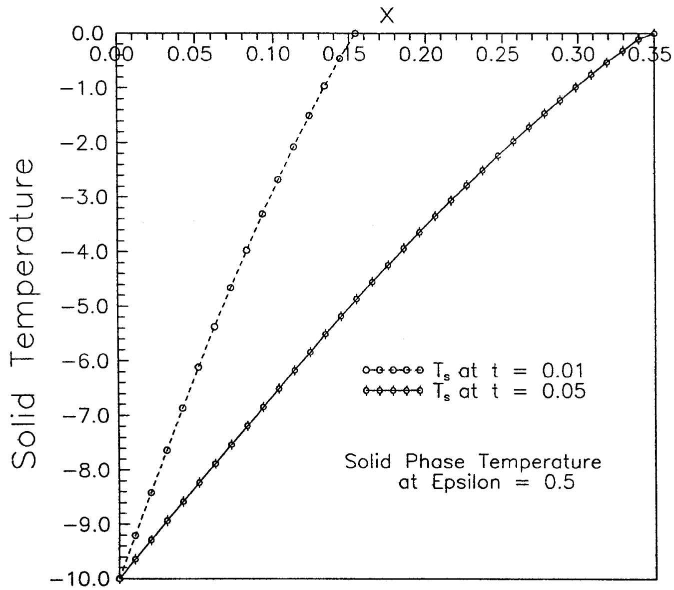

Figure 7.
Solid phase temperature

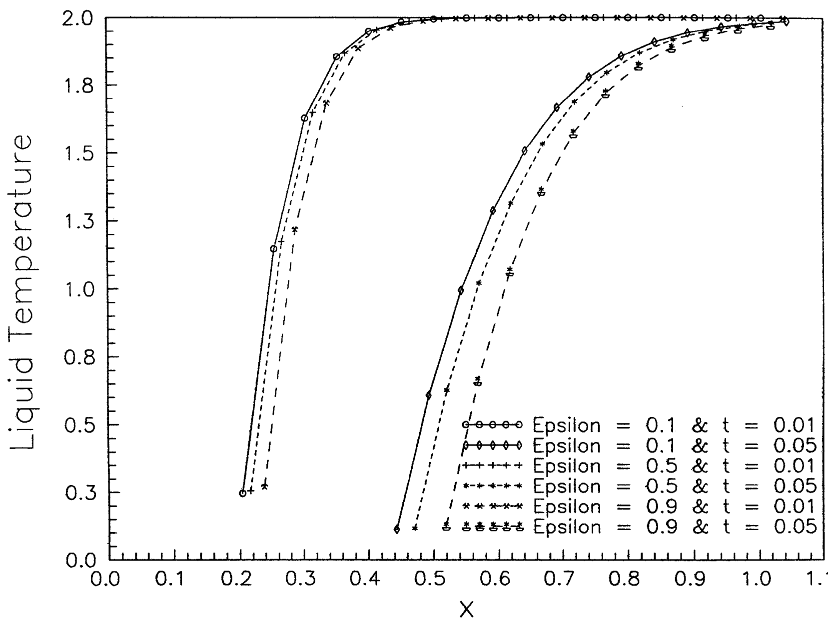

Figure 8.
Liquid phase temperature

6. Conclusion

The phase change problem herein is formulated using the simple mushy zone model and the boundary integral technique. A new numerical algorithm is developed based on the model and the method used.

The present algorithm includes a brief discussion of the assumptions made on the simple mushy zone model. Also the algorithm has the flexibility to handle and analyze each parameter, which has an effect on the movement of the moving boundaries that appear throughout the process. Finally, the present algorithm has the flexibility to handle multiphase problems.

References

Ahmed, S.G. and Wrobel, L.C. (1995) "Numerical solution of solidification problems using integral equations", 3rd Int. Conference on Free and Moving Boundary Problems, Bled, Slovenia.

Alexiades,V. and Solomon, A.D. (1993), *Mathematical Modeling of Melting and Freezing Processes*, Hemisphere Publishing Corp., Washington, DC.

Chuang, Y.K. and Szekely, J. (1972) "On the use of Green's functions for solving melting or solidification problems", *Int. J. Heat Mass Transfer*, Vol. 14, pp. 1285-94.

DeLima-Silva, W. Jr and Wrobel, L.C. (1993), "A boundary element formulation for multi-dimensional ablation problems", *Boundary Element XIV*, Computational Mechanics Publication, Southampton and Elsevier, London.

Heinlein, M., Mukherjee, S. and Richmond, C. (1986),"'A boundary element method analysis of temperature fields and stress during solidification", *Acta Mechanica*, Vol. 59, pp. 59-81.

Hsieh, C.K., Choi, C.-Y. and Kassab, A.J. (1992), "Solution of Stefan problems by a boundary element method", *Boundary Element Technology VII*, Computational Mechanics Publication, Southampton and Elsevier, London.

Lunardini, V.J. (1991), *Heat Transfer with Freezing and Thawing*, Elsevier, Amsterdam.

Rubinstein, L.I. (1971), "*The Stefan Problem*: translations of mathematical monographs", *Amer. Math. Soc.*, Vol. 27, Providence, RI.

Shaw, R.P. (1982), "A boundary integral equation approach to the one-dimensional ablation problem", *Boundary Element Methods in Engineering*, Springer-Verlag, Berlin.

Tarzia, D.A. (1981), "Una revision sobre problemas de frontera movil y libra para la ecuacion del calor. El problema de Stefan", *Math. Notae*, Vol. 29, pp. 147-241.

Tarzia, D.A. (1995), "On the determination of the unknown coefficients through phase change process", 3rd Int. Conference on Free and Moving Boundary Problems, Bled, Slovenia.

Wrobel, L.C. (1983), "A boundary element solution to Stefan's problem", *Boundary Elements V*, Springer-Verlag, Berlin.

Zabaras, N., Mukherjee, S. and Richmond, O. (1988), "An analysis of inverse heat transfer problems with phases using an integral method", *J. Heat Transfer*, Vol. 110, pp. 554-61.