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An efficient approach to isotherm migration method in two dimensions

RADHEY S. GUPTA and AMBREESH KUMAR
Department of Mathematics, University of Roorkee, Roorkee 247667, India

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NOMENCLATURE

B	radial distance of the fixed boundary
n	outward normal to the solid–liquid interface
r	radial coordinate
r_t, r_u, r_{uu}	partial derivatives of r
Δr	increment in r during the time step Δt
S	radial distance of the moving interface
S_t, S_θ, S_u	partial derivatives of S
t	time
Δt	time step
u	temperature
$u_t, u_r, u_{rr}, u_\theta, u_{\theta\theta}$	partial derivatives of u
Δu	temperature step
v_n	velocity of the interface in the direction of n
x, y	Cartesian coordinate.

Greek symbols

β	physical constant
θ	angular coordinate
$\Delta\theta$	angular step.

Subscript

i, j	location in u–θ plane.

Superscript

k	time level.

INTRODUCTION

THE ISOTHERM migration method (IMM), pioneered by Chernous'ko [1] and Dix and Cizek [2], is one of the most powerful techniques for solving moving boundary problems (MBPs). The greatest advantage of the IMM is that, as the moving boundary is essentially an isotherm its movement can be traced directly as part of the solution. Initially, the IMM was presented by its originators for problems in one dimension only. Later on, it was extended for solving a two-dimensional (2-D) solidification problem by Crank and Gupta [3]. In their method, the movement of the isotherms is followed along the fixed vertical or horizontal lines, i.e. parallel to the axes in Cartesian coordinates. However, this method calls for a lot of interpolations–extrapolations on the axis and on the diagonal at each time step. Crank and Crowley [4, 5] further investigated the IMM, also in 2-D, by choosing the orthogonal flow lines to be the path for the movement of the isotherms. But, since the movement of a point on an isotherm may not always be along the radial line (as the isotherms are not circles), the centre of curvature and the radius of curvature, for every point on each isotherm, have to be computed at each time step. This should naturally increase the amount of computations tremendously and would therefore reduce the scope of the method.

In this note the movement of the isotherms has been tracked along the fixed radial lines, i.e. θ = const. in the cylindrical coordinates system (r, θ). As the movement is always along fixed lines, the need for determining the centre and radius of curvature is avoided. Consequently, the present procedure becomes more economical computationally in comparison to its predecessors. Further, it may be mentioned that the previous approaches of the IMM [3, 4], break down near the end of the solidification–melting process because of too few mesh points, whereas, the present one goes through nicely. We illustrate the method by taking a sample problem already discussed in refs. [3, 4]. Both the explicit and implicit schemes are implemented through a DEC 2050 computer.

MATHEMATICAL STATEMENT OF THE PROBLEM

An infinitely long square prism, extending between $-1 \leqslant x, y \leqslant 1$, is initially filled with a fluid at the fusion temperature $u = 1$. The temperature on its surface is subsequently maintained constant at $u = 0$, below the fusion temperature, so that inward solidification starts taking place. Because of symmetries, about the axes and the diagonal $y = x$, it is sufficient to work in the triangular region R defined by $R = \{x, y|y \leqslant x \leqslant 1,\ 0 \leqslant y \leqslant 1\}$. In cylindrical coordinates it can be written as $R = \{r, \theta|0 \leqslant r \leqslant B(\theta),\ 0 \leqslant \theta \leqslant \pi/4\}$, where $B(\theta)$ is the fixed boundary of the prism. Therefore, we require a solution of the equation

$$u_t = u_{rr} + u_r/r + u_{\theta\theta}/r^2 \quad \text{in } D \tag{1}$$

where D is the domain bounded by the fixed boundary $r = B(\theta) = 1/\cos\theta$, on which $u = 0$, and by the moving interface defined as $r = S(\theta, t)$, on which $u = 1$, for $0 \leqslant \theta \leqslant \pi/4$. Also due to various symmetries, the additional conditions to be satisfied are

$$u_\theta = 0 \quad \text{at} \quad \theta = 0 \quad \text{and} \quad \pi/4. \tag{2}$$

The familiar condition arising due to phase change on the interface is given by

$$\frac{\partial u}{\partial n} = -\beta v_n \tag{3}$$

where v_n denotes the velocity of the interface in the direction of n, the outward normal to it, and β depends on the properties of the material undergoing phase change (which is constant for the present problem and taken to be 1.5613, the same as used by Crank and Gupta [3] and others).

The transformation of $u(r, \theta, t)$ to $r(u, \theta, t)$ renders equations (1) and (3) respectively to the following IMM form of equations

$$r_t = r_{uu}/r_u^2 - 1/r - r_u(u_{\theta\theta}/r^2) \tag{4}$$

and

$$S_t = \frac{1}{\beta}[1 + S_\theta^2/S^2]/S_u. \tag{5}$$

The derivations of equations (4) and (5) have been obtained by using results of Patel [6], Crank and Gupta [3], Crank and Crowley [4] and Saitoh [7].

DISCRETIZATION OF EQUATIONS

Working on the u–θ grid, we compute the movements of some selected points on the isotherm u = const. along the radial lines θ = const. at successive intervals of time Δt. Let us choose Δu and $\Delta\theta$ such that $u_i = u_0 + i\Delta u$, $i = 0(1)N$ ($u_0 = 0$, $u_N = 1$) and $\theta_j = \theta_0 + j\Delta\theta$, $j = 0(1)M$ ($\theta_0 = 0$, $\theta_M = \pi/4$). Assuming that $r_{i,j}^k$ denotes the position of a point on the isotherm $u = u_i$ along the radial line $\theta = \theta_j$ and at $t = t_k = k\Delta t$ and that values of r on various isotherms are already known at $t = t_k$, we describe below the explicit and implicit schemes for determining the values of r at t_{k+1}, i.e. $r_{i,j}^{k+1}$, $i = 0(1)N$ and $j = 0(1)M$.

A general finite difference replacement of equation (4) gives

$$\frac{r_{i,j}^{k+1}-r_{i,j}^{k}}{\Delta t} = \alpha\Bigg[\frac{r_{i-1,j}^{k+1}-2r_{i,j}^{k+1}+2r_{i+1,j}^{k+1}}{(r_{i,j}^{k+1}-r_{i-1,j}^{k+1})^2} - 1/r_{i,j}^{k+1} - 1/(r_{i,j}^{k+1})^2\left(\frac{r_{i,j}^{k+1}-r_{i-1,j}^{k+1}}{\Delta u}\right)(u_{\theta\theta})_{i,j}^{k+1}\Bigg] + (1-\alpha)\Bigg[\frac{r_{i-1,j}^{k}-2r_{i,j}^{k}+r_{i+1,j}^{k}}{(r_{i,j}^{k}-r_{i-1,j}^{k})^2} - 1/r_{i,j}^{k} - 1/(r_{i,j}^{k})^2\left(\frac{r_{i,j}^{k}-r_{i-1,j}^{k}}{\Delta u}\right)(u_{\theta\theta})_{i,j}^{k}\Bigg],$$

$$i = 1(1)N-1, \quad j = 0(1)M. \tag{6}$$

It gives an explicit scheme for $\alpha = 0$ and an implicit scheme for $\alpha = 0.5$. We describe below the details of implementing the implicit scheme. The other scheme, i.e. the explicit one, can be followed with much greater ease.

Let $\Delta r_{i,j}^k$ denote the displacement of the isotherm u_i along θ_j in the time interval Δt, i.e.

$$r_{i,j}^{k+1} = r_{i,j}^k + \Delta r_{i,j}^k. \tag{7}$$

Expressing equation (6) in terms of Δ and retaining only the first-order terms, we get

$$A_i\Delta r_{i-1,j}^k + B_i\Delta r_{i,j}^k + C_i\Delta r_{i+1,j}^k = D_i, \tag{8}$$
$$i = 1(1)N-1, \quad j = 0(1)M$$

where

$$A_i = -\Delta t\frac{r_{i-1,j}^k-2r_{i,j}^k+r_{i+1,j}^k}{(r_{i,j}^k-r_{i-1,j}^k)^3} - \frac{\Delta t}{2(r_{i,j}^k-r_{i-1,j}^k)^2} - \frac{\Delta t}{2\Delta u}\frac{1}{(r_{i,j}^k)^2}(u_{\theta\theta})_{i,j}^{k+1}$$

$$B_i = 1+\Delta t\frac{r_{i-1,j}^k-2r_{i,j}^k+r_{k+1,j}^k}{(r_{i,j}^k-r_{i-1,j}^k)^3} - \frac{\Delta t}{2(r_{i,j}^k)^2} + \frac{\Delta t}{2(r_{i,j}^k-r_{i-1,j}^k)^2} + \frac{\Delta t}{\Delta u}\left\{\frac{r_{i,j}^k-r_{i-1,j}^k}{(r_{i,j}^k)^3} + \frac{1}{2}\frac{1}{(r_{i,j}^k)^2}\right\}(u_{\theta\theta})_{i,j}^{k+1}$$

$$C_i = -\frac{\Delta t}{2(r_{i,j}^k-r_{i-1,j}^k)^2}$$

and

$$D_j = \Delta t\frac{r_{i-1,j}^k-2r_{i,j}^k+r_{i+1,j}^k}{(r_{i,j}^k-r_{i-1,j}^k)^2} - \frac{\Delta t}{r_{i,j}^k} - \frac{\Delta t}{2\Delta u}\frac{r_{i,j}^k-r_{i-1,j}^k}{(r_{i,j}^k)^2}[(u_{\theta\theta})_{i,j}^{k+1}+(u_{\theta\theta})_{i,j}^k].$$

Equation (8) can be solved provided $\Delta r_{0,j}^k$ and $\Delta r_{N,j}^k$ are known. As the isotherm $u = u_0$ always coincides with the fixed surface of the prism, we have

$$\Delta r_{0,j}^k = 0. \tag{9}$$

Although the condition at the interface given by equation (5) can be discretized implicitly to obtain an extra equation in order to solve equation (8), it gives rise to unnecessary complications. We, instead compute $\Delta r_{N,j}^k$ from the explicit discretization of equation (5)

$$\Delta r_{N,j}^k = \frac{\Delta t}{\beta}\left[1+\frac{1}{(r_{N,j}^k)^2}\left(\frac{r_{N,j+1}^k-r_{N,j-1}^k}{2\Delta\theta}\right)\right]\frac{\Delta u}{r_{N,j}^k-r_{N-1,j}^k}. \tag{10}$$

Further, expanding $u_{\theta\theta}$ in time direction by Taylor's series we can write

$$u_{\theta\theta}^{k+1} = u_{\theta\theta}^k + \Delta t\frac{\partial}{\partial t}(u_{\theta\theta}^k) + \ldots$$

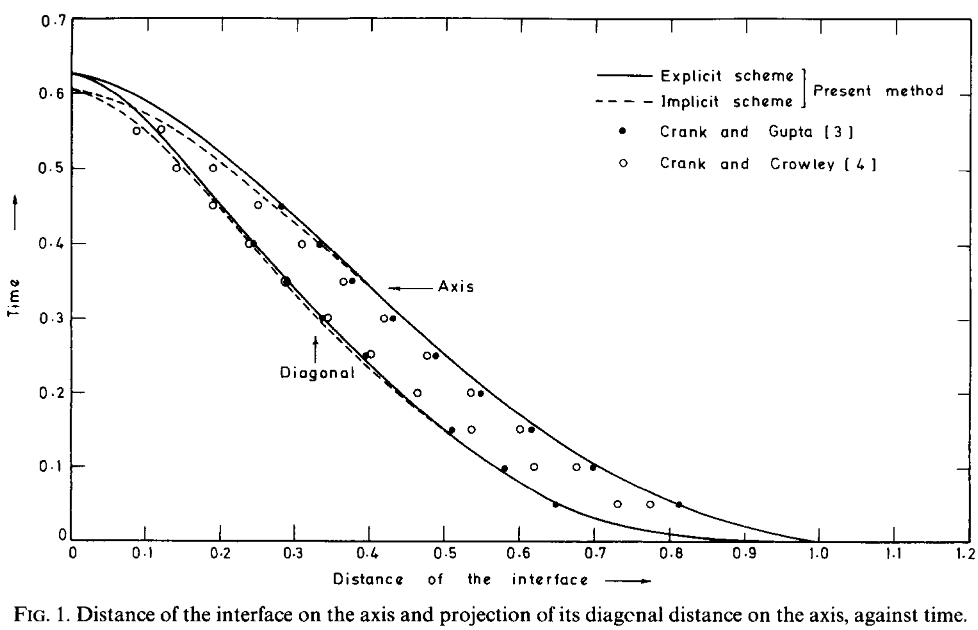

FIG. 1. Distance of the interface on the axis and projection of its diagonal distance on the axis, against time.

For small Δt and also realizing that the behaviour of u is smooth, we may assume that $u_{\theta\theta}^{k+1} \simeq u_{\theta\theta}^{k}$.

The term $u_{\theta\theta}$ appearing in equation (6) is computed in the following manner. We interpolate (or extrapolate) linearly the values of u corresponding to $r_{i,j}^k$ at $\theta = \theta_{j-1}$ and θ_{j+1}.

If we denote the value of u corresponding to $r_{i,j}^k$ at θ_{j-1} by $u_{i,j}^-$ and at θ_{j+1} by $u_{i,j}^+$ then $(u_{\theta\theta})_{i,j}^k$ can be expressed as

$$(u_{\theta\theta})_{i,j}^k = \frac{u_{i,j}^- - 2u_{i,j}^k + u_{i,j}^+}{(\Delta\theta)^2} \tag{11}$$

where $u_{i,j}^-$ and $u_{i,j}^+$ may be computed by the following interpolation formulae

$$u_{i,j}^- = u_{i-1} + \frac{r_{i,j}^k - r_{i-1,j-1}^k}{r_{i,j-1}^k - r_{i-1,j-1}^k}(u_i - u_{i-1}), \tag{12}$$

$$i = 1(1)N, \quad j = 1(1)M$$

and

$$u_{i,j}^+ = u_{i+1} + \frac{r_{i,j}^k - r_{i+1,j+1}^k}{r_{i,j+1}^k - r_{i+1,j+1}^k}(u_i - u_{i+1}), \tag{13}$$

$$i = 0(1)N-1, \quad j = 0(1)M-1.$$

NUMERICAL RESULTS AND DISCUSSION

As an IMM is not self starting, one has to commence the computations after adopting the initial positions of the isotherms from some other source. In the present problem the relevant values, i.e. the position vectors of various points on the isotherms, are taken as in ref. [3], from the one parameter integral method of Poots [8] at $t = 0.0461$. We have selected $\Delta u = 0.1$ and $\Delta\theta = \pi/40$ for both the explicit and implicit schemes. The time step for the explicit scheme it taken to be $\Delta t = 0.00005$ and for the implicit scheme to be $\Delta t = 0.0001$. The distance of the interface on the axis and the projection of its radial distance along the diagonal on the axis, at various times has been plotted in Fig. 1. Corresponding results from the IMMs of refs. [3, 4] are also shown for comparison. As can be seen, the values obtained from the present method are very near to those due to earlier authors so far as the distance of the interface on the axis is concerned. However, the values pertaining to the distance along the diagonal, computed from the present method, tend to agree more with ref. [3] rather than with ref. [4]. Interface contours are also plotted in one quarter of the prism at various times in Fig. 2 along with the corresponding figures of ref. [3]. A close agreement is clearly observed between the two. The results obtained from the explicit and implicit schemes are almost identical except with a little variation near the end. The time for complete solidification of the prism is obtained to be 0.6252 and 0.6052 from the explicit and implicit schemes, respectively. The corresponding figures from Crank and Gupta [3] and Crank and Crowley [4] are not available for comparison.

As the isotherm is expected to assume a circular shape gradually near the end of the process, we keep computing the difference between the distances of the interface along the axis and along the diagonal for each isotherm. As soon as it becomes negligible within the desired accuracy (10^{-4} in the present problem), we fix the centre of the isotherm at the origin. At this stage the displacement of the circular isotherm need not be calculated for all θ's. It has been calculated at the point on the axis only.

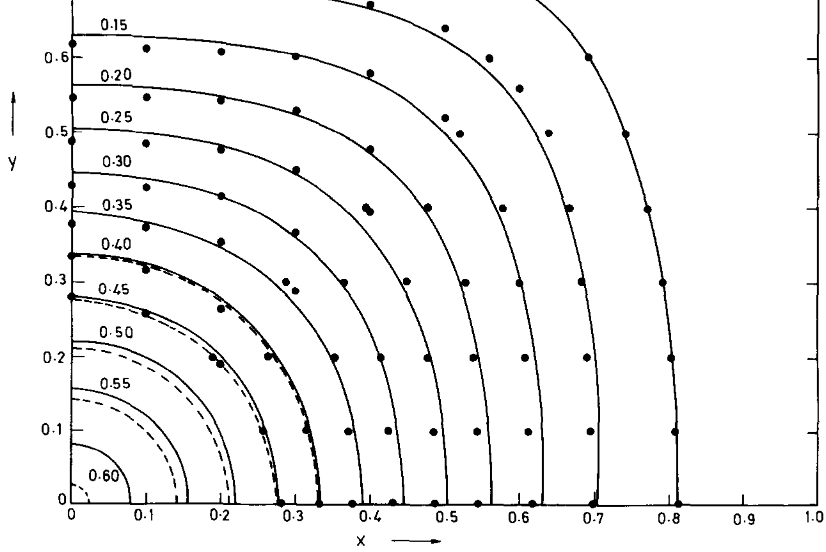

FIG. 2. Interface contours at $t = 0.05\ (0.05)\ 0.60$.

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