MAKING CURVED INTERPHASES STRAIGHT IN PHASE-CHANGE PROBLEMS

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RESUMEN

This paper presents a method for straighten curved interphases arising in phase-change problems. The method works on isoparametric finite elements, performing a second transformation which the interphase looks as a straight line. This allows using the current Gaussian integration technique for squares to evaluate the integrals over each phase. Several numerical examples are presented to show the performance of the method.

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INTRODUCTION

During the latest years very much interest has been devoted to the numerical solution of phase-change problems. This phenomenon takes place in many processes of technological interest such as soil freezing, steel and glass industry, thermal protection of heated devices, nuclear safety analysis and many others[1,2]. This problem is characterized by a geometric-type nonlinearity due to the moving boundaries of the regions where the heat transfer equation must be solved[3]. Regarding this fact, many authors have developed algorithms which track the position of the moving front. There are a number of works which use a deforming grid formulation[4-6]. In these methods the interphase always lies on one side of some determined elements. The grid moves to adapt to the displacements of the interphase, remaining the same elements in the solid and liquid phases. As an alternative to reduce the number of degrees of freedom, O'Neill[7] discretizes only the boundary of each phase, using Green functions to eliminate the volume integrals. This boundary element method is applied to the quasisteady form of the heat transfer equation (low Stefan number) in materials where the thermal coefficients are not temperature-dependant. Although tracking methods are a "natural" approximation to this problem, there are a number of drawbacks that induce using fixed domain methods. Between them one can address that they need starting solutions and they cannot cope with appearing/disappearing phases and multiple or no-smooth interphases.

Fixed domain methods use weak formulations[8,9] and implicitely contain the interphase moving condition in the integrated form of the heat transfer equation. Atthey[10] uses the enthalpy as the nodal unknown

and an explicit scheme for the time integration. Once the enthalpy is determined for a given time step, he obtains the temperature applying the inverse enthalpy-temperature relation. Comini et al.[11] replace the effect of the latent heat by an equivalent heat capacity valid in a narrow range of temperatures around the melting temperature. In this way, this equivalent heat capacity method removes the discontinuity at the phase-change front, allowing using the temperature as the main unknown. However this class of method has the drawback that the time step used must be small enough to prevent the interphase from advancing more than one element per time step, otherwise the algorithm loses part of the latent heat involved. Meyers[12] instead, splits the interphase into a phase-change region within which the enthalpy varies linearly with the temperature. But when this mushy region moves in-between two nodes, the algorithm does not realize its motion. A way to circumvent this objection is to use a large regularization parameter so that the phase-change region contains several elements. Hence the solution is strongly dependent on the size of the regularizaton parameter whose proper magnitude is unknown a priori. Rolph et al.[13] and Roose et al.[14] use a fictitious heat source applied to those elements which are changing phase, until such elements are completely melted. The features of these algorithms resemble those of the enthalpy-based methods. Fredmond and Blanchard[15] integrate the heat transfer equation with respect to time, defining a freezing index as the main unknown. Furthermore they regularize the enthalpy to treat mushy regions.

To avoid the neccessity of an explicit smoothing in the temperature formulation, it has been proposed using discontinuous finite elements[16]. In this way, it is possible to accurately integrate the

latent heat contribution to the equilibrium equation. When an interphase traverses an element, it is split off and the integrations over each phase are perfomed separately over each part. The discontinuous integration concept was previously used by Steven[17] to solve the Poisson equation in materials where the physical properties have a jump discontinuity at a specified internal boundary, as in a non-homogeneous medium. However in both algorithms of References 16 and 17, the interphase is considered straight, which is obviously not true in most practical cases, as when using linear quadrilateral finite elements.

In this paper, the two-dimensional phase-change problem is analized. The discretization process is achieved via quadrilateral finite elements. We use the linear isoparametric coordinate transformation to evaluate the element matrices and a second mapping in those elements where an interphase lays across to obtain a new representation of the elements in which the interphase looks as a straight line. Then the integrals can be accurately calculated using numerical integration for triangles or quadrilaterals. Finally, the nonlinear system of equations is solved by a modified Newton scheme to improve convergence and avoid numerical instability of the iterative scheme. Several numerical examples are presented to show the behavior of the method. It is worth mentioning that this procedure may be straightforwardly applied to other physical problems where there can be elements with an abrupt internal interphase.

GOVERNING EQUATIONS AND FINITE ELEMENT FORMULATION

The heat conduction process is ruled by the partial differential equation

$$\nabla^T k \nabla T + Q = \rho \frac{\partial H}{\partial t} \qquad (1)$$

in a domain Ω, with appropriate boundary and initial conditions. In equation (1) k is the thermal conductivity, T the temperature, Q the internal heat source, ρ the density, H the specific enthalpy and t the time.

For phase-change problems the entalpy has a jump discontinuity at the melting temperature T_m, equal to the latent heat content per unit volume L. Therefore H attains a discontinuity at the free boundary. The integral weak form[8,16] of equation (1) takes into account this discontinuity and is the basis for a finite element analysis[18]. Integrating equation (1) weighted by some functions $N_i(x)$ and applying an α-method[19] for the time derivative of the entalpy, we have

$$- \int_\Omega \nabla N_i(x) \, k \, (T_{n+\alpha-1}) \, \nabla T_{n+\alpha-1} \, dV - \int_\Omega N_i(x) \frac{H_{n+\alpha-1} - H_{n-1}}{\alpha \, \Delta t} \, dV +$$

$$+ \int_\Omega N_i(x) \, Q_{n+\alpha-1} \, dV + \int_{\partial\Omega_q} N_i(x) \, q_{n+\alpha-1} \, dS = 0 \qquad (2)$$

with $0 < \alpha < 1$. In equation (2), n is the outward-drawn normal to the boundary surface, and q is the prescribed heat flux on the portion $\partial\Omega_q$ of the boundary. The subscript n denotes values evaluated at specific times of the time interval. We shall concentrate here on implicit methods, more precisely when $\alpha = 1$. Equation (2) may be rewritten in a compact form as

$$i_j + f_j - g_j = 0 \qquad (3)$$

where f_j is the heat conduction contribution to node j, g_j is the external flux and i_j is the nodal enthalpy. Applying Galerkin's method, that is, using the same weighting functions as shape functions for the temperature discretization, i.e.

$$T = \sum_{i=1}^{N} N_i(x)\, u_i(t)$$

we obtain the system of N equations

$$K_n\, u_n + i\,(u_n) = g_n \qquad (4)$$

where K is the stiffness matrix, i is the enthalpy vector, g is the force vector and u is the vector of nodal unknowns u_i. Equation (3) stands for a single equation of the system (4) where we have

$$[K]_{ij} = \int_{\Omega} \nabla N_i\, k\, \nabla N_j\, dV \qquad (5.1)$$

$$[i]_i = \int_{\Omega} \frac{1}{\Delta t} N_i\, H_n\, dV \qquad (5.2)$$

$$[g]_i = \int_{\Omega} N_i\, Q_n\, dV + \int_{\Omega} \frac{1}{\Delta t} N_i\, H_{n-1}\, dV + \int_{\partial\Omega_q} N_i\, q_n\, ds \qquad (5.3)$$

When the interphase traverses an element, the enthalpy becomes discontinuous inside it and equation (5.2) cannot be adequately integrated using a numerical technique such as the Gaussian rule[16].

Applying the isoparametric transformation[18] to the two-phase element of Figure 1 (a), i.e.

$$x = \sum_{i=1}^{N} N_i\,(\xi,\eta)\, x_i$$

where N_i, $i = 1,\ldots,N$ are the same linear shape functions used for the discretization of the temperature and x_i are nodal coordinates, this element is mapped onto a master which in the (ξ,η) plane looks as in Figure 1 (b). Then the integrals (5) can be perfomed in the master. The nodal enthalpy contribution from equation (5.2) reads as

$$[i]_j = \int_{-1}^{1}\int_{-1}^{1} N_j\,(\xi,\eta)\, H_{(T(x))}\, \det J\, d\xi\, d\eta \qquad (6)$$

where J is the jacobian of the isoparametric transformation.

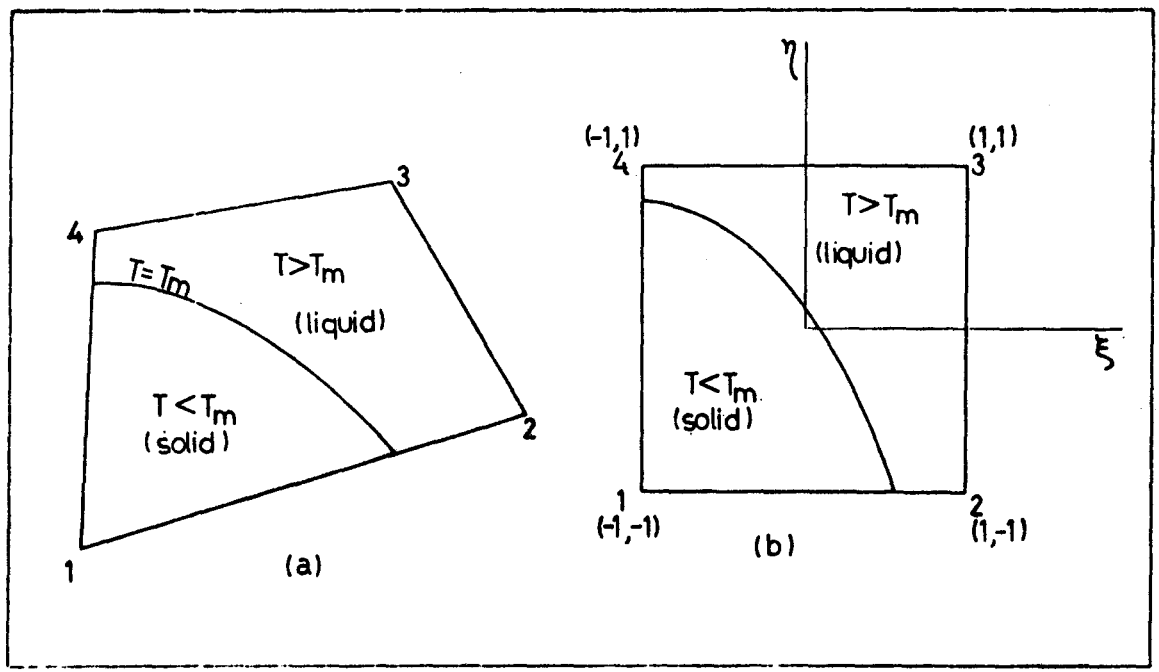

FIGURE 1: Two-phase elements and its isoparametric representation.

In order to integrate the discontinuity accurately , equation (6) may be evaluated separately in both regions, frozen and unfrozen, of the master, i.e.[16]

$$[i]_j = \int_{\Omega_\ell^m} N_j \, H \det J \, d\xi \, d\eta + \int_{\Omega_s^m} N_j \, H \det J \, d\xi \, d\eta \qquad (7)$$

where the subscripts s and ℓ denote solid and liquid phases and the superscript m refers to the master element. Considering the functions H_s and H_ℓ defined as in Figure 2, that is, as extensions of the smooth portions of H , equation (7) may be written in the two following alternative ways

$$[i]_j = \int_{-1}^{1}\int_{-1}^{1} N_j \, H_\ell \det J \, d\xi \, d\eta + \int_{\Omega_s^m} N_j \, (H_s - H_\ell) \det J \, d\xi \, d\eta \qquad (8.1)$$

$$[i]_j = \int_{-1}^{1}\int_{-1}^{1} N_j \, H_s \det J \, d\xi \, d\eta + \int_{\Omega_\ell^m} N_j \, (H_\ell - H_s) \det J \, d\xi \, d\eta \qquad (8.2)$$

As, the integrands in each of the first right-hand side terms in equations (8) are smooth and the integration domain is a square, the problem is reduced to evaluating the integrals of the difference between H_s and H_ℓ in any of the regions into which the master element is divided.

THE SPECIAL ELEMENT

Since the solid and liquid regions have arbitrary curved boundaries, there are no simple numerical integration schemes to evaluate the second integrals in equation (8). The solution proposed in this paper is to find a mapping of the (ξ,η) plane onto another (ξ',η') , in which these regions are transformed into a triangle or a quadrilateral, according to whether the interphase cuts two adjacent or two

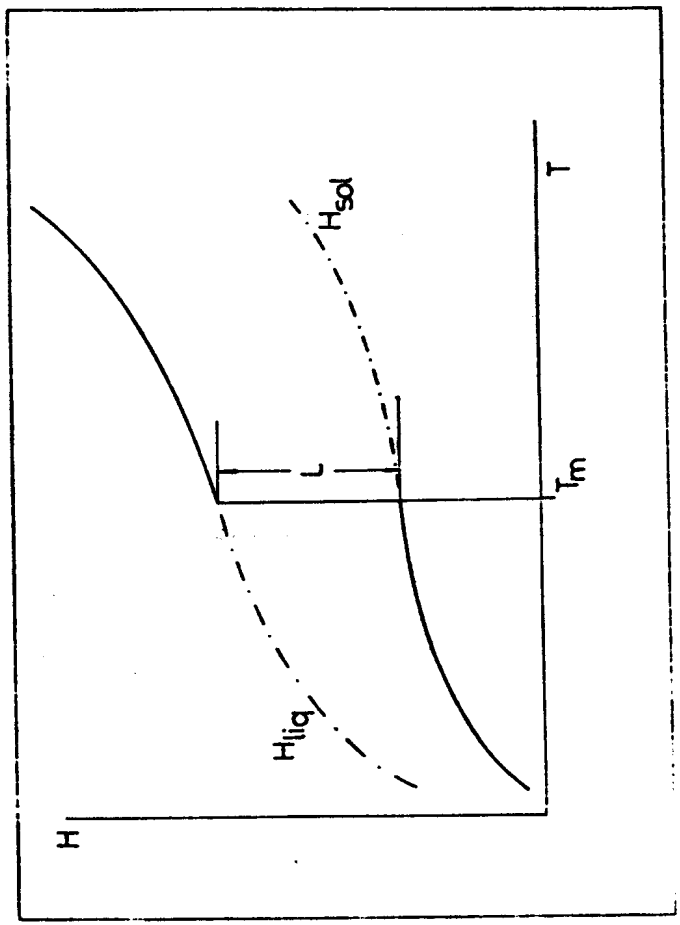

FIGURE 2: Extended enthalpy function for the solid and the liquid.

opposite sides, as shown in Figure 3. Once this transformation is obtained (and may be easily inverted), the problem is solved by integrating in the hatched area of the elements of Figure 3. A first trial may be the mapping $(\xi,\eta) \rightarrow (\xi,T)$ where in each element T is given by

$$T = N_1 u_1 + N_2 u_2 + N_3 u_3 + N_4 u_4 \tag{9}$$

Figure 4 shows the result of this transformation. It is trivial that under this mapping, the interphase is a straight line T = constant, parallel to the ξ axis. Furthermore all the sides of the quadrilateral remain straight because at ξ or η constant, T is a linear function of the remaining variable. However a problem arises when $T_1 = T_4$ or/and $T_2 = T_3$ because this transformation is not one to one but the element is mapped onto a triangle or a line in the (ξ,T) plane. This mapping may be modified to override this drawback. Let us note that the temperature may be written as

$$T = \bar{T} + \left.\frac{\partial T}{\partial \xi}\right|_0 \xi + \left.\frac{\partial T}{\partial \eta}\right|_0 \eta + \left.\frac{\partial^2 T}{\partial \xi\, \partial \eta}\right|_0 \xi\,\eta$$

where $\bar{T}$ is the aritmetic mean of the four nodal temperatures and

$$\left.\frac{\partial T}{\partial \xi}\right|_0 = \frac{T_2 + T_3 - T_1 - T_4}{4}$$

$$\left.\frac{\partial T}{\partial \eta}\right|_0 = \frac{T_4 + T_3 - T_1 - T_2}{4} \tag{10}$$

$$\left.\frac{\partial^2 T}{\partial \xi\, \partial \eta}\right|_0 = \frac{T_3 + T_1 - T_2 - T_4}{4}$$

the subscript 0 denoting values evaluated at the origin of coordinates. Hereinafter we shall use a superimposed dash for denoting such values. Therefore a second trial reads

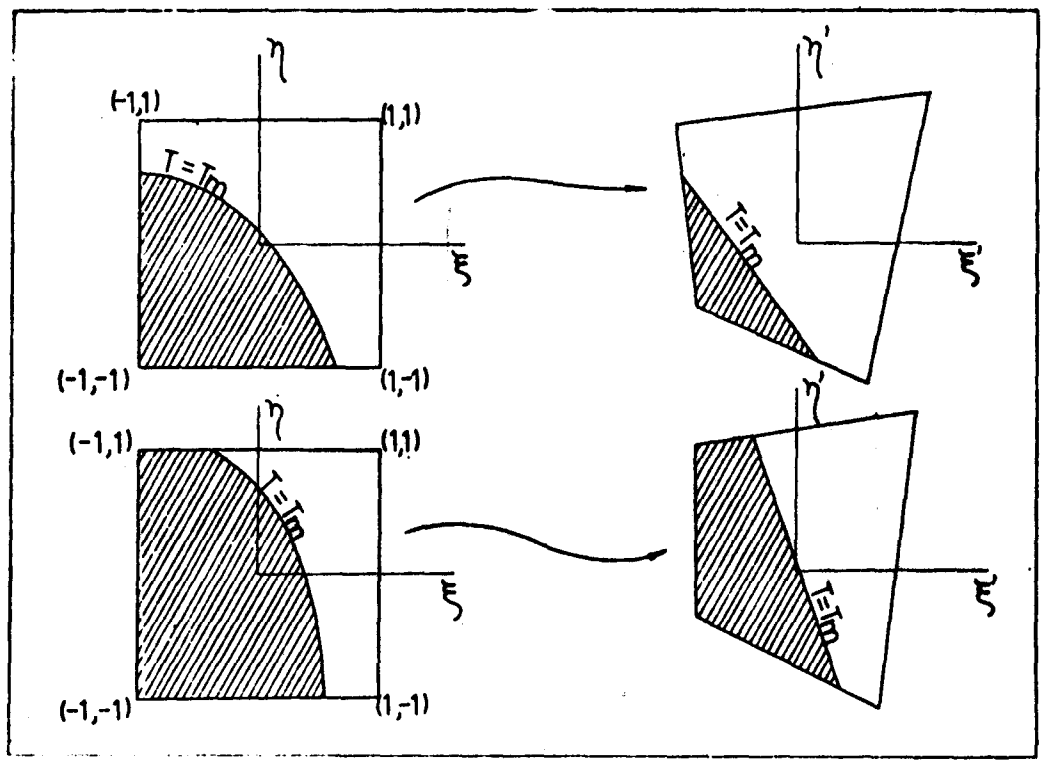

FIGURE 3: Two-phase elements. Integration regions.

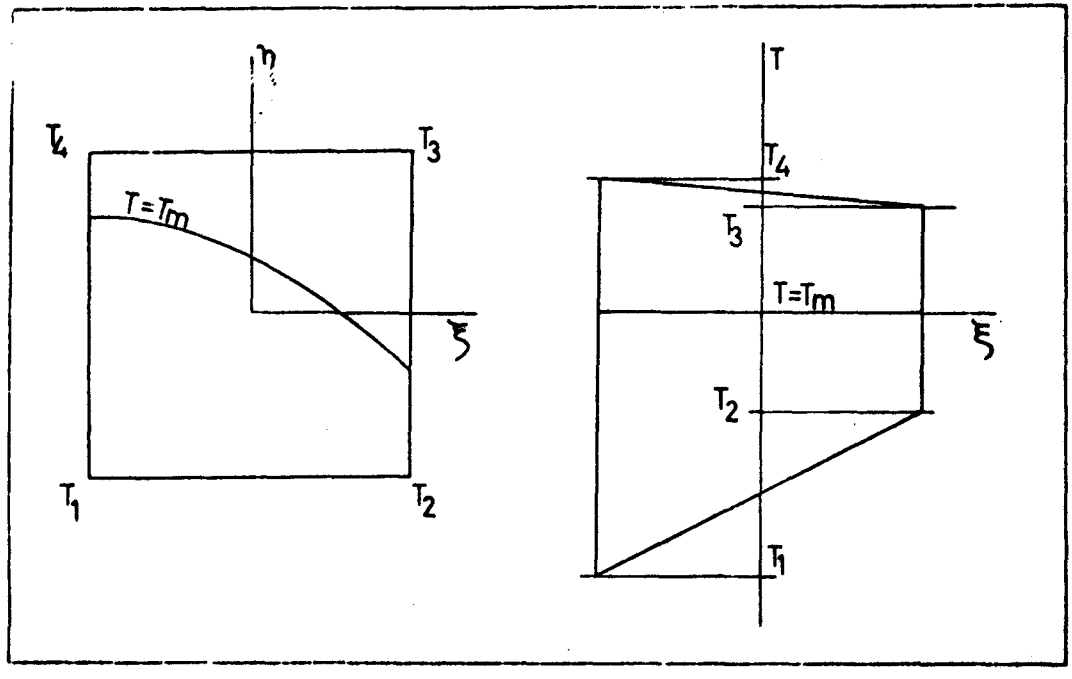

FIGURE 4: Transformation of the master element under the mapping $(\xi,\eta) \rightarrow (\xi,T)$.

$$\begin{bmatrix} \xi \\ \eta \end{bmatrix} + \begin{bmatrix} T \\ V \end{bmatrix} = \begin{bmatrix} \bar{T} + \overline{\frac{\partial T}{\partial \xi}}\,\xi + \overline{\frac{\partial T}{\partial \eta}}\,\eta + \overline{\frac{\partial^2 T}{\partial \xi\,\partial \eta}}\,\xi\,\eta \\ -\overline{\frac{\partial T}{\partial \eta}}\,\xi + \overline{\frac{\partial T}{\partial \xi}}\,\eta \end{bmatrix}$$

The new coordinate system may be written as

$$\begin{bmatrix} T \\ V \end{bmatrix} = M \begin{bmatrix} \xi \\ \eta \end{bmatrix} + \begin{bmatrix} \bar{T} + \overline{\frac{\partial^2 T}{\partial \xi\,\partial \eta}}\,\xi\,\eta \\ 0 \end{bmatrix}$$

where M is the matrix of the transformation

$$M = \begin{bmatrix} \overline{\frac{\partial T}{\partial \xi}} & \overline{\frac{\partial T}{\partial \eta}} \\ -\overline{\frac{\partial T}{\partial \eta}} & \overline{\frac{\partial T}{\partial \xi}} \end{bmatrix}$$

As we shall see later, this transformation solves many of the problems of the previous one. However when the temperature varies linearly within the element giving a straight interphase, it would be elegant that this transformation becomes the identity. This may be reached by writing

$$\begin{bmatrix} \xi' \\ \eta' \end{bmatrix} = M^{-1} \begin{bmatrix} T - \bar{T} \\ V \end{bmatrix}$$

where

$$M^{-1} = \frac{1}{\| \overline{\nabla T} \|^2} \begin{bmatrix} \overline{\frac{\partial T}{\partial \xi}} & -\overline{\frac{\partial T}{\partial \eta}} \\ \overline{\frac{\partial T}{\partial \eta}} & \overline{\frac{\partial T}{\partial \xi}} \end{bmatrix} = \frac{1}{\| \overline{\nabla T} \|^2} M^T$$

Hence

$$\begin{bmatrix} \xi' \\ \eta' \end{bmatrix} = \begin{bmatrix} \xi \\ \eta \end{bmatrix} + \frac{\overline{\frac{\partial^2 T}{\partial \xi \, \partial \eta}}}{\| \overline{\nabla T} \|^2} \xi \, \eta \, \overline{\nabla T} \qquad (11)$$

Equation (11) satisfies the previous requirements. First, for ξ = constant equation (11) gives the parametric equation of one side of the quadrilateral in the (ξ',η') plane with η as the parameter. But ξ' and η' are linear functions of η alone. The same holds for a side with η = constant. Hence the transformation maps quadrilaterals with sides parallel to the axes (ξ,η) onto quadrilaterals in the (ξ',η') plane. Additionally, when the temperature varies linearly within the element, the second derivative in equation (10) is null and the transformation (11) becomes the identity. Furthermore multiplying equation (11) by $\overline{\nabla T}$, we can see that every isotherm $T = T_p$ transforms into a straight line in the (ξ',η') plane since

$$(\overline{\nabla T})^T \begin{bmatrix} \xi' \\ \eta' \end{bmatrix} = (\overline{\nabla T})^T \begin{bmatrix} \xi \\ \eta \end{bmatrix} + \overline{\frac{\partial^2 T}{\partial \xi \, \partial \eta}} \xi \, \eta = T_p - \bar{T} = \text{constant}$$

Denoting

$$A_\xi = \overline{\frac{\partial T}{\partial \xi}} \, \overline{\frac{\partial^2 T}{\partial \xi \, \partial \eta}} \Big/ \| \overline{\nabla T} \|^2$$

$$A_\eta = \overline{\frac{\partial T}{\partial \xi}} \, \overline{\frac{\partial^2 T}{\partial \xi \, \partial \eta}} \Big/ \| \overline{\nabla T} \|^2 \qquad (12)$$

equation (11) reduces to

$$\begin{bmatrix} \xi' \\ \eta' \end{bmatrix} = \begin{bmatrix} \xi \\ \eta \end{bmatrix} + \begin{bmatrix} A_\xi \\ A_\eta \end{bmatrix} \xi \, \eta$$

We can take as a measure of the deformation of the element

the coefficient

$$A_\xi^2 + A_\eta^2 = \left(\frac{\overline{\partial^2 T}}{\partial \xi \, \partial \eta} \right)^2 / \| \overline{\nabla T} \|^2$$

which is the relation between the curvature and the temperature gradient. The determinant of the jacobian J' of this transformation reads

$$\det J' = (1 + A_\xi \eta)(1 + A_\eta \xi) - A_\xi \xi A_\eta \eta = 1 + A_\xi \eta + A_\eta \xi \quad (13)$$

From equation (13) we can see that the determinant of J' is a linear function of ξ and η. Therefore, for the jacobian to be positive everywhere in the quadrilateral, it is neccessary and sufficient that the jacobian be positive in the four corners of the element. Thus this condition reads

$$1 \pm A_\xi \eta \pm A_\eta \xi > 0$$

which is equivalent to

$$1 - (|A_\xi| + |A_\eta|) > 0$$

or applying equation (12)

$$\| \overline{\nabla T} \|^2 > \left| \frac{\overline{\partial^2 T}}{\partial \xi \, \partial \eta} \right| \left(\left| \frac{\overline{\partial T}}{\partial \xi} \right| + \left| \frac{\overline{\partial T}}{\partial \eta} \right| \right) \quad (14)$$

Replacing the derivatives by their definition and after some algebraic manipulations, condition (14) reads

$$|\Delta| \, |\Delta_1| < \Delta_1^2 + \Delta_2^2$$

$$|\Delta| \, |\Delta_2| < \Delta_1^2 + \Delta_1^2$$

where

$$\Delta = T_1 + T_3 - T_2 - T_4$$

$$\Delta_1 = T_3 - T_1$$

$$\Delta_2 = T_2 - T_4$$

Figure 5 shows the plot of these equations in the Δ_1, Δ_2 plane, being the jacobian negative inside the area enclosed by the circles. The square ploted in the same figure is defined by the equation

$$|\Delta_1| + |\Delta_2| = |\Delta|$$

whose interior represents the region where, for a given temperature, there are two isotherms going through the element. This occurs when

$$\min(T_1, T_3) > \max(T_2, T_4) \quad \text{or} \quad \max(T_1, T_3) < \min(T_2, T_4)$$

Thus taking a temperature T^* such that $\min(T_1, T_3) > T^* > \max(T_2, T_4)$ or $\max(T_1, T_3) < T^* < \min(T_2, T_4)$, the isotherm $T = T^*$ cuts the four sides of the quadrilateral as shown in Figure 6. We can see that the region of negative jacobian almost coincide with the region where the two-phase element has two interphases, but this situation is very rare in a numerical computation. Hence we can conclude that in a large number of problems the mapping (11) will behave adequately.

To verify the accuracy of this mapping, we can set $H_1 - H_3 = 1$ in the second integrals of equation (8) and evaluate the area of the hatched regions shown in Figure 7 for several values of β. In Table 1 is depicted the comparison between a.) the method described above to map the region into a triangle, integrating numerically within the triangle with 9 points of Gauss, b.) the straightline-interphase method and c.) the analytical value given by

$$\text{Area} = \tfrac{1}{4} + \left[\frac{1}{2} - \frac{T_3 - T_1}{T_3 + T_1} - \frac{1}{4} \frac{T_3 T_1}{(T_3 + T_1)^2} \ln\left(\frac{T_3}{T_1}\right) \right]$$

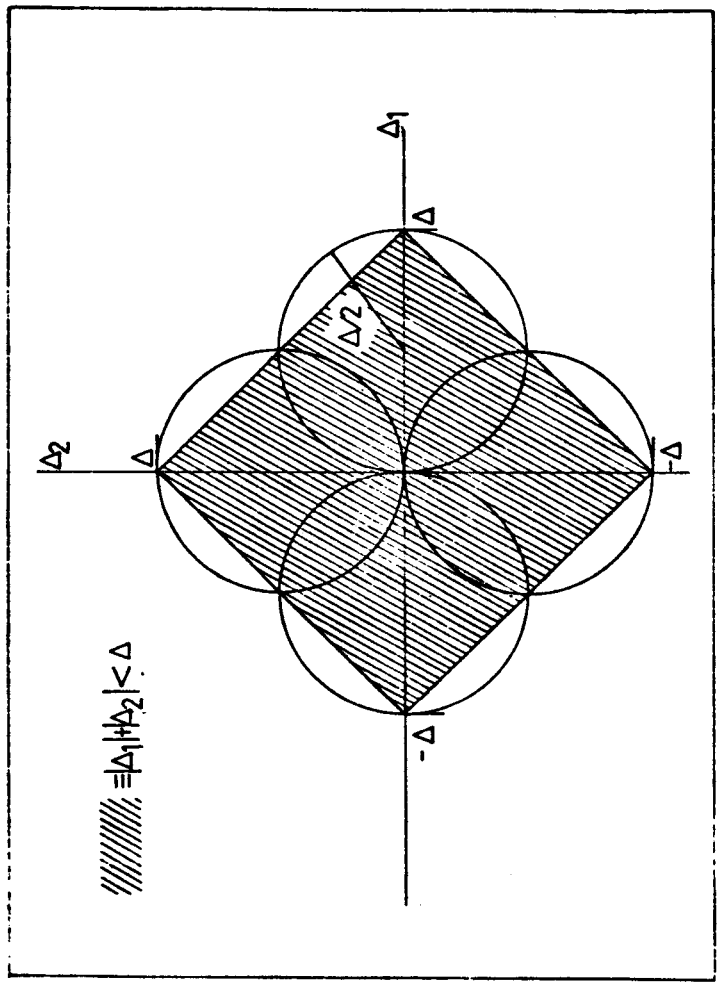

FIGURE 5: Analysis of the mapping. Region of negative Jacobian.

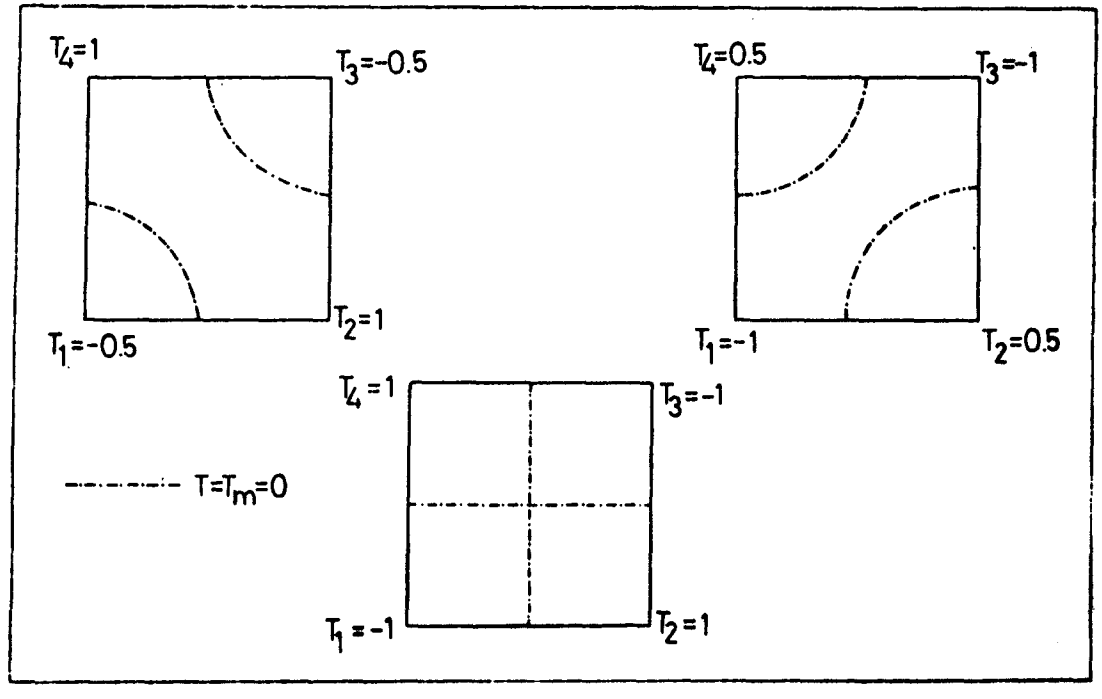

FIGURE 6: Sketch of the two phase element with two interphases within.

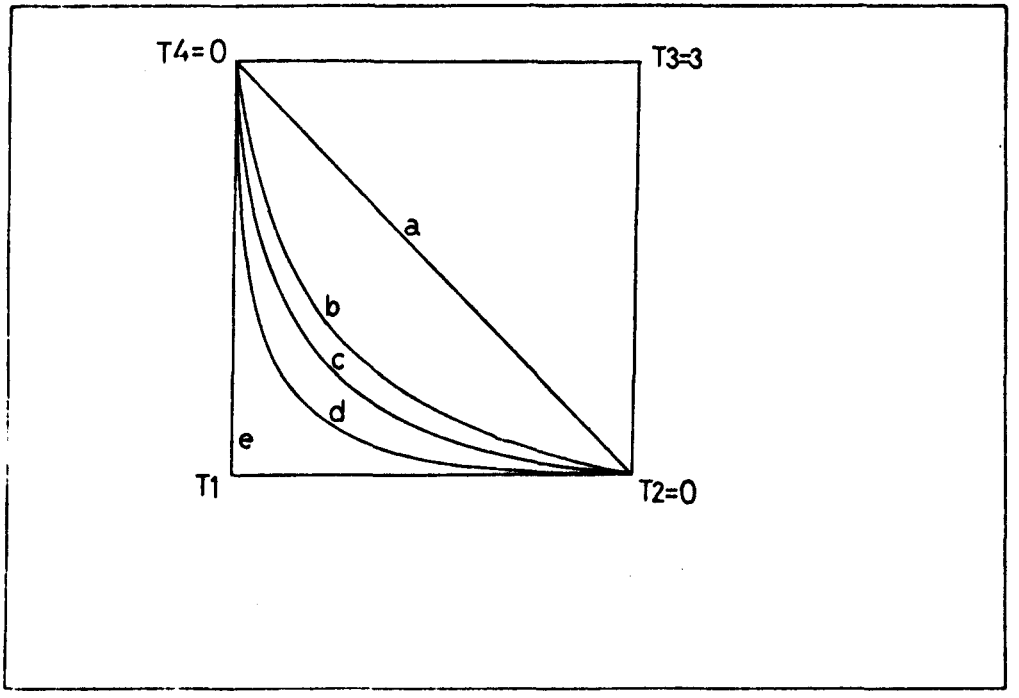

FIGURE 7: Interphase position at various nodal temperatures.

It remains to analyse the ease of the invertion of coordinates, that is to go from (ξ',η') to (ξ,η). With some algebraic manipulations we can write

$$A_\eta\,\xi^2 + (1 + (A_\xi\,\eta' - A_\eta\,\xi'))\,\xi - \xi' = 0$$

Dividing by ξ^2 and solving the quadratic equation in $1/\xi$, we find

$$\xi = 2\,\xi' / \left[(1 + A_\xi\,\eta' - A_\eta\,\xi') + \sqrt{1 + (A_\xi\,\eta' - A_\eta\,\xi')^2 + 2\,(A_\xi\,\eta' + A_\eta\,\xi')}\right]$$

Furthermore, the jacobian of the transformation is

$$\left|\frac{\partial(\xi',\eta')}{\partial(\xi,\eta)}\right| = \sqrt{1 + (A_\xi\,\eta' - A_\eta\,\xi')^2 + 2\,(A_\xi\,\eta' + A_\eta\,\xi')}$$

Thus we can see that, at any point of Gauss used for the numerical integration, we need to evaluate only one square root for the coordinate inversion and the computation of the jacobian.

THE INCREMENTAL SOLUTION ALGORITHM

The next step is the solution of the nonlinear system (4). This process may be viewed as finding a root of the residual

$$r(u) = Ku + i(u) - g = 0 \qquad (15)$$

This is not an easy task due to the step-like behaviour of the residual in this type of problem. Moreover when no special care is devoted to the solution scheme, the temperature in those nodes associated with phase-changing elements may jump above or below the melting value during the iterative process. The explanation of these oscilations is found in the amount of latent heat involved in each rearrangement of

the intephase position. Currently in a finite element context, the search process is achieved in an incremental form, i.e.

$$S\Delta u_n^j = - r(u_n^j)$$

$$u_n^{j+1} = u_n^j + \Delta u_n^j$$

where S is an appropriate iteration matrix, usually the jacobian matrix of (15) and the superscript j stands for the iteration number. However the residual in equation (15) is not differentiable and some skill must be used to obtain an adequate iteration matrix. The main duty of this matrix is to damp the spurious oscilations aforementioned. As the information of the interphase movement is enclosed in the residual vector, one manner to accomplish this task is to appropriately include this vector in S . Quasi-Newton methods[20] provide a systematic way to do this job. In Reference 16 is developed an algorithm of this type that makes a diagonal correction of S that has shown to be adequate to handle this type of instabilities. During the iterative process it is useful to use underrelaxtion in the first iterations to enhance stability and overrelaxation to improve the convergence rate at the last ones. The relaxation parameter can be properly determined using a line search technique[16] which determines the size of the increment which vanishes the projection of the residual in the search direction, i.e. find σ so that

$$(\Delta u_n^j)^T \; r(u_n^j + \sigma \, \Delta u_n^j) = 0 \qquad (16)$$

updating the unknown as

$$u_n^{j+1} = u_n^j + \sigma \, \Delta u_n^j$$

Performing exact line searches satisfying precisely equation (16) is rather an expensive task. However, numerical experimentation has shown

that it suffices to satisfy a less restrictive relation of the form

$$\left| \frac{(\Delta u_n^j)^T \; r(u_n^j + \sigma \Delta u_n^j)}{(\Delta u_n^j)^T \; r(u_n^j)} \right| < \epsilon_l$$

where the parameter ϵ_l is set to say 0.9.

To stop the iteration we measure the magnitud of the out-of-balance of the solution, that is, iteration proceeds until

$$\frac{|| \; r(u) \; ||}{|| \; Ku \; ||} < \epsilon_R$$

where ϵ_R is the required threshold for the normalized residual.

NUMERICAL EXAMPLES

The performance of the formulation above described has been examined in several numerical problems. In the following we present the solution for three examples. The first one concerns the solidification of a simi-infinite region defined by $x > 0$, $y > 0$. The initial temperature is 0.3°C and the half plane is frozen by lowering the temperature on the sides $x = 0$ and $y = 0$ to -1°C. The thermal properties are

$$k_s = k_l = 1 \text{ Kcal/m sec °C} \qquad \rho c_s = \rho c_l = 1 \text{ Kcal/m}^3 \text{ °C}$$

$$\rho L = 2 \text{ Kcal/m}^3 \qquad T_m = 0°C$$

The finite element mesh used is depicted on Figure 8, where only a 45° section has been discretized. To simulate the infinite half plane, adiabatic conditions has been imposed on the sides AB and BC. The same holds on the side OA because of the simmetry of the problem. The one-hundred element mesh is refined near the origen to reproduce better the transient condition at $t = 0$. The time step used is 0.01 sec. Figures

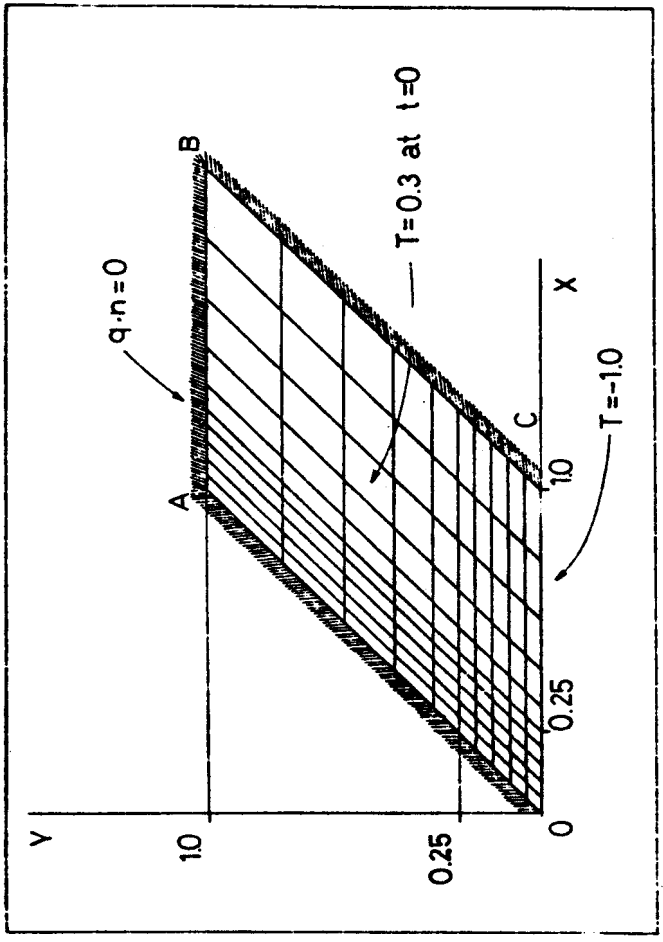

FIGURE 8: Finite element mesh for model problem one.

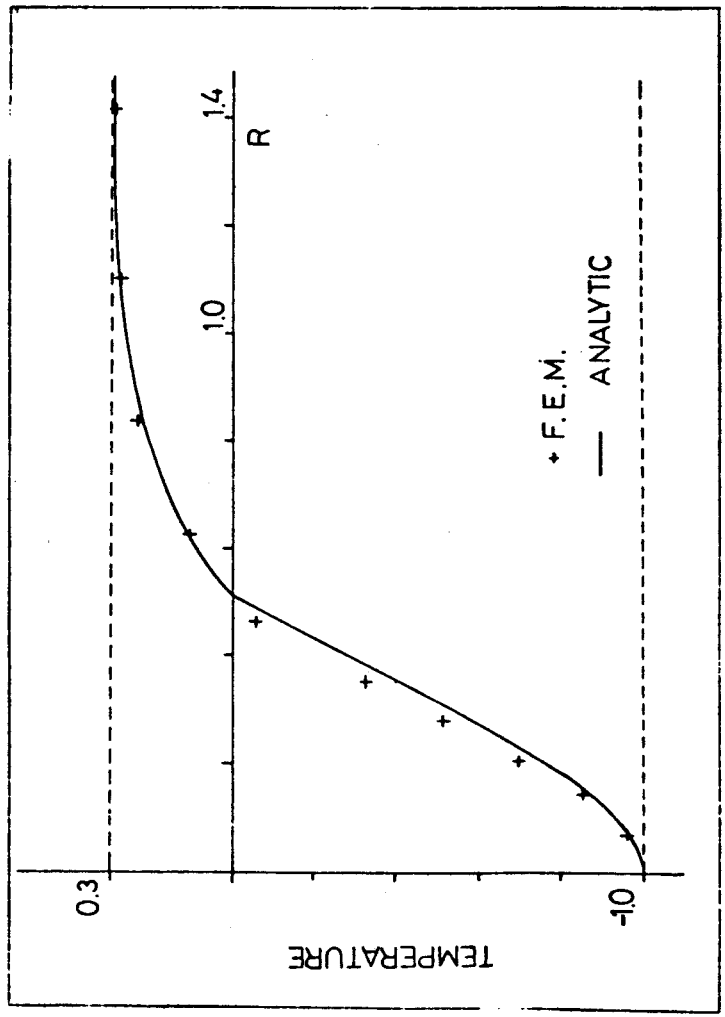

FIGURE 9: Temperature distribution for time = 0.04 sec.

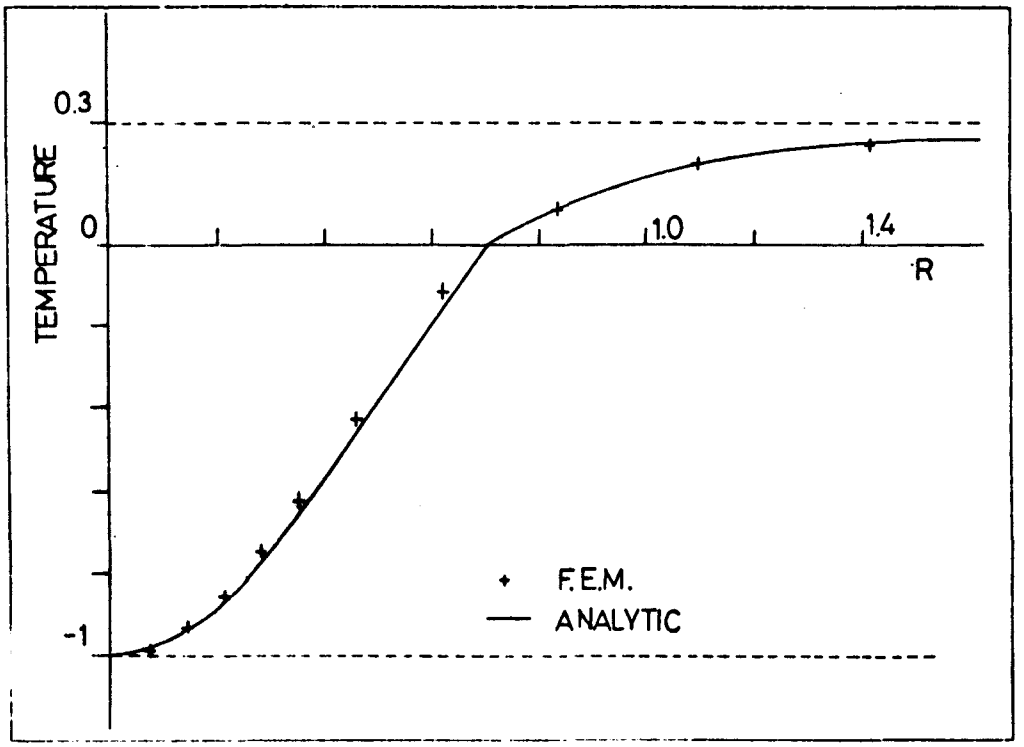

FIGURE 10: Temperature distribution for time = 0.08 sec.

9 and 10 show the temperature profile along the line $x = y$ as a function of the distance to the origin R, for two time steps. The numerical solution is compared with the analytical solution of Budhia and Krieth[21]. Figure 11 shows the time evolution of the interphase position. The mean CPU time needed for computing the residual vector in the first time step was 6.158 sec. This is the time step when more elements change phase. For the same mesh in the linear case (without phase-change and discontinuous integration) the mean CPU time was 5.825 sec. For the straight-interphase assumption the mean CPU time was 5.906 sec. The curved-interphase method is 4% more expensive than the straight-intephase algorithm and 5.7% than the linear case. Runs were performed on a VAX 11/780. The additional cost due to the new formulation is irrelevant.

The second example uses a coarser mesh for the same problem. The mesh depicted on Figure 12 uses one-hundred equally-spaced elements to discretize the 90° corner region of the half plane. The time step used in this example is 0.02 sec. Figures 13 and 14 show the temperature profile along the line $x = y$ for two different time steps. In Figure 15 the interphase locus is plotted for $t = 0.04$ sec.

The third example involves an internal heat source. The temperature distribution is given by

$$T = \begin{cases} 2\ f\ (x,y,t) & f > 0 \\ \\ 1.5\ f\ (x,y,t) & f < 0 \end{cases} \qquad (17)$$

where

$$f = R + 0.25\ t - 1$$

being R the distance measured from the point $P = (0.1,0)$. The interphase locus is an arc of circumference at any time. It is represented

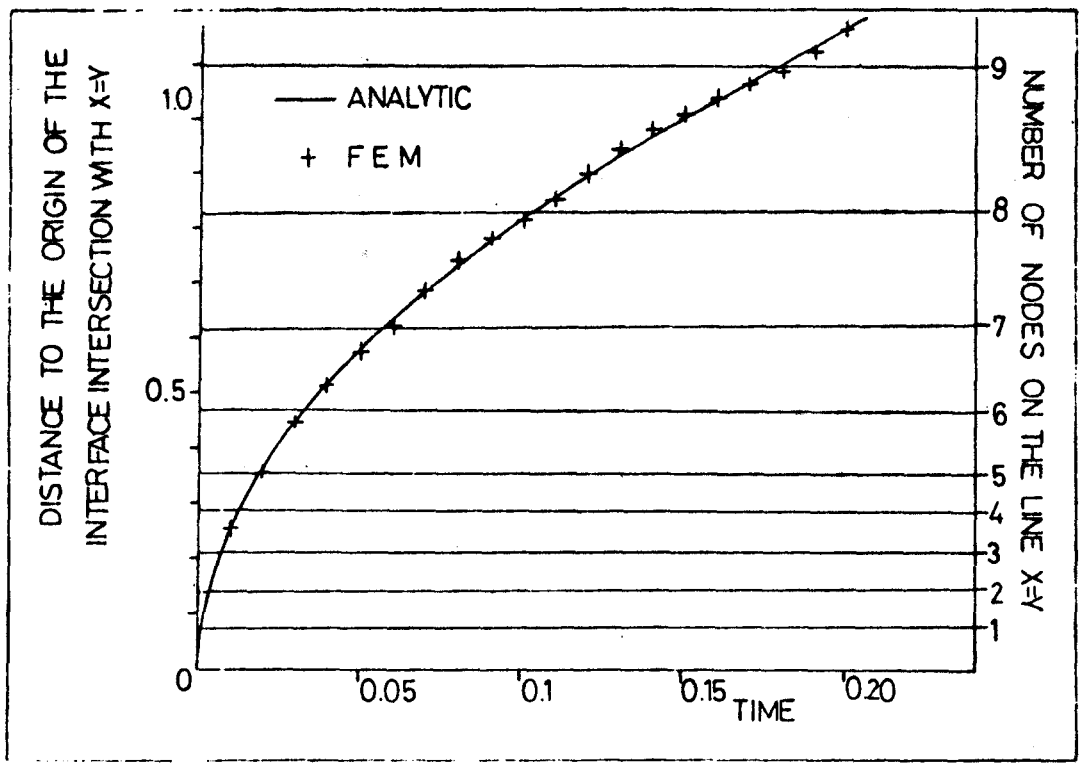

FIGURE 11: Evolution of the front position for model problem one.

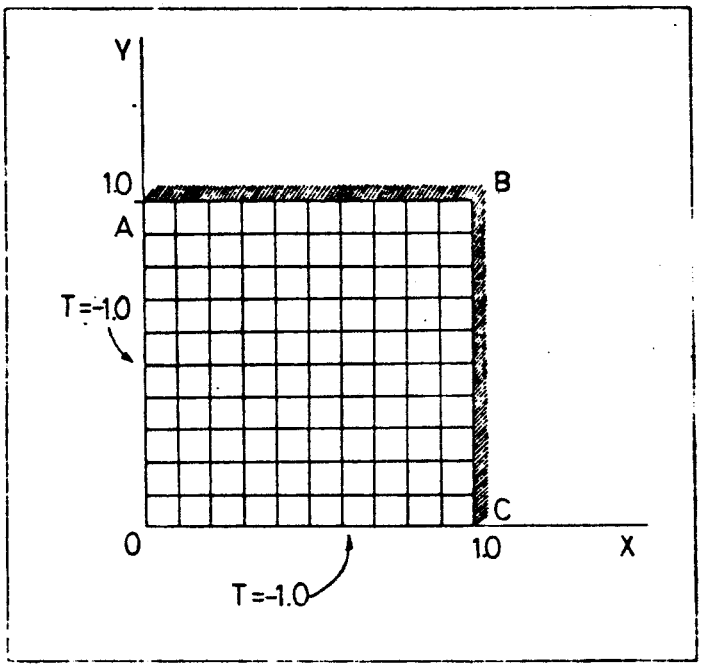

FIGURE 12: Finite Element mesh for model problem two.

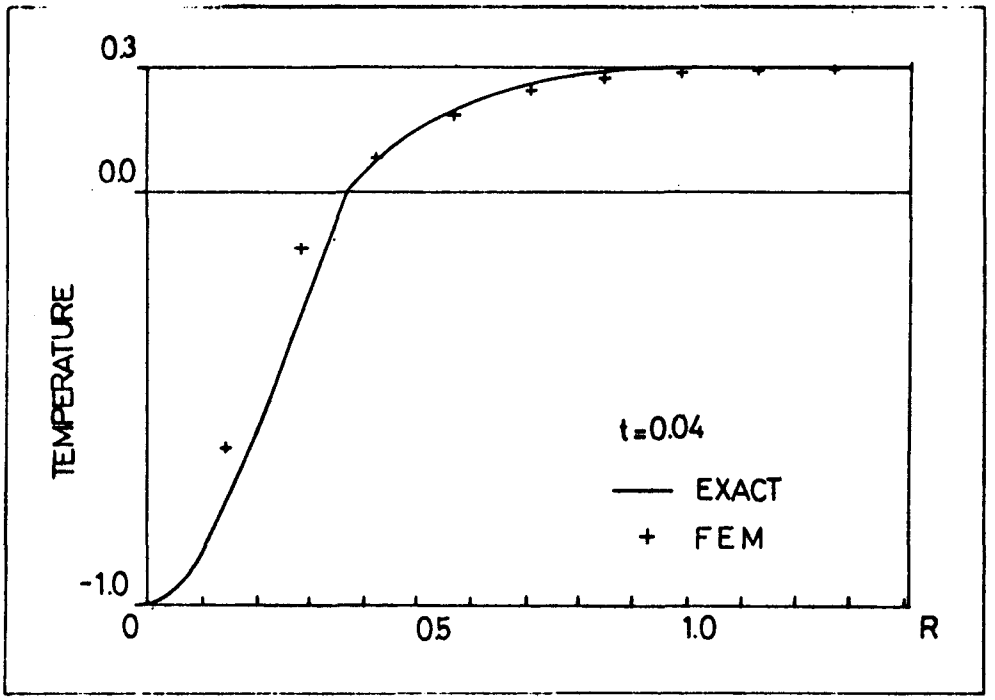

FIGURE 13: Temperature distribution for time = 0.04 sec.

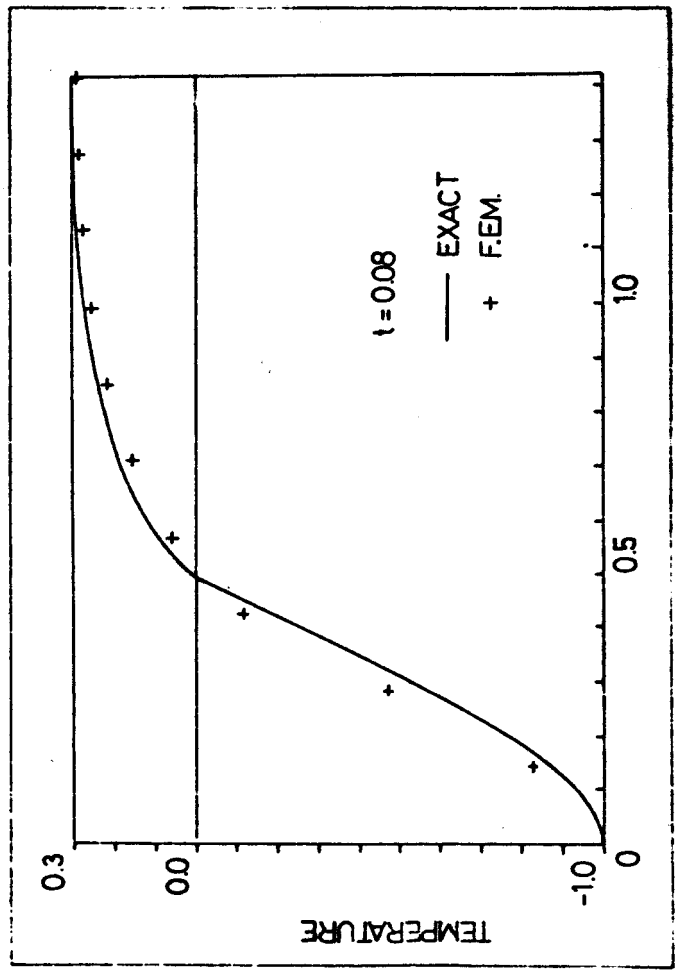

FIGURE 14: Temperature distribution for time = 0.08 sec.

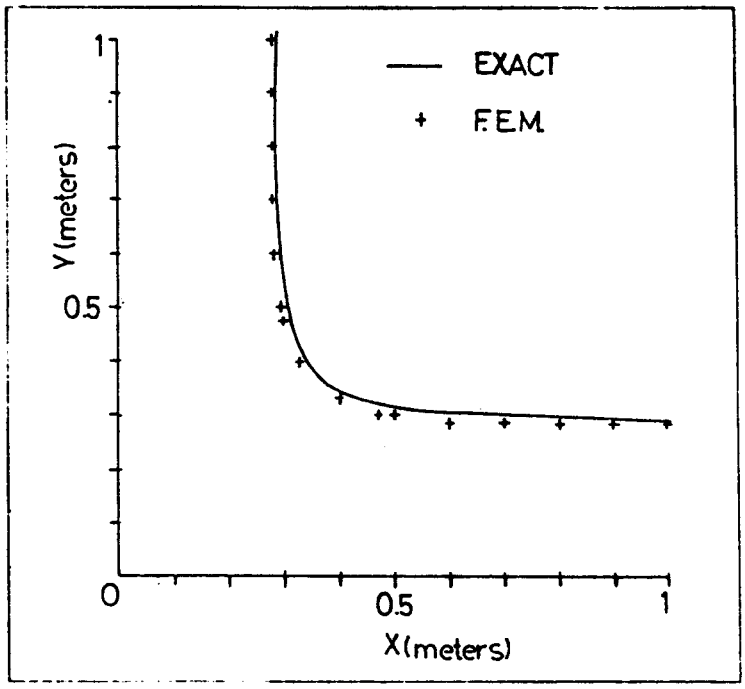

FIGURE 15: Interphase location at time = 0.04 sec.

phase locus is an arc of circumference at any time. It is represented by the equation

$$R = 1 - 0.25\ t$$

and thus its normal is the radial unit vector. The thermal properties are the same as for the first example.

This temperature distribution is achieved by using the internal heat source given by[22]

$$Q(x,y,t)\begin{cases} 2\ (0.25 - \frac{1}{R}) & f > 0 \\ 1.5\ (0.25 - \frac{1}{R}) & f < 0 \end{cases}$$

and the corresponding boundary conditions arising from equation (17).

Figure 16 depicts the 272 finite-element mesh used for the discretization of the region enclosed by the line ABCDEFGOA. On the whole boundary the temperature is imposed according to (17). The time step used is 0.25 sec. Figure 17 plots the intephase position for two time steps. Figure 18 shows the temperature profile at $t = 1$ sec. for several lines of constant y.

CONCLUSIONS

A new procedure for dealing with curved interphases was presented. It allows an improved integration of discontinuous functions within the elements which are traversed by such interphases. The procedure was applied to model two-dimensional phase-change problems. The solution is obtained in terms of temperature, without the current requirement of an explicit smoothing of the temperature-enthalpy rela-

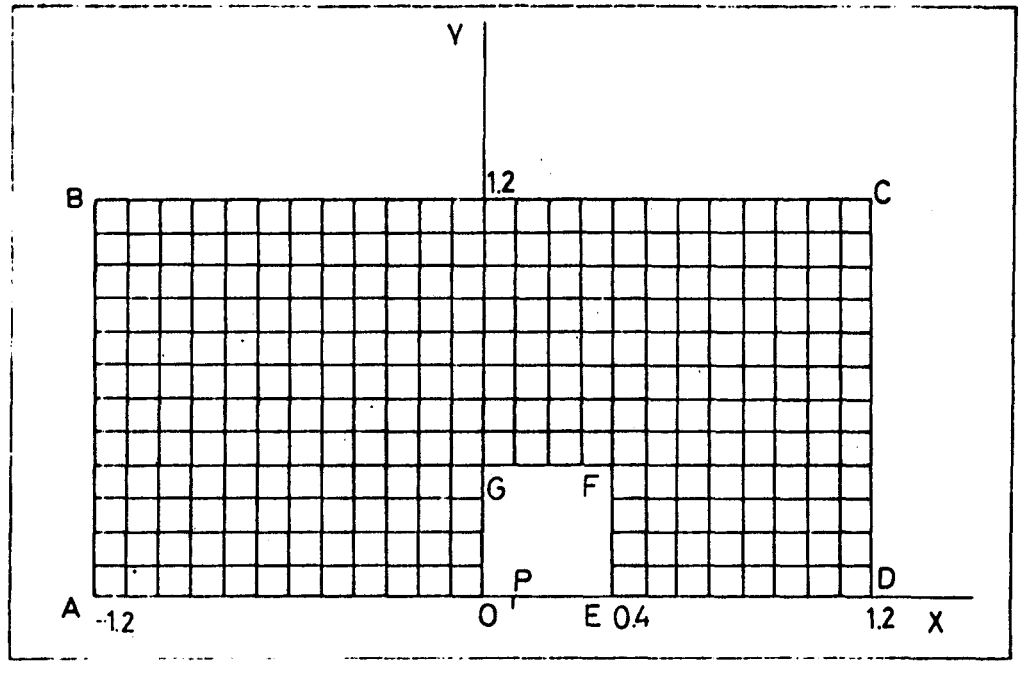

FIGURE 16: Finite Element Mesh for model problem three.

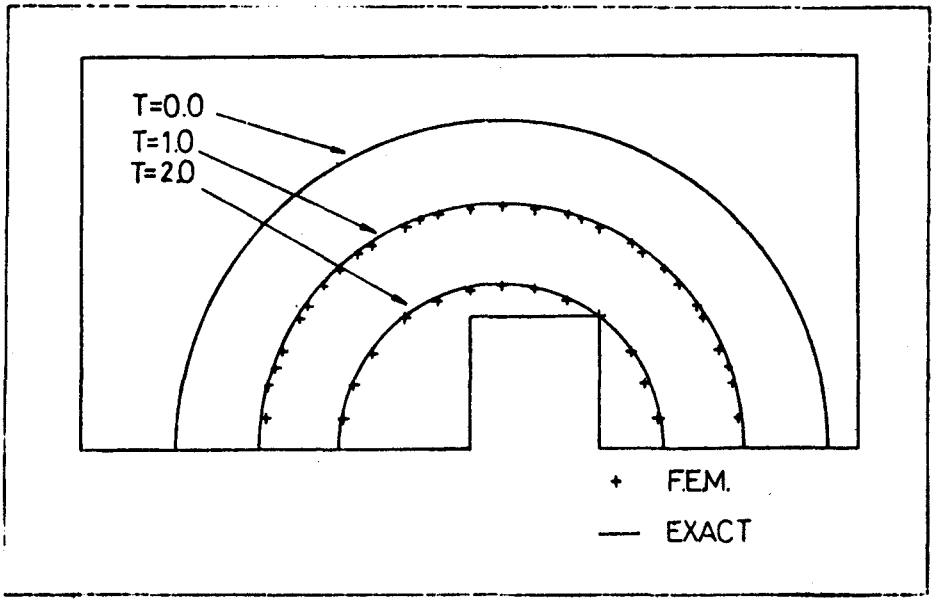

FIGURE 17: Interphase location for several time steps.

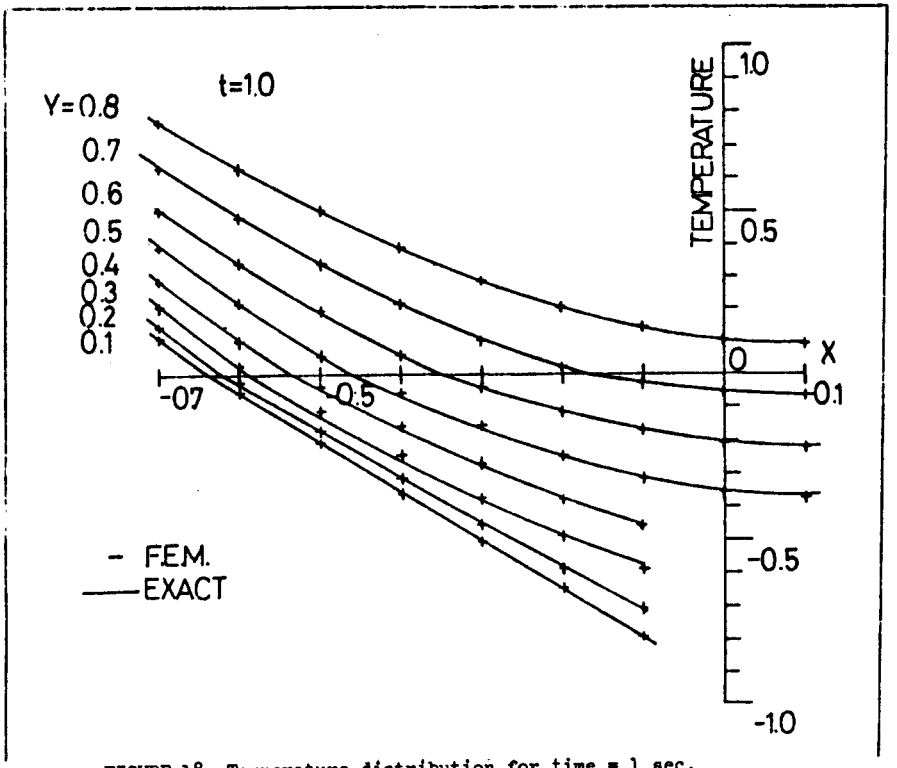

FIGURE 18: Temperature distribution for time = 1 sec.

$\beta = \frac{T_1 + T_3}{T_1 - T_3}$	AREA		
	PRESENT METHOD (a)	STRAIGHTLINE INTERPHASE (b)	ANALYTICAL SOLUTION (c)
0	2	2	2
0.82	0.173125	2	0.1731586
0.875	0.1358975	2	0.13582017
0.936	0.087365	2	0.08684
0.967	0.054804	2	0.053622

Tabla I

tion. The algorithm features an accurate integration of the enthalpy contribution to the residual vector. Furthermore, the convergence criterion is ruled by the norm of this residual vector.

The iteration process is handled by a careful strategy to avoid spurious oscilations and lack of convergence. It combines a proper modification of the iteration matrix with an approximate line search.

This algorithm may be readily implemented in finite element packages without any major modification of the program. Little additional calculation is required to evaluate the proposed transformation, only a square root at each Gaussian point is needed to compute the jacobian and to invert the coordinate system. The computation of the integrals in those elements travesed by the interphase does not produce relevant extra cost. The method behaves encouragingly in the examples performed.

Acknowledgements

M. Storti and L.A. Crivelli would like to thank the Consejo Nacional de Investigaciones Cientificas y Tecnicas (CONICET), Argentina, for the support given via a research fellowship provided for this work.

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