

# Treatment of multi-dimensional moving boundary problems by coordinate transformation

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**Abstract**—A method based on coordinate transformation which transforms the time-varying domain into an invariant one, is given for solving multi-dimensional solidification/melting problems. The present method differs from its predecessors in that it transforms one space variable only while others remain unchanged. This results in tremendous amounts of saving in computations in comparison to methods proposed by earlier authors. Two sample problems are treated by the method in two dimensions one concerned with solidification of the square prism and the other with melting in a rectangular prism. The numerical results obtained by the present method are found to be in good agreement with those due to earlier authors. The method is further extended to three dimensions through a problem of cuboid solidification. Obtained in the present paper are perhaps the only available results for the complete solidification of the cuboid.

## 1. INTRODUCTION

THE STUDY of moving boundary problems (MBPs) arising in the heat conduction and diffusion has become a highly popular subject in recent years due to its vast applications in a variety of problems of practical importance (see refs. [1] and [2]). These problems are characterised by the presence of a moving boundary (MB) giving rise to solution domains that vary with time. The analytical solutions to MBPs are restricted to a very few particular cases and those too in one dimension only (see ref. [3]). As each practical problem presents its own complexity, recourse is generally made to numerical methods. The description of various numerical and other methods with useful bibliography may be found in the surveys of Furzeland [4] and Crank [5].

In an earlier but interesting method for dealing with one-dimensional (1-D) MBPs, Landau [6] fixed the moving boundary by making some suitable transformation. This novel idea was further exploited by Beaubouff [7] and Ferris and Hill [8] for solving MBPs in one dimension. The use of coordinate transformation for immobilising the boundary in case of two-dimensional (2-D) MBPs has also been reported by some of the authors. For example, Furzeland [9] uses body-fitted curvilinear coordinate transformation for transforming a curved-shaped region into a fixed rectangular domain; Saitoh [10] and Duda *et al.* [11] discuss problems by reducing them to polar form and make the subsequent transformation on it. More recently Sparrow and Hsu [12] also use coordinate transformation for their control volume formulation.

In their formulation, Furzeland [9] and Saitoh [10] transform both of the space variables, thereby involving the first and the second derivatives of one space variable with respect to the other along the fixed boundaries as well as along the moving boundary. The numerical evaluation of these derivatives creates a lot of problems since special attention is paid in computing

them. Moreover, it may be noted that immobilisation of the boundary in polar form as suggested by Saitoh [10] is not possible when two ends of the MB move along two parallel lines, as will be a case discussed here.

In the present paper we suggest a methodology based on coordinate transformation for solving two- and three-dimensional MBPs. The procedure differs from those of its predecessors in the sense that only one of the space variables is transformed while the other is kept unchanged. As a result not only a much simpler formulation is obtained in comparison to those of Furzeland [9] and Saitoh [10] but the space derivatives appearing along the interface and the fixed boundaries are also eliminated. The problems of solidification of square prism and melting in a rectangle are taken as test problems which have already been discussed by other authors, namely, Poots [13], Crank and Gupta [14], Saitoh [10], Crank and Crowley [15, 16], Jamet and Bonnerot [17] and Furzeland [9]. The method has been further extended to three dimensions by solving the problem of solidification of a cuboid which has been previously dealt with by Riley and Duck [18] through an approximate analytical method. Lazaridis [19] also treated the problem by a numerical technique but could not go far in time. The results obtained in the present paper for the complete solidification of cuboid appear to be the only ones available so far.

## 2. TWO-DIMENSIONAL PROBLEMS

### Problem I

An infinitely long, square prism is initially filled with a fluid at its fusion temperature of unity, say. The temperature on its surface is suddenly dropped to zero and is maintained constant throughout. The process of solidification starts from the surface inwards. We shall be interested in finding the temperature distribution in the solidified region along with the determination of the interface position at any instant of time.

Let us assume that the square cross-section of the



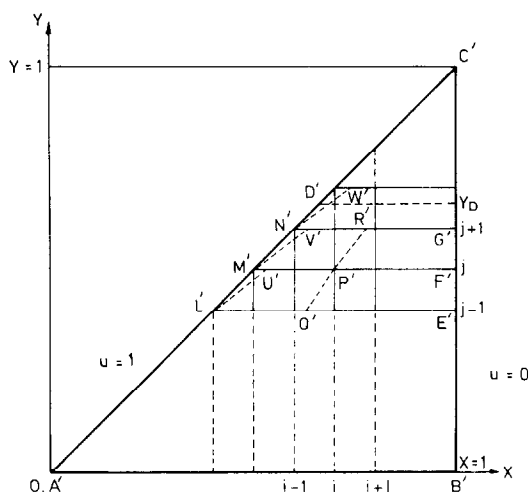


FIG. 2. Domain of reference after transformation (Problem I).

and

$$X = 1 - \frac{(1-x)(1-y)}{1-s(y,t)}, \quad s(y,t) \leq x \leq 1, \\ Y \leq X \leq 1, \quad t > 0 \quad (8)$$

where  $s(y, t)$  satisfies the following

$$s(y, t) = \begin{cases} \varepsilon(y, t) & \text{if } \varepsilon(y, t) > y \\ y & \text{otherwise} \end{cases}$$

where  $x = \varepsilon(y, t)$  is an alternative form of the interface  $\phi = 0$ . By applying the above transformations, equation (1) becomes

$$u_t = \frac{1-X}{1-s} s_t(u_x)_{Y,t} + \frac{(1-Y)^2}{(1-s)^2} (u_{xx})_{Y,t} + (u_{yy})_{x,t} \text{ in } R. \quad (9)$$

$(u_{YY})_{x,t} = (u_{yy})_{x,t}$  denotes the second partial derivative of  $u(x, y, t)$  with respect to  $Y$  at constant  $x$  and constant  $t$  in the untransformed domain;  $(u_x)_{Y,t}$  and  $(u_{XX})_{Y,t}$  denote the first and the second partial derivatives respectively of  $u(X, Y, t)$  at constant  $Y$  and constant time in the transformed domain. The condition (5) at the interface transforms to

$$s_t = \frac{1}{\beta} \left[ \frac{(1-Y)^2}{(1-s)^2} (u_x)_{Y,t}^2 + (u_Y)_{x,t}^2 \right] / \frac{(1-Y)}{(1-s)} (u_x)_{Y,t}, \quad (10)$$

since  $s_i = \varepsilon_i$  at  $X = Y$  for  $Y \leq Y_D$ , and is zero otherwise.  $Y_D$  being the point where the interface cuts the diagonal (Fig. 2). The boundary conditions (2) and (3) respectively transform to

$$u = 0 \quad \text{on the surface} \quad X = 1 \quad (11)$$

and

$$u = 1 \quad \text{on} \quad X = Y, \quad Y \leq Y_n. \quad (12)$$

*Discretization of transformed equations.* As usual, we subdivide the domain  $R \equiv [X, Y | 0 \leq Y \leq 1, Y \leq X \leq 1]$ , choosing a suitable  $\Delta X$  and  $\Delta Y$ , such that

$X_i = X_0 + i\Delta X$ ,  $i = 0(1)N$  with  $X_0 = 0$ ,  $X_N = 1$  and  $Y_j = Y_0 + j\Delta Y$ ,  $j = 0(1)N$  with  $Y_0 = 0$ ,  $Y_N = 1$ . We evaluate the  $us$  on this grid at successive time steps  $t_m = t_0 + m\Delta t$ , where  $t_0$  is the time when numerical computations are commenced and  $\Delta t$  is the time interval.

As has been stated earlier, because of the symmetry we need to calculate the values of  $u$  in the lower triangle  $A'B'C'$  (Fig. 2), i.e. at grid points  $(X_i, Y_j)$ , where

$$Y_i = Y_0 + j\Delta Y, \quad j = 0(1)N$$

$$X_i = X_0 + i\Delta X, \quad i = j(1)N.$$

The temperature in the upper triangle can be known by symmetry.

Let us assume that the temperatures and the positions of the interface are known at the  $m$ th time level; then an explicit finite-difference replacement of (9) at a general point  $(X_i, Y_j, t_m)$  in the space-time grid, where the temperature is denoted by  $u_{i,j}^m$ , can be made in the following way,

$$\begin{aligned} \frac{u_{i,j}^{m+1} - u_{i,j}^m}{\Delta t} &= \frac{1 - X_i}{1 - s_j^m} \cdot \frac{u_{i+1,j}^m - u_{i-1,j}^m}{2\Delta X} \\ &\times \frac{s_j^{m+1} - s_j^m}{\Delta t} + \frac{(1 - Y_j)^2}{(1 - s_j^m)^2} \\ &\times \frac{u_{i-1,j}^m - 2u_{i,j}^m + u_{i+1,j}^m}{(\Delta X)^2} + (u_{YY})_{i,j}^m \end{aligned} \quad (13)$$

for  $j = 0(1)N$  and

$$i = \begin{cases} j(1)N-1, & \text{if } Y_j > Y_D \\ j+1(1)N-1, & \text{if } Y_i \leq Y_D \end{cases}$$

with  $u_{N,j} = 0, j = 0(1)N$  and  $u_{j,j} = 1, Y_j \leq Y_D$ . The value of  $u_{i,j}^{m+1}$ , i.e. the value of  $u_{i,j}$  at the advanced level of time, can be determined explicitly from (13) provided  $s_j^{m+1}$  is known. For computing  $s_j^{m+1}$ , we make use of (10) whose finite-difference replacement can be written as,

$$\frac{s_j^{m+1} - s_j^m}{\Delta t} = -\frac{2}{\beta} \left[ \frac{(1 - Y_j)^2}{(1 - s_j^m)^2} \left( \frac{u_{j+1,j}^m - u_{j,j}^m}{\Delta X} \right)^2 + (u_r)_{j,j}^2 \right] \frac{(1 - Y_j)}{(1 - s_j^m)} \frac{u_{j+1,j}^m - u_{j,j}^m}{\Delta X} \quad (14)$$

giving  $s_j^{m+1}$  explicitly for  $Y_j \leq Y_D$ . For  $Y > Y_D$ , i.e. for the region which does not undergo transformation,

$$s_j^{m+1} = s_j^m = (1 - Y_j)^2. \quad (15)$$

In order to evaluate the  $u_Y$  and  $u_{YY}$  appearing in the right side of equations (13) and (14), we proceed as follows :

Again, referring to Fig. 1, let us assume that at any time  $t$ , L, M and N are the positions of the interface at different  $y$ s in the  $x$ - $y$  plane. The distances  $d(L, E)$ ,  $d(M, F)$  and  $d(N, G)$  are transformed to  $d(L', E')$ ,  $d(M', F')$  and  $d(N', G')$  respectively in Fig. 2. Consider an internal mesh point  $P'$  at  $Y = Y_j$  in the  $X$ - $Y$  plane. Let  $P$  be its corresponding position at  $y = Y_j$  in the untransformed plane  $x$ - $y$  (Fig. 1). Let the points  $Q$  and  $R$ , in Fig. 1, correspond to fixed  $x$  at  $y = Y_{j-1}$  and

$y = Y_{j+1}$ , respectively. The transformed positions of Q and R are denoted by Q' and R' in the  $X$ - $Y$  plane in Fig. 2. The values of  $u$  at Q' and R' are computed by linear interpolation, for the present purpose, using two nearest mesh points. For example, when P' is  $(X_i, Y_j)$ , we compute

$$u_{Q'} = u_{i-1,j-1}^m + \frac{u_{i,j-1}^m - u_{i-1,j-1}^m}{\Delta X} \times \left[ 1 - X_{i-1} - \frac{(1-s_j^m)(1-Y_{j-1})}{(1-s_{j-1}^m)(1-Y_j)} (1-X_i) \right] \quad (16)$$

for  $j = 1(1)N-1$  and

$$i = \begin{cases} j(1)N-1, & Y_j > Y_D \\ j+1(1)N-1, & Y_j \leq Y_D \end{cases}$$

Similarly

$$u_{R'} = u_{i,j+1}^m + \frac{u_{i+1,j+1}^m - u_{i,j+1}^m}{\Delta X} \times \left[ 1 - X_{i+1} - \frac{(1-s_j^m)(1-Y_{j+1})}{(1-s_{j+1}^m)(1-Y_j)} (1-X_i) \right] \quad (17)$$

for

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

Using the above values,  $u_{YY}$  at the internal mesh point P' may be obtained by the usual three point formula,

$$(u_{YY})_{P'} = \frac{u_{Q'} - 2u_{P'} + u_{R'}}{(\Delta Y)^2}. \quad (18)$$

The first derivative w.r.t.  $Y$ , needed at the interface points, e.g. at M' (Fig. 2), is computed in a similar manner using a forward difference formula,

$$(u_Y)_{M'} = \frac{u_{V'} - u_{M'}}{\Delta Y}. \quad (19)$$

the value of  $u_{V'}$  is computed using a formula similar to (17) and is given by

$$u_{V'} = u_{j+1,j+1}^m + \frac{u_{j+2,j+1}^m - u_{j+1,j+1}^m}{\Delta X} \times \left[ 1 - X_{j+2} - \frac{(1-s_j^m)(1-Y_{j+1})}{(1-s_{j+1}^m)(1-Y_j)} (1-X_{j+1}) \right] \quad (20)$$

for  $Y_j \leq Y_D$ .

### Numerical results and discussion

In order to assess the accuracy of the results obtained from the present method, we also make a start, like the IMM [14], by taking the initial values of the temperature and interface positions from Poots [13] one parameter integral method at  $t = 0.0461$ . Two sets of results have been obtained—one with  $\Delta X = \Delta Y = 0.1$  and the other with  $\Delta X = \Delta Y = 0.05$ ; the size of  $\Delta t$  is chosen to meet the stability criterion of the explicit scheme. In the present problem the value of  $\Delta t$  has been chosen to be 0.0001 and 0.00004 for the first and the second sets respectively.

The positions of the interface for different  $Y$ s are

evaluated using equations (14) and (15) at various times. To compare our results with those of [14] and [15], the point where the interface cuts the diagonal is obtained by fitting a circle through the two neighbouring points like [14]. The symmetry of the problem suggests that towards the end of the solidification process, the interface should become a circle and once the circle is formed, it should persist till the end. In view of this fact, we keep on making a comparison between the distances of the interface on the axis and on the diagonal from the origin. As soon as the difference between these two becomes negligible, within the desired accuracy ( $10^{-4}$  in our case), the centre of circle is fixed at the origin. In doing so the position of the interface has to be computed at the axis only. Its location at different  $Y$ s can then be ascertained using simple arithmetic. The distances of the interface along the  $x$ -axis as well as the  $x$ -coordinates of its position on the diagonal are given in Table 1 along with the comparative figures from the earlier authors, viz. Crank and Gupta [14] and Crank and Crowley [15]. The figures corresponding to distance of the interface on the axis agree in all the three methods from the beginning to the end. However, so far as the figures corresponding to the distance along the diagonal is concerned, the results obtained from the present method agree better with those of IMM [14]. In any case, the present results tend to agree with those of Crank and Crowley also [15] as time goes by.

It is worthwhile to note that the present method can be carried right up to the end of the solidification process. The total time for the complete solidification has been found to be 0.6302 and 0.6258, when  $\Delta X = \Delta Y = 0.1$  and  $\Delta X = \Delta Y = 0.05$  respectively. Since other methods can not be pursued until complete solidification takes place, such figures are not available for them.

### Problem II

The present numerical technique is now applied to another problem defined in a rectangular region. This problem has also been solved by Jamet and Bonnerot [17], Furzeland [9] and Crank and Crowley [16]. Since the method has already been elaborated in connection with Problem I, we would like to deal with the computational aspect of the present problem in brief only.

The problem concerns melting of ice contained in a rectangular cylinder of infinite length with a cross-section,  $0 \leq x \leq 1$ ,  $0 < y \leq 4$ . Initially the part of the cylinder  $y > 2 + \cos \pi x$  contains ice at the melting temperature zero while the remaining portion,  $y \leq 2 + \cos \pi x$ , is occupied by water with a temperature distribution given by,

$$u(x, y, 0) = 1 - \frac{y}{2 + \cos \pi x}, \quad y \leq 2 + \cos \pi x. \quad (21)$$

All the sides of the cylinder, except  $y = 0$  where the temperature  $u = 1$  is maintained for  $t > 0$ , are insulated. Thus the equation to be solved, in non-

Table 1. Comparison of  $x$ -coordinate of the solid-liquid interface on the  $x$ -axis and on the diagonal

Time, $t$	On the $x$ -axis				On the diagonal			
	Crank and Gupta [14]	Crank and Crowley [15]	Present method		Crank and Gupta [14]	Crank and Crowley [15]	Present method	
			$\Delta X = \Delta Y = 0.1$ $\Delta t = 0.0001$	$\Delta X = \Delta Y = 0.05$ $\Delta t = 0.00004$			$\Delta X = \Delta Y = 0.1$ $\Delta t = 0.0001$	$\Delta X = \Delta Y = 0.05$ $\Delta t = 0.00004$
0.05	0.8125	0.775	0.8125	0.8125	0.6483	0.732	0.6476	0.6527
0.10	0.6979	0.676	0.6982	0.6993	0.5812	0.619	0.5642	0.5746
0.15	0.6157	0.601	0.6156	0.6175	0.5103	0.535	0.4935	0.5046
0.20	0.5473	0.536	0.5463	0.5489	0.4428	0.463	0.4264	0.4395
0.25	0.4865	0.477	0.4837	0.4874	0.3948	0.399	0.3642	0.3791
0.30	0.4302	0.420	0.4244	0.4295	0.3351	0.342	0.3130	0.3273
0.35	0.3766	0.364	0.3663	0.3731	0.2831	0.283	0.2590	0.2765
0.40	0.3337	0.308	0.3078	0.3162	0.2332	0.237	0.2176	0.2236
0.45	0.2816	0.249	0.2495	0.2569	0.1947	0.188	0.1764	0.1817
0.50	—	0.188	0.1894	0.1953	—	0.139	0.1339	0.1381
0.55	—	0.119	0.1271	0.1290	—	0.087	0.0899	0.0912
0.60	—	—	0.0562	0.0513	—	—	0.0398	0.0363
Time of complete-freezing		—	0.6302	0.6258				

The dashes indicate that the corresponding figures are not available.

dimensional form, is

$$u_t = u_{xx} + u_{yy} \quad \text{in } \Omega \quad (22)$$

where  $\Omega = [x, y | y \leq 2 + \cos \pi x, \quad 0 \leq x \leq 1]$ . The corresponding boundary conditions are given by,

$$u = 1 \quad \text{on } y = 0$$

$$u_x = 0 \quad \text{on } x = 0 \quad \text{and} \quad x = 1$$

and

$$u_y = 0 \quad \text{on } y = 4, \quad \text{for } t > 0. \quad (23)$$

The conditions at the interface, which arise due to continuity of the temperature and discontinuity in its first derivative along the interface, may be written as

$$u = 0, \quad \frac{\partial u}{\partial n} = -v_n \quad \text{on } \phi(x, y, t) = 0 \quad \text{for } t > 0, \quad (24)$$

where  $\phi(x, y, t)$  denotes the position of the interface at any time  $t$ ;  $v_n$  the velocity of the interface along the outward drawn normal  $n$ , of the interface.

#### Transformation of equations

Figure 3 shows the regions of ice and water separated by the interface  $AB$  at any time  $t$ . By making use of the appropriate change of variables the interface is transformed to coincide with  $y = 4$ , resulting in  $OABC$  (Fig. 3) to be mapped onto the complete rectangle  $OA'B'C'$  (Fig. 4). Following transformations are used in order to achieve the desired objective.

$$t = t, \quad X = x \quad \text{and}$$

$$Y = \frac{4y}{s(x, t)} \quad 0 \leq y \leq s, \quad 0 \leq Y \leq 4, \quad (25)$$

where  $s(x, t)$  is the  $y$ -coordinate of the interface for fixed  $x$  at any time  $t$ .

Using these variables the heat conduction equation (25) transforms to,

$$u_t = \frac{Y}{s} (u_Y)_{X,t} s_t + \frac{16}{s^2} (u_{YY})_{X,t} + (u_{XX})_{Y,t}. \quad (26)$$

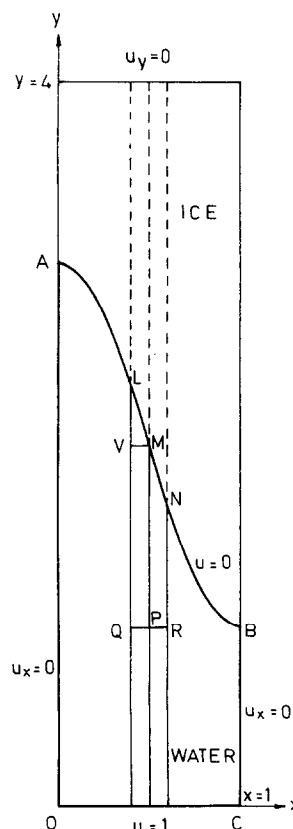
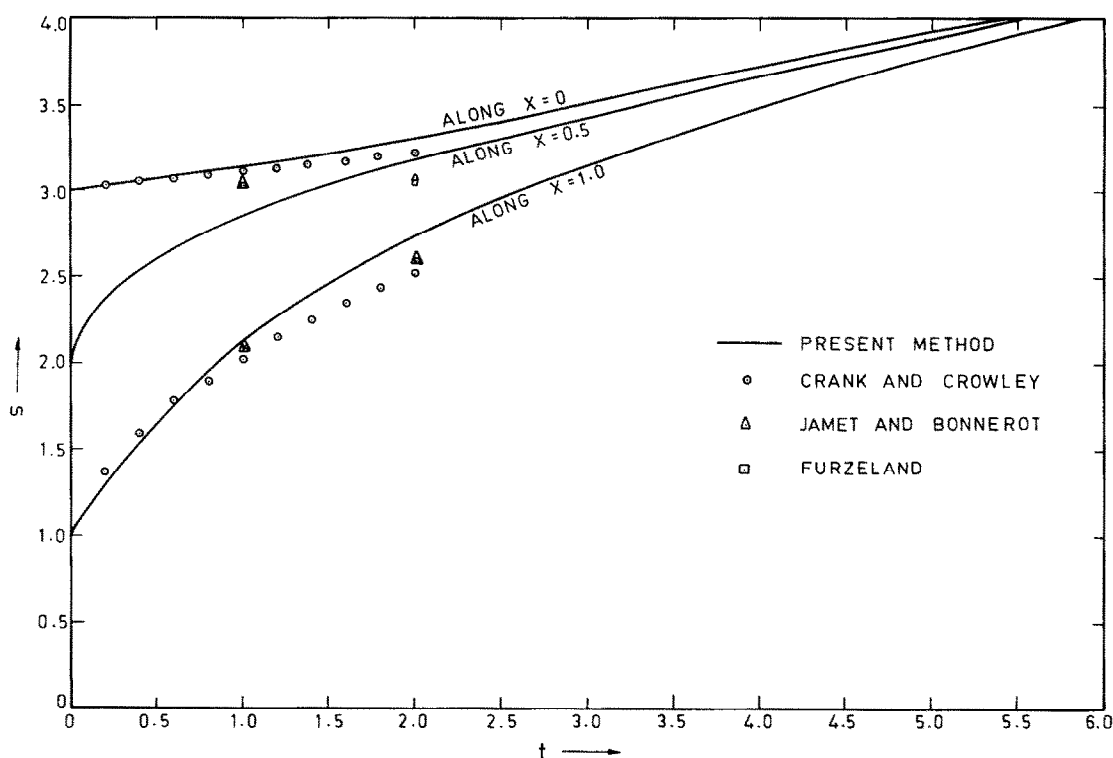


FIG. 3. Domain of reference before transformation (Problem II).



FIG. 5. Graph of the interface position against time along  $x = 0.0, 0.5$  and  $1.0$ .

(26) may be written as,

$$\begin{aligned} \frac{u_{i,j}^{m+1} - u_{i,j}^m}{\Delta t} = & \left[ \frac{Y_j}{s_i^m} \cdot \frac{u_{i,j+1}^m - u_{i,j-1}^m}{2\Delta Y} \right. \\ & \times \left. \frac{s_i^{m+1} - s_i^m}{\Delta t} \right] + \left[ \frac{16}{(s_i^m)^2} \right. \\ & \times \left. \frac{u_{i,j-1}^m - 2u_{i,j}^m + u_{i,j+1}^m}{(\Delta Y)^2} \right] + (u_{xx})_{i,j}^m \end{aligned} \quad (29)$$

$j = 1(1)M-1 \quad \text{and} \quad i = 0(1)N$

with  $u_{i,0} = 1$  and  $u_{i,M} = 0$ ;  $i = 0(1)N$ .

It may be noted that  $s_i^{m+1}$  is not known in the above equation. It can, however, be calculated from the equation (28) after replacing it by the following difference formula

$$\begin{aligned} \frac{s_i^{m+1} - s_i^m}{\Delta t} = & \left[ (u_x)_{i,M}^2 + \frac{16}{(s_i^m)^2} \right. \\ & \times \left. \left( \frac{u_{i,M}^m - u_{i,M-1}^m}{\Delta Y} \right) \right] \left/ \frac{4}{s_i^m} \frac{u_{i,M}^m - u_{i,M-1}^m}{\Delta Y} \right., \end{aligned} \quad (30)$$

$i = 0(1)N$ .

Having calculated  $s_i^{m+1}$  from (30) the value of  $u_{i,j}^{m+1}$  can be obtained explicitly from (29).  $u_{xx}$  and  $u_x$  appearing in (29) and (30) are computed using a similar interpolation technique as used in Problem I.

#### Numerical results and discussion

It is conventional in a finite-difference method to subdivide the domain into square meshes. However, it

may be noticed in the present problem that there is a very steep temperature gradient everywhere at zero time (Fig. 3). On account of this the selection of equal meshes in  $X$  and  $Y$  directions gives rise to inaccurate results. Therefore we make the numerical computations after subdividing the interval  $0 \leq X \leq 1$  into 20 equal parts and interval  $0 \leq Y \leq 4$  into 10 equal parts, which is equivalent to taking  $\Delta X = 0.05$  and  $\Delta Y = 0.4$ . In order to meet the stability criterion the time step  $\Delta t$  is taken to be 0.0001.

Table 2 gives the positions of the interface along the edges  $X = 0$  and  $X = 1$ . As already mentioned, this problem has also been solved in refs. [9, 16 and 17]. Their results, as far as available, are also given side-by-side for comparison. A good deal of consistency can be observed in the present results (Fig. 5).

### 3. THREE-DIMENSIONAL PROBLEM

#### Mathematical statement

Consider a cuboid, bounded by planes parallel to the coordinate planes

$$f(x, y, z) \equiv (1 - x^2)(1 - y^2)(1 - z^2) = 0, \quad (31)$$

filled with a liquid at its fusion temperature  $u = 1$ . At time  $t = 0$  a temperature  $u = 0$  is imposed and maintained at the outer boundary. As the liquid starts solidifying, at any time during the period of solidification, let the location of the three-dimensional

solidification front be given by,

$$\phi(x,y,z,t) = 0 \tag{32}$$

an isothermal surface at temperature  $u = 1$ .

The equation describing the heat conduction process (in non-dimensional form) is given by,

$$u_t = u_{xx} + u_{yy} + u_{zz} \text{ in } D \tag{33}$$

where  $D$  is the domain enclosed by the surfaces (31) and (32). The associated boundary conditions are,

$$u = 0 \text{ on } f(x,y,z) = 0, \quad t > 0 \tag{34}$$

and

$$u = 1 \text{ on } \phi(x,y,z,t) = 0, \quad t > 0. \tag{35}$$

The initial condition is given by,

$$u = 1 \text{ and } \phi \equiv f = 0 \text{ at } t = 0. \tag{36}$$

Another familiar condition to be satisfied at the interface is,

$$\frac{\partial u}{\partial n} = -\beta v_n \text{ on } \phi(x,y,z,t) = 0 \tag{37}$$

where  $n$  is the outward normal with respect to liquid to  $\phi = 0$ ;  $v_n$  is the velocity of the moving interface in the direction of  $n$  and  $\beta$  is a constant depending on the thermal properties of the material undergoing phase change.

As there is symmetry about the coordinate planes we may work in a single octant, say, formed by the planes  $x = 1, y = 1, z = 1$ , where  $u = 0$ , and the coordinate planes  $x = 0, y = 0, z = 0$ , where normal fluxes are zero (due to symmetry). We can further divide this octant into three symmetrical portions. One of these portions, a pentahedron  $O, ABCD$  shown in Fig. 6, may be defined by,

$$R = [x,y,z | p(y,z) \leq x \leq 1, 0 \leq y,z \leq 1] \tag{38}$$

where  $p(y,z)$  is defined as,

$$p(y,z) = \begin{cases} y, & \text{if } y \geq z \\ z, & \text{if } y \leq z. \end{cases}$$

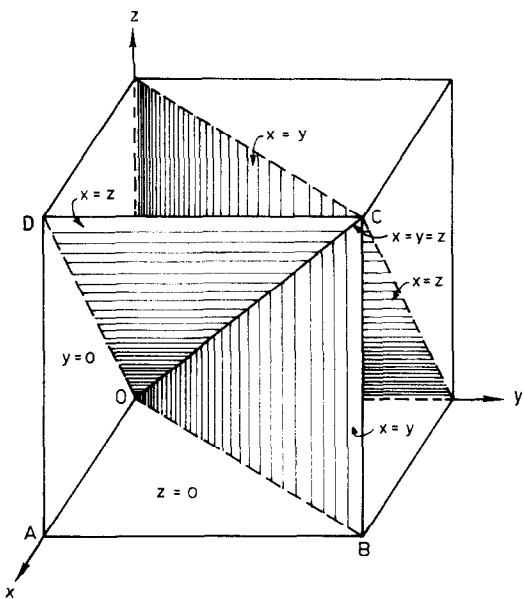


FIG. 6. One of the three symmetrical pentahedron.

The other portions can be drawn in analogous manner.

Now we shall be concerned with solving (33) over  $\Omega \subset R$ , where  $\Omega$  is bounded by the plane  $ABCD$ , which remains at a temperature  $u = 0$  for  $t > 0$ , the interface  $A'B'C'D'$ , where  $u = 1$ , and the four planes which are given by,

- $ADD'A \quad \text{i.e. } y = 0$
- $ABB'A \quad \text{i.e. } z = 0$
- $DCC'D' \quad \text{i.e. } x = z$

and

- $BCC'B' \quad \text{i.e. } x = y \text{ (see Fig. 7).}$

It may be noted that due to symmetry the normal fluxes to these planes will be zero. Mathematically, the domain  $\Omega$  may be represented as,

$$\Omega = [x,y,z | s(y,z,t) \leq x \leq 1, 0 \leq y,z \leq 1] \tag{39}$$

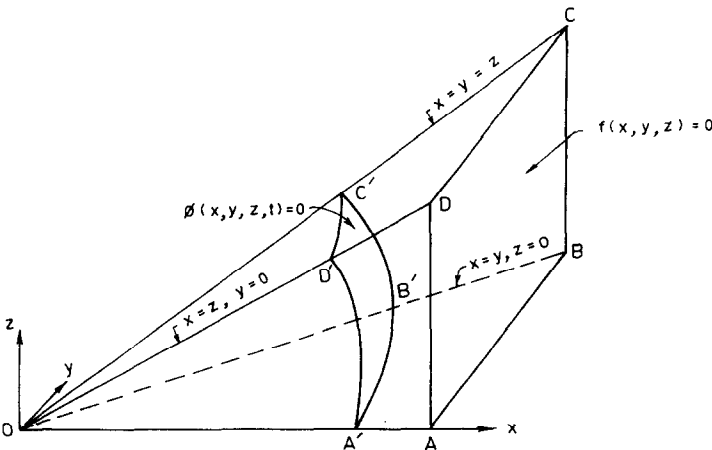


FIG. 7. Domain of reference before transformation (3-D).



where  $s(y, z, t)$  satisfies the following,

$$s(y, z, t) = \begin{cases} \varepsilon(y, z, t) & \text{if } \varepsilon(y, z, t) \geq p(y, z) \\ p(y, z) & \text{otherwise} \end{cases}$$

where  $x = \varepsilon(y, z, t)$  is an alternative form of the solid/liquid interface  $\phi = 0$ .

#### Transformation of equations

We transform the time-dependent domain to an invariant domain by making a change in one space variable only. For some fixed values of  $y, z$  and  $t$ , say,  $t = t$ ,  $y = Y$  and  $z = Z$ , let us consider the following transformation on  $x$ ,

$$X = 1 - \frac{(1-x)[1-p(Y, Z)]}{1-s(Y, Z)}. \quad (40)$$

Obviously, the foregoing transformation maps the variable domain onto  $R$ , which remains fixed for all times. As a result of the above, equation (33) becomes,

$$u_t = \frac{1-X}{1-s} (u_x)_{Y,Z,t} s_t + \frac{(1-p)^2}{(1-s)^2} (u_{xx})_{Y,Z,t} + (u_{yy})_{x,z,t} + (u_{zz})_{x,y,t} \quad (41)$$

where  $s_t$  denotes the partial derivative of  $s$  with respect to  $t$ ,  $(u_{yy})_{x,z,t} = (u_{yy})_{x,z,t}$  and  $(u_{zz})_{x,y,t} = (u_{zz})_{x,y,t}$  are the second derivatives of  $u(x, y, z, t)$  with respect to  $Y$  and  $Z$  at constant  $x, z, t$  and constant  $x, y, t$  respectively.

The associated boundary conditions now become,

$$u = 0 \quad \text{on} \quad X = 1 \quad (42)$$

and

$$u = 1 \quad \text{on} \quad X = p(Y, Z) \quad (43)$$

where  $s(Y, Z, t) = \varepsilon(Y, Z, t)$

while on the portion where  $s(Y, Z, t) \neq \varepsilon(Y, Z, t)$ , the condition of zero normal flux holds.

The interface condition (37) can also be written in an alternative manner as

$$s_t = \frac{1}{\beta} [(u_x)^2 + (u_y)^2 + (u_z)^2] / u_x. \quad (44)$$

In terms of the new variables above becomes,

$$\varepsilon_t = \frac{1}{\beta} \left[ \frac{(1-p)^2}{(1-\varepsilon)^2} (u_x)_{Y,Z,t} + (u_y)_{x,z,t}^2 + (u_z)_{x,y,t}^2 \right] \left[ \frac{1-p}{1-\varepsilon} (u_x)_{Y,Z,t} \right] \quad (45)$$

since  $s_t(Y, Z, t) = \varepsilon_t(Y, Z, t)$ , at  $X = p(Y, Z)$ , and is zero otherwise.

#### Discretization of the transformed equations

Let us define a cubical grid in the octant, choosing suitable  $\Delta X, \Delta Y$  and  $\Delta Z$ . A point  $(X_i, Y_j, Z_k)$  on this grid is given by  $X_i = X_0 + i\Delta X$ ,  $Y_j = Y_0 + j\Delta Y$  and  $Z_k = Z_0 + k\Delta Z$ ,  $i, j, k = 0(1)N$ , where  $(X_0, Y_0, Z_0)$  is the origin  $(0, 0, 0)$  and  $(X_N, Y_N, Z_N)$  is the farthest vertex of the cuboid from the origin. We compute the values of  $u$  on

this grid at time  $t_m = t_0 + m\Delta t$ , where  $t_0$  is the initial time,  $\Delta t$  is the time step and  $m$  is a positive integer. However, due to symmetry as already discussed, we need computing  $u$  only for

$$k, j = 0(1)N \quad \text{and} \quad i = \omega(1)N$$

$$\text{where } \omega = \begin{cases} j, & \text{if } j \geq k \\ k, & \text{if } j < k \end{cases}$$

Assuming that the temperatures and the position of the interface are known up to time  $t_m = m\Delta t$ , the finite-difference replacement of equation (41) by explicit method at point  $(X_i, Y_j, Z_k, t_m)$ , where the temperature is denoted by  $u_{i,j,k}^m$ , may be written as

$$\begin{aligned} \frac{u_{i,j,k}^{m+1} - u_{i,j,k}^m}{\Delta t} &= \frac{1-X_i}{1-s_{j,k}^m} \frac{u_{i+1,j,k}^m - u_{i-1,j,k}^m}{2\Delta X} \cdot \frac{s_{j,k}^{m+1} - s_{j,k}^m}{\Delta t} \\ &+ \frac{(1-p_{j,k})^2}{(1-s_{j,k}^m)^2} \frac{u_{i-1,j,k}^m - 2u_{i,j,k}^m + u_{i+1,j,k}^m}{(\Delta X)^2} \\ &+ (u_{yy})_{i,j,k}^m + (u_{zz})_{i,j,k}^m \quad (46) \end{aligned}$$

$$i = \begin{cases} \omega + 1(1)N - 1, & \text{if } s_{j,k}^m = \varepsilon_{j,k}^m \\ \omega(1)N - 1, & \text{if } s_{j,k}^m = p_{j,k} \end{cases} \quad j, k = 0(1)N - 1$$

with  $u_{\omega,j,k}^m = 1$ .

The values of  $u_{i,j,k}^{m+1}$  may be computed explicitly provided  $s_{j,k}^{m+1}$  is known. To determine it we make use of the finite-difference replacement of equation (44), which gives,

$$\begin{aligned} \frac{\varepsilon_{j,k}^{m+1} - \varepsilon_{j,k}^m}{\Delta t} &= \frac{1}{\beta} \left[ \frac{(1-p_{j,k})^2}{(1-\varepsilon_{j,k}^m)^2} \right. \\ &\times \frac{u_{\omega+1,j,k}^m - u_{\omega,j,k}^m}{\Delta X} + (u_y^2)_{\omega,j,k}^m \\ &+ (u_z^2)_{\omega,j,k}^m \left. \right] \left[ \frac{(1-p_{j,k})}{(1-\varepsilon_{j,k}^m)} \right] \\ &\times \frac{u_{\omega+1,j,k}^m - u_{\omega,j,k}^m}{\Delta X}. \quad (47) \end{aligned}$$

This provides  $\varepsilon$  explicitly. For  $j, k$  where  $s_{j,k}^m = p_{j,k}$ , we have

$$s_{j,k}^{m+1} = s_{j,k}^m = p_{j,k}. \quad (48)$$

The values of  $u_{yy}$  and  $u_{zz}$  are computed at constant  $x, z, t$  and  $x, y, t$  respectively. The procedure is given below.

Let us denote by  $v_j^-$  the temperature at a point on grid line  $Y = Y_{j-1}, Z = Z_k$  corresponding to the mesh point  $(X_i, Y_j, Z_k)$  for constant  $x, z, t$  and  $v_j^+$  on  $Y = Y_{j+1}, Z = Z_k$ . Similarly  $v_k^-$  on  $Y = Y_j, Z = Z_{k-1}$  and  $v_k^+$  on  $Y = Y_j, Z = Z_{k+1}$  for constant  $x, y, t$ . Then we can write,

$$(u_{yy})_{i,j,k}^m = \frac{v_j^- - 2u_{i,j,k}^m + v_j^+}{(\Delta Y)^2} \quad (49)$$

and

$$(u_{zz})_{i,j,k}^m = \frac{v_k^- - 2u_{i,j,k}^m + v_k^+}{(\Delta Z)^2} \quad (50)$$

where  $v_j^-, v_j^+, v_k^-$  and  $v_k^+$  are computed from the

following interpolation formulae,

$$v_j^- = u_{i-1,j-1,k}^m + \left[ (1-X_{i-1}) - \frac{1-p_{j-1,k}}{1-p_{j,k}} \cdot \frac{1-s_{j,k}}{1-s_{j-1,k}} (1-X_i) \right] \times \frac{u_{i,j-1,k}^m - u_{i-1,j-1,k}^m}{\Delta X}$$

$$v_j^+ = u_{i,j+1,k}^m + \left[ (1-X_i) - \frac{1-p_{j+1,k}}{1-p_{j,k}} \cdot \frac{1-s_{j,k}}{1-s_{j+1,k}} (1-X_i) \right] \times \frac{u_{i,j+1,k}^m - u_{i,j+1,k}^m}{\Delta X}$$

$$v_k^- = u_{i-1,j,k-1}^m + \left[ (1-X_{i-1}) - \frac{1-p_{j,k-1}}{1-p_{j,k}} \cdot \frac{1-s_{j,k}}{1-s_{j,k-1}} (1-X_i) \right] \times \frac{u_{i,j,k-1}^m - u_{i-1,j,k-1}^m}{\Delta X}$$

$$v_k^+ = u_{i,j,k+1}^m + \left[ (1-X_i) - \frac{1-p_{j,k+1}}{1-p_{j,k}} \cdot \frac{1-s_{j,k}}{1-s_{j,k+1}} (1-X_i) \right] \times \frac{u_{i,j,k+1}^m - u_{i,j,k+1}^m}{\Delta X}$$

Similar expressions for  $u_y$  and  $u_z$  appearing in (46) may be written as,

$$(u_y)_{\omega,j,k}^m = \frac{v_j^+ - u_{\omega,j,k}^m}{\Delta Y} \quad (51)$$

$$(u_z)_{\omega,j,k}^m = \frac{v_k^+ - u_{\omega,j,k}^m}{\Delta Z} \quad (52)$$

where,

$$v_j^+ = u_{\omega,j+1,k}^m + \left[ (1-X_{\omega+1}) - \frac{1-p_{j+1,k}}{1-p_{j,k}} \cdot \frac{1-s_{j,k}}{1-s_{j+1,k}} (1-X_{\omega}) \right] \times \frac{u_{\omega+2,j+1,k}^m - u_{\omega+1,j+1,k}^m}{\Delta X}$$

$$v_k^+ = u_{\omega+1,j,k+1}^m + \left[ (1-X_{\omega+1}) - \frac{1-p_{j,k+1}}{1-p_{j,k}} \cdot \frac{1-s_{j,k}}{1-s_{j,k+1}} (1-X_{\omega}) \right] \times \frac{u_{\omega+2,j,k+1}^m - u_{\omega+1,j,k+1}^m}{\Delta X}$$

#### Numerical computations

As the present method is not self-starting we have to adopt the initial values of temperatures and interface locations from some other sources at a small time. This we have chosen from the one-parameter heat-balance

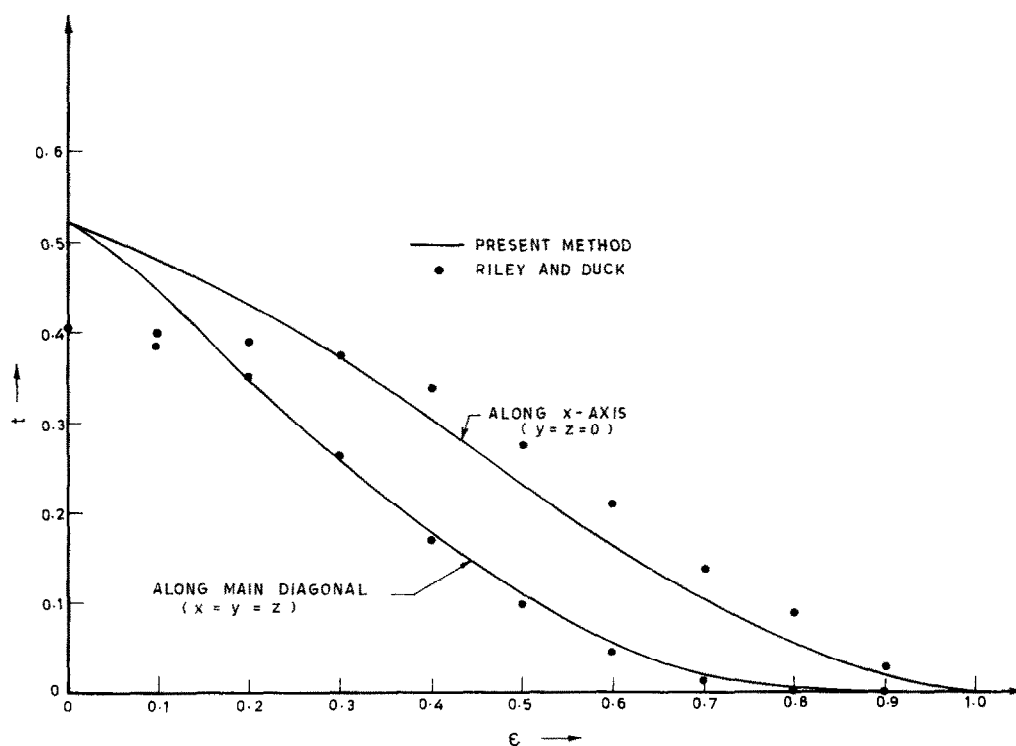


FIG. 8. Comparison of  $x$ -coordinates of the interface positions along the  $x$ -axis and the main diagonal at various times.

integral method of Riley and Duck [18] at  $t \approx 0.03$ . The space mesh sizes are taken to be  $\Delta X = \Delta Y = \Delta Z = 0.1$  and the time step to be  $\Delta t = 0.00005$ .

Due to symmetry of the problem the shape of the solidification front will be a cube with rounded corners at small times which should gradually become spherical. In view of this fact, we keep on making a check between the distances of the interface at the  $x$ -axis and the main diagonal. As soon as the difference between the two becomes negligible within the desired accuracy ( $10^{-5}$  in our case), we assume the interface to be of spherical shape with centre at the origin. From here onwards, we compute the movements of the interface on the axis only.

In Fig. 8 we have shown the movements of the interface along the  $x$ -axis and the main diagonal  $x = y = z$ . Corresponding figures of [18] are also shown for comparison.

It must be pointed out that the distances of the interface along the main diagonal  $x = y = z$  and also along the diagonal  $x = y, z = \text{constant}$ , are not readily available since they do not lie on a mesh point generally. These are computed by assuming circular interface profile on the diagonal  $y = x$  for planes  $z = k\Delta z$ . Through these points, is projected the position along the main diagonal considering a spherical shape of the solid-liquid interface on this diagonal.

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## TRAITEMENT DES PROBLEMES MULTIDIMENSIONNELS DE FRONTIERE MOBILE PAR UNE TRANSFORMATION DE COORDONNEES

**Résumé**—Une méthode basée sur une transformation de coordonnées qui transforme le domaine variable dans le temps en un autre invariant, est donnée pour résoudre les problèmes multidimensionnels de solidification ou fusion. La présente méthode diffère des précédentes en ceci qu'elle transforme une seule variable d'espace tandis que les autres restent inchangées. Ceci économise le temps de calcul numérique. Deux exemples de problème bidimensionnels sont traités, l'un concernant la solidification d'un prisme carré, l'autre la fusion d'un prisme rectangulaire. Les résultats numériques obtenus sont en bon accord avec ceux d'auteurs antérieurs. La méthode est étendue ensuite à trois dimensions à travers un problème de solidification cubique. Les résultats de ce dernier cas sont probablement uniques car il ne semble pas que des données soient disponibles.

## LÖSUNG VON MEHRDIMENSIONALEN PROBLEMEN MIT BEWEGTEN GRENZEN DURCH KOORDINATENTRANSFORMATION

**Zusammenfassung**—Eine Methode, welcher die Transformation des zeitvarianten Gebietes in ein zeitinvariantes zugrundeliegt, wird für die Lösung von mehrdimensionalen Erstarrungs/Schmelzproblemen vorgeschlagen. Die vorgestellte Methode unterscheidet sich von vorhergehenden, indem sie nur eine Raumvariable transformiert, während die anderen unverändert bleiben. Dies hat eine enorme Einsparung an Rechenaufwand zur Folge, verglichen mit Methoden, die von früheren Autoren vorgeschlagen wurden. Zwei zweidimensionale Beispielaufgaben werden mit dieser Methode bearbeitet—eine behandelt den Erstarrungsvorgang eines quadratischen Prismas, die andere den Schmelzvorgang in einem rechteckigen Prisma. Die mit dieser Methode erhaltenen numerischen Ergebnisse stimmen gut mit denen von früheren Autoren überein. Diese Methode wird durch ein Problem des kubischen Erstarrens auf drei Dimensionen erweitert. Der vorgestellte Artikel enthält die vielleicht einzigen verfügbaren Ergebnisse der vollständigen kubischen Erstarrung.

## РЕШЕНИЕ МНОГОМЕРНЫХ ЗАДАЧ С ДВИЖУЩЕЙСЯ ГРАНИЦЕЙ МЕТОДОМ ПРЕОБРАЗОВАНИЯ КООРДИНАТ

**Аннотация**—Для решения многомерных задач затвердевания/плавления используется метод, основанный на преобразовании координат. Представленный метод отличается от предложенных ранее тем, что изменяется только одна пространственная переменная, а все остальные остаются неизменными. При расчетах это приводит к большой вычислительной экономии по сравнению с методами других авторов. Рассматриваются две двумерные задачи: одна—о затвердевании квадратной призмы и другая—о плавлении прямоугольной призмы. Установлено, что численные результаты, полученные этим методом, хорошо согласуются с данными других авторов. Далее метод распространяется на решение трехмерных задач в случае затвердевания прямоугольного параллелепипеда. Данные, полученные в настоящей работе, являются, пожалуй, единственными по затвердеванию прямоугольного параллелепипеда.