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FINITE DIFFERENCE FRONT-TRACKING ALGORITHMS FOR STEFAN PROBLEMS ARISING IN REACTOR SAFETY STUDIES

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ABSTRACT

Assessments of the residual risk from nuclear power plants require the modelling of highly unlikely accidents in which part of the reactor core melts, and so it is necessary to consider thermal attack on reactor structures. It is useful to divide the problems that arise into two groups. In the first group heat penetrates the whole medium before significant melting occurs (e.g. thermal attack on a thin steel slab). A method based on a modification of a standard finite difference scheme (alternating direction implicit method) to include tracking the melt-front between mesh points provides an efficient scheme for this group. The second group of problems is characterized by the propagation of a thermal front, associated with the melt-front, into an essentially ambient medium. The growth of a melt-pool in a reactor substrate is a good example of this type of problem (here the scale-length may be less than one centimetre initially in a medium that occupies many cubic metres). A conservative form of the isotherm migration method has proved to be well-suited for this group, provided that a co-ordinate system exists in which the isotherm positions are single-valued. This method handles the temperature-dependent thermophysical properties, which often occur in real problems, in a simple form.

In this paper these two algorithms are described and results given for test problems.

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1. INTRODUCTION

Assessments of the residual risk from nuclear power plants require the modelling of highly unlikely accidents in which part of the reactor core melts. The molten material, in which heat is generated by the decay of unstable fission products, contacts structures within the reactor vessel, and if the vessel is penetrated, could interact with the basemat. Large computer codes exist that predict the response of reactor containments to such accidents and these require algorithms for the various melting interactions. It is necessary that the algorithms contain sufficient detail to avoid gross inaccuracy, but should not lead to large increases in running time for the codes in which they are incorporated. (In some cases simple heat balances are sufficient.)Various approximate analytic [1]and numerical procedures have been investigated. For efficient numerical algorithms we require (i) good conservation properties (ii) good discretization of the thermal flux, particularly close to the melt front, and (iii)engineering accuracy (i.e.$\sim$3% in front propagation speed) with a limited number of nodes and reasonably large timesteps.

The problems to be solved can be divided into two groups. In the first, heat penetrates the whole medium before significant melting occurs and convective cooling of the far boundary of the medium is significant (e.g.thermal attack on a thin steel slab). An algorithm (the 'gamma' method) based on modifications to a standard finite difference approximation of the heat equation on a fixed domain has been developed for this group of problems (see section 2). In the second group a thermal front, associated with the moving melt-front, propagates into an ambient medium (e.g.growth of a melt-pool in the basemat), and a conservative form of the isotherm migration method (IMM) suited to this group is presented in section 3. Solutions for test problems demonstrate the efficiency of these algorithms.

2. THE 'GAMMA' METHOD : FRONT-TRACKING ON A FIXED MESH IN TWO DIMENSIONS

Consider the melting (ablation) problem shown in Fig 1. ϕ_z is a heat flux density applied to the upper surface which, once melting has started, is at temperature T_m. The DI method [2] is the basis of this algorithm for solving the heat equation and modifictions required to account for the varying domain are outlined below. The computational esh is shown in Fig 2. The melt-front position $z = \zeta(x,t)$ must be a single valued function of x at all times, and at time t it is discretized as ζ_i, from which two sets of arameters Γ_i, γ_i are derived:

$$\zeta_i = (\Gamma_i - \gamma_i)\delta z \qquad (2.1)$$

here Γ_i is an integer and $0.2 \leq \gamma_i < 1.2$ to restrict the size of the coefficients ppearing in equation (2.2) below.

The key to the method is to note that the discretized sets of equations for the

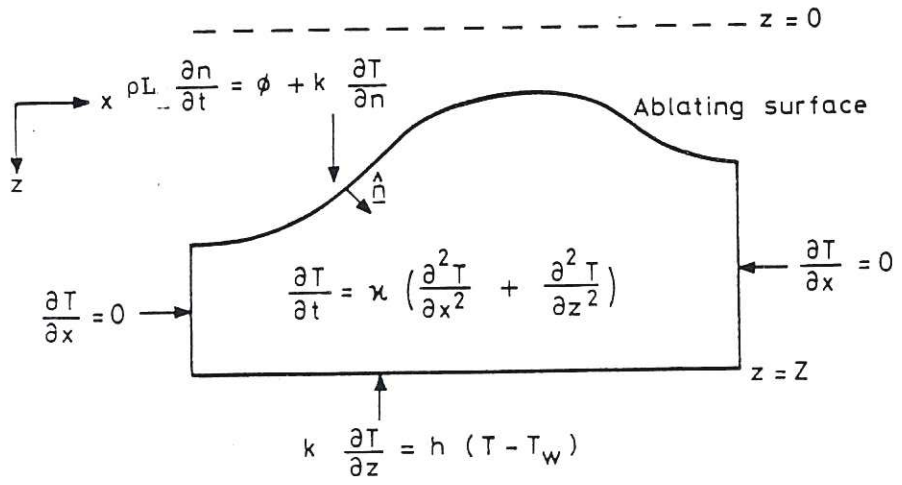

Fig.1 Typical ablation problem.

domain interior (i.e. for all $i, \Gamma_i < j \leq J$) may be closed by using the usual guard values on the fixed boundaries and by using guard values at nodes (i,j) where $j=\Gamma_i$ obtained by a quadratic extrapolation of the temperature profile through points $(i,j+2)$, $(i,j+1)$ and noting that $T=T_m$ when $z=\zeta_i$. (This is the Lagrange interpolation of Crank [3].) Using (2.1) the following relationship for the guard point is obtained:

$$T_{i,j} = a[\gamma_i]\, T_m + b[\gamma_i]\, T_{i,j+1} + c[\gamma_i]\, T_{i,j+2}; \quad j = \Gamma_i \qquad (2.2)$$

where $$a[\gamma] = 2/(\gamma+\gamma^2);\ b[\gamma] = -2(1-\gamma)/\gamma;\ c[\gamma] = (1-\gamma)/(1+\gamma) \qquad (2.3)$$

The Stefan condition on the ablation front may be re-written in the form

$$\rho L \frac{\partial \zeta}{\partial t} = \phi_z + k\left(1 + \left(\frac{\partial \zeta}{\partial x}\right)^2\right) \left.\frac{\partial T}{\partial z}\right|_{z=\zeta} \quad ; \text{ where } \phi_z = \phi\left(1+\left(\frac{\partial \zeta}{\partial x}\right)^2\right)^{\frac{1}{2}} \qquad (2.4)$$

The discretized form of this equation is always advanced explicitly at the beginning of each half timestep to obtain values of ζ_i, γ_i and Γ_i at the end of the half step. A second-order discretization of $\partial T/\partial z$ is used:

$$\frac{\partial T}{\partial z} \approx \frac{T_{i,j+2} - T_{i,j}}{\delta z} - \frac{\gamma}{\delta z}\left(T_{i,j+2} - 2T_{i,j+1} + T_{i,j}\right); \quad j = \Gamma_i \qquad (2.5)$$

The half of the ADI with z-discretization implicit uses previously calculated temperature values for x-discretization including old guard point values, but uses the updated values of γ_i and Γ_i to close the tridiagonal system of equations. $\partial\zeta/\partial t$ may then be re-evaluated for the end of the half time step using previously calculated values of γ and Γ. At this stage an iteration on γ and Γ is possible, however, the chosen procedure is to make corrections for changes in $\partial\zeta/\partial t$ during the timestep, and use timestep control to ensure that these correction terms remain small.

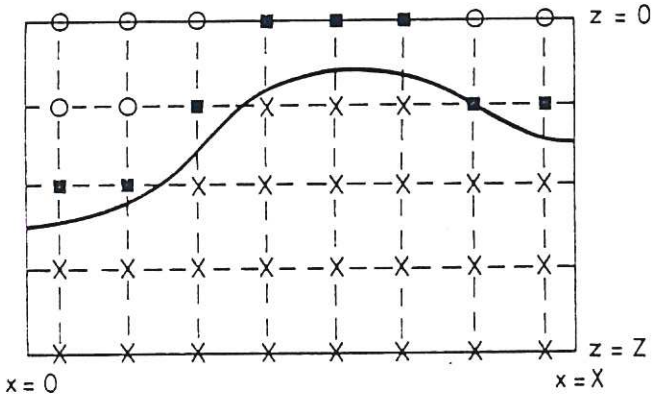

Fig.2 The mesh used in the 'gamma' method.
x are normal mesh points in the slab; ■ are guard points, which incorporate the moving boundary condition, and o are not used in the calculation.

The second half of the ADI (x-discretization implicit) is performed in a similar manner. First, equation 2.4 is discretized to obtain an estimate of the domain at the end of the timestep. The tridiagonal systems are then solved sequentially, starting with j=

reducing j by one each time. This allows updated guard point values (calculated on the estimated domain) to be used when they are required. This effectively masks out the points shown o in Fig.2. At the end of the timestep $\partial\zeta/\partial t$ is re-evaluated, and γ and Γ are recalculated as above.

Further details of the method will be published elsewhere. A one-dimensional version [4] which uses a Crank-Nicolson discretization has proved to be successful and efficient for practical problems [5]. The two-dimensional code has been tested using ablation problems and encouraging results obtained, however results are only given in this paper for the Bonnerot-Jamet problem [6].

3. CONSERVATION FORM OF THE ISOTHERM MIGRATION METHOD (IMM).

The IMM in one dimension [7,8] may be interpreted as a co-ordinate transformation, whereby temperature is replaced as the dependent variable by a spatial co-ordinate (the position of the isotherm). Turland has shown that if the resulting non-linear equation is discretized in a conservative manner the method works well for Stefan problems involving the propagation of a thermal front into an ambient medium [9]. The IMM can be extended to two and three dimensions in a number of ways [10,11,9]. One way is to choose an appropriate orthogonal curvilinear co-ordinate system, denoted (u,v,w), and enact a change of variable making one spatial co-ordinate (u, say) the dependent variable by treating temperature as an independent variable [9].

It can be shown that the heat equation

$$\rho c \frac{\partial T}{\partial t} = \underset{\sim}{\nabla}.(k \underset{\sim}{\nabla} T) \tag{3.1}$$

where ρ is constant but c and k may be functions of temperature, transforms to

$$\frac{\partial \psi}{\partial t} = -\left(\frac{\partial \Phi^T}{\partial T} + \frac{\partial \Phi^v}{\partial v} + \frac{\partial \Phi^w}{\partial w}\right) \tag{3.2}$$

where

$$\psi(v,w,T,t) = \rho c(T) \int_o^u h_1 h_2 h_3 \, du' \tag{3.3}$$

for $h_1 = h_1(u',v,w)$ etc

$$\Phi^T = \frac{h_2 h_3}{h_1} \frac{k}{u_T} \left[1 + \frac{h_1^2}{h_2^2} u_v^2 + \frac{h_1^2}{h_3^2} u_w^2\right] \tag{3.4}$$

$$\Phi^v = -\frac{h_1 h_3}{h_2} k u_v \; ; \; \Phi^w = -\frac{h_1 h_2}{h_3} k u_w \tag{3.5}$$

and

$$h_1 = \left(\frac{\partial s}{\partial u}\right)_{v,w} \; ; \; h_2 = \left(\frac{\partial s}{\partial v}\right)_{u,w} \; ; \; h_3 = \left(\frac{\partial s}{\partial w}\right)_{u,v} \tag{3.6}$$

where s is a measure of distance. Non-numeric subscripts denote partial differentiation. The Stefan condition

$$\rho L(\partial n/\partial t) = \underset{\sim}{\phi}.\hat{\underset{\sim}{n}} + k(\partial T/\partial n) \tag{3.7}$$

transforms to

$$\frac{L}{c} \frac{\partial \psi}{\partial t} = F\phi + \Phi^T; \; F = h_2 h_3 \left(1 + \frac{h_1^2}{h_2^2} u_v^2 + \frac{h_1^2}{h_3^2} u_w^2\right) \tag{3.8}$$

where quantities are evaluated at the melting temperature.

If w is an ignorable co-ordinate the appropriate forms of ψ, Φ^T, Φ^v and F are given in Table 1. From equation 3.2 a conservative scheme for the quantity ψ (closely related to the heat content) can be constructed using a control volume method in (v,T) space.

	CARTESIAN ($u\equiv y,\ v\equiv x$)	CYLINDRICAL ($u\equiv r,\ v\equiv\theta$)	SPHERICAL ($u\equiv r,\ v\equiv\theta$)
ψ	ρcy	$\rho cr^2/2$	$\rho cr^3\sin\theta/3$
ϕ^T	$k(1+y_x^2)/y_T$	$k(r^2+r_\theta^2)/rr_T$	$k(r^2+r_\theta^2)\sin\theta/r_T$
ϕ^V	$-ky_x$	$-kr_\theta/r$	$-kr_\theta\sin\theta$
F	$(1+y_x^2)^{\frac{1}{2}}$	$(r^2+r_\theta^2)^{\frac{1}{2}}$	$r\sin\theta(r^2+r_\theta^2)^{\frac{1}{2}}$

TABLE 1. Form of ψ, ϕ^T, ϕ^V and F used in CONIMM.

This has been implemented for problems in two spatial variables in the CONIMM code which uses the three co-ordinate systems given in Table 1. Rather than use an explicit scheme CONIMM uses a time-centred discretization (alternating direction implicit method) with appropriate linearization in the evaluation of some of the derivatives of u. (Linearization is not needed for the temperature dependence of the thermal properties.) This removes the timestep constraint imposed by an explicit method, but also destroys exact conservation: however, in practice this scheme gives answers close to those from an explicit scheme.

4. RESULTS FOR TEST PROBLEMS.

It is instructive to determine the performance of these methods and codes on problems already in the literature or with analytic solutions. Three such problems are considered here. The first does not involve melting, but demonstrates the performance of the CONIMM code on a thermal front propagation problem. (In the IMM the movement of the melt-front is simple: the test demonstrates that the method does not degrade the solution of the heat equation.) It is solved using CONIMM's spherical polar option. The second problem is the freezing of a square prism, which is solved with CONIMM's cylindrical option. The third problem is that of Bonnerot and Jamet [6], which can be envisaged as a freezing problem with the liquid at the freezing point. The main difficulty lies in the chosen initial conditions and the steep gradient the melt-front makes with the cartesian co-ordinate system at early times. This problem has been solved using both CONIMM's cartesian option and by the gamma method.

Problem 1: Diffusion of heat from a hot sphere into an ambient medium with temperature dependent thermal properties.

It is required to solve numerically

$$\rho c \frac{\partial T}{\partial t} = \frac{1}{R^2} \frac{\partial}{\partial R}\left(R^2 k \frac{\partial T}{\partial R}\right) \qquad (4.1)$$

in $1 < R < \infty$ with initial conditions $T = 1$ at $t = 0$ for $R > 1$, and boundary conditions $T = 2$ at $R = 1$ for $t > 0$, and $T \to 1$ as $R \to \infty$ for $t > 0$, where $\rho = 1$ and $c(T)=k(T)=T$. The analytic solution is

$$T(R,t) = \left[1 + \frac{3}{R}\,\mathrm{erfc}\left\{\frac{R-1}{2t^{\frac{1}{2}}}\right\}\right]^{\frac{1}{2}} \qquad (4.2)$$

This problem may be solved using one spatial variable, but if the co-ordinate system is offset by R_s it provides a test of two dimensional spherical polar algorithms. The mesh used in the IMM is obtained by the intersection of a set of radial lines with the iso-

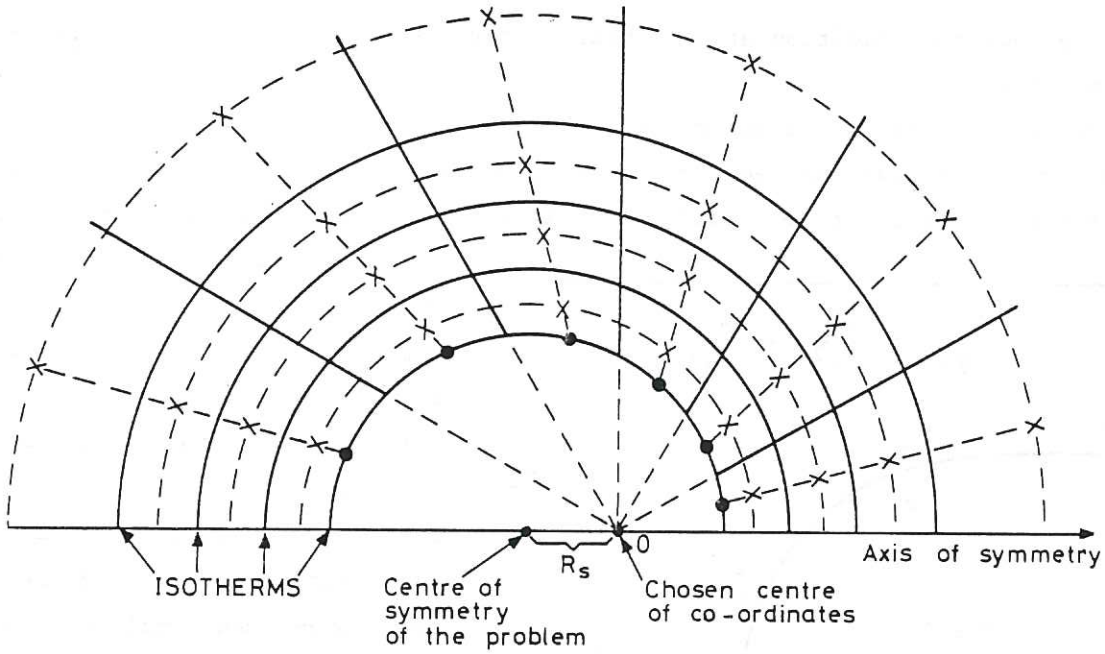

Fig.3 IMM mesh for problem 1. The solid isotherms and radial lines define cells for the method. The mesh points (x) used in the calculation are located at the centre of these blocks in temperature-angle space. Boundary conditions are imposed at nodes •.

herms (see Fig.3). The calculated isotherm positions are for the centres of mesh cells nd correspond to block averages. Equation 4.1 was inverted numerically to give R(T,t) or the chosen isotherms at t = 0.005. CONIMM was run with 16 isotherms until t = 1.0 ith (a) $R_s = 0$ and (b) $R_s = 0.5$ using 10 radial lines. The numerical results are compred in Table 2 with (i) the analytic solution obtained from (4.1) and (ii) block averges calculated from the analytic solution for the mesh that was used (denoted $\overline{R}_{16}$). (In ONIMM the position of the outermost isotherm is determined by conservation and by seting $\phi^T = 0$ at the outer (ambient) boundary. There is no need for the penetration distnce introduced in [7].) The main source of error arises because of the difference betzen the spot value and block average in the outermost block. Run (b) shows good agreeent with run (a) indicating that CONIMM handles the varying curvature of the isotherms

Temperature T	Starting Profile R(t=0.005)	Analytic Solution R(t=1.0)	Numerical Solutions R(t=1.0)	Analytic Solution $\overline{R}_{16}$(t=1.0)
1.969	1.0046	1.0271	1.0273±0.0002	1.0276
1.844	1.0230	1.147	1.148±0.001	1.147
1.656	1.051	1.368	1.371±0.001	1.369
1.344	1.092	1.920	1.932±0.002	1.922
1.094	1.177	2.864	2.918±0.005	2.881
1.031	1.223	3.522	3.636±0.020	3.700

TABLE 2: Results for problem 1. Numerical solution is given for $R_s=0$, and the maximum difference between the $R_s=0$ and $R_s=0.5$ solutions is shown. $\overline{R}_{16}$ is a block average.

fectively. Run (a) required 85 timesteps and took 12 seconds of CPU on the PRIME 500, n (b) required 89 timesteps and used 40 seconds of CPU. This example demonstrates e efficiency of CONIMM for problems involving temperature dependent thermal properties d propagation into an ambient medium. A relatively minor modification (an option in

the code) allows the condition at the inner surface (T = 2, R = 1) to be replaced by th Stefan condition.

Problem 2: The freezing of a square prism.

This problem (see Fig.4) has been solved using a variety of numerical techniques [10,11 12]. At t = 0 the whole prism is liquid at its freezing point. The boundary temperature is then depressed and held constant while the liquid solidifies. The IMM solution employs a cylindrical polar co-ordinate system centred on x = 0, y = 0. From symmetry the temperatur field need only be solved over one-eighth of the prism. The IMM require a starting solution, and the most su table one-dimensional solution to us is that of Neumann [13]for freezing from a plane wall. At short times th is accurate everywhere except in the corners. The Neumann solution for L 1.561 (other properties being set to one) was discretized to find isother positions at t = 0.001. The IMM gives a good discretization of the temperature profile at all times, but may lead to penalties arising from the limited timestep if neighbouri points are too close.

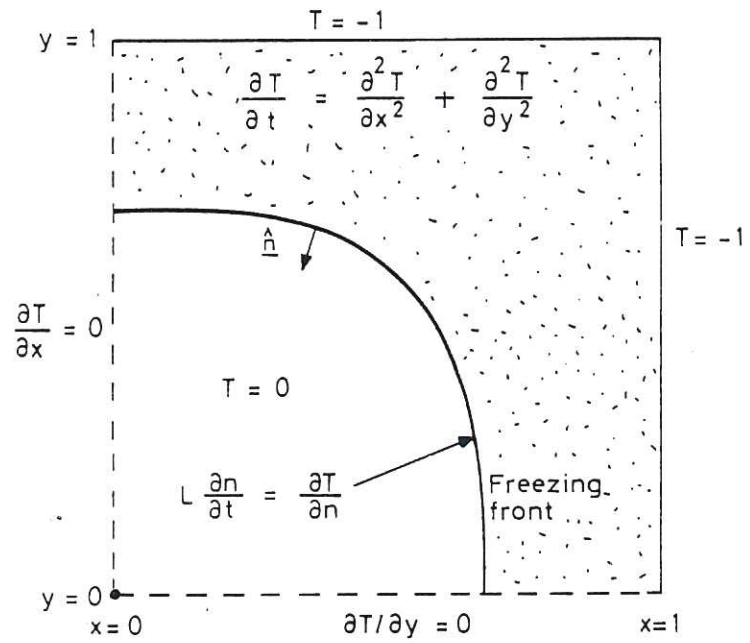

Fig.4 The freezing of a square prism.

	5 x 4 mesh			10 x 10 mesh		
TIME	x_A^F	x_D^F	N	x_A^F	x_D^F	N
0.001	0.967	0.912	0	0.967	0.939	0
0.1	0.673	0.634	121	0.673	0.630	241
0.3	0.426	0.358	205	0.426	0.352	420
0.5	0.209	0.157	265	0.208	0.154	518
0.6	0.066	0.047	299	0.067	0.048	575
0.61	0.043	0.032	304	0.046	0.033	584

TABLE 3. Freezing of a square prism. x_A^F and x_D^F are the values of the x-co-ordinate of the freezing front on axis and diagonal respectively. N is the number of timesteps (this depends on a user specified accuracy parameter).The discrepancy in the initial values of x_D^F arises from the interpretation of the starting solution.

Results for a coarse mesh (4 isotherms and 5 radial lines) and for a finer mesh (10 iso therms and 10 radial lines) are given in Table 3. These agree well with each other,whe differences in the interpretation of the starting solution have decayed, and with Crowl ey's enthalpy method results [12]. They show greater consistency on mesh refinement tha the results obtained with the IMM of Crank and Crowley [11], whose results are consiste with those presented here. No stability problems were encountered in the present calcu ations. The predicted time for complete freezing is 0.6296±0.0005 (coarse mesh) and 0.6327±0.0002 (finer mesh), compared with Crowley's value of ∿0.625. The run for the

finer mesh took seconds CPU time on a PRIME 500.

Problem 3 : The Bonnerot - Jamet problem [6].

This is illustrated in Fig 5. The problem involves a rapid redistribution of the initial temperature profile which leads to little movement of the boundary near x = 0 and rapid movement near x = 1 at early times. Both methods described above have been applied to this problem. For the 'gamma' method a fixed mesh on the domain $0<x<1$, $0<y<4$ was used with a fixed timestep $\delta t=0.01$. No stability difficulties were encountered. Results are given in Table 4. The cartesian version of CONIMM was also used to solve this problem. The selection of small timesteps by the code for the early part of the evolution was indicative of difficulties at this stage. Results are given in Table 4. Furzeland [14] has compiled a set of results for this problem, obtained using transform

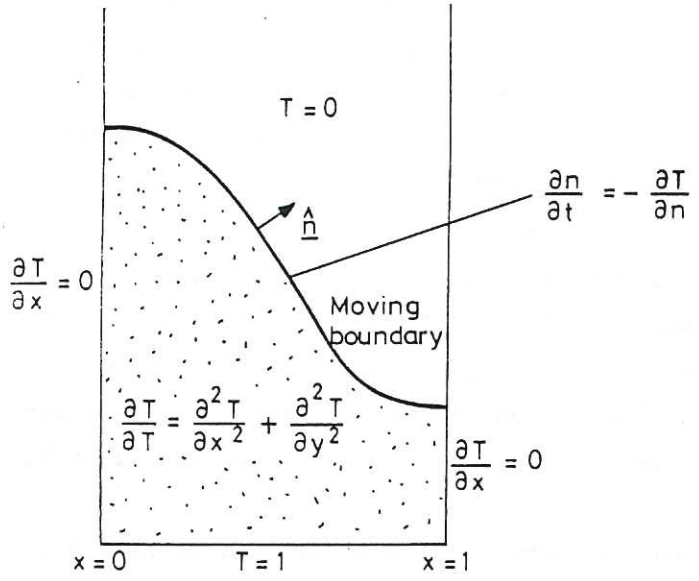

Fig.5 Problem 3: The initial position of the boundary is $y = 2 + \cos\pi x$ and the initial temperature distribution is linear in y.

	'GAMMA' METHOD			FINITE-ELEMENTS [6]		
x	δx=1/10	δx=1/15	δx=1/20	δx=1/8	δx=1/16	δx=1/64
0	3.030	3.037	3.042	3.181	3.122	3.068
0.5	2.770	2.774	2.779	2.978	2.902	2.810
1.0	2.583	2.596	2.601	2.712	2.635	2.610

x	δx=1/5	δx=1/8	δx=1/10	δx=1/12	
0	3.161	3.132	3.120	3.111	CONIMM
0.5	2.888	2.856	2.836	2.822	(Cartesian option)
1.0	2.487	2.513	2.529	2.540	

TABLE 4. Moving boundary position at t=2 for problem 3. The CONIMM calculations were done with equal numbers of isotherms and radial lines (δx is the spacing in x).

and enthalpy methods, which may be compared with Table 4. Combining all these studies, the best approximation to the position of the front at t = 2 appears to be y = 3.055 (x = 0), y = 2.795 (x = 0.5), and y = 2.600 (x = 1), where the error in assessment is likely to be less than 0.015. Using this solution as a basis for comparison, the transform methods [14] and the 'gamma' method perform well, as does the enthalpy method (although the interpolation used to obtain the frontal position in the enthalpy solution is not discussed). The IMM gives reasonable solutions, even on a coarse mesh but appears to be less accurate than the solutions discussed above (the use of block averages may degrade the solution and conservation is unimportant). All methods compare favourably with the original finite element method of Bonnerot and Jamet [6].

DISCUSSION AND CONCLUSIONS.

Two methods of solving ablation and Stefan-like problems in 2 space dimensions

using finite difference methods have been presented. The IMM is best suited to problems with constant temperature boundary conditions (including the Stefan condition) and requires monotonicity of the temperature field in one of the chosen spatial variables. It is efficient for problems with propagating thermal fronts, and the conservative formulation outlined above removes any arbitrariness in the condition on the outermost isotherm. The formulation implemented in CONIMM treats temperature dependent properties and requires no interpolation. The examples discussed above illustrate the range of problems that can be treated by CONIMM and show that in all cases reasonable accuracy can be obtained with a limited amount of computation. The performance on problem 1 is particularly impressive, compared with conventional methods (although the accuracy is no better than 1%). Although this example did not include melting, the addition of an ablation condition does not lead to additional complications or sources of inaccuracy. Problem 2 illustrates the high accuracy that can be achieved when the temperature profiles are relatively simple: the main source of inaccuracy here is the initial singularity caused by the corner. Problem 3 is less suited to the IMM, but again reasonable results were obtained.

The 'gamma' method is related to a number of other finite difference methods for moving boundary problems. In practice the equations solved are identical to those arising in the enthalpy method except close to the moving boundary where knowledge of the intercept of the front should, in principle, lead to better discretizations of the thermal fluxes in this region. Ablation examples (not discussed here) and problem 3 illustrate the potential of this method, which per timestep requires only a small amount of additional computation over enthalpy schemes, and less than any transform method. The main drawback, as with most front tracking schemes, is that the moving boundary must be a single valued function of one of the co-ordinates; but this can often be arranged in practical problems. The method is suitable for problems that cannot be treated by the enthalpy method such as ablation problems, and can be generalized in many ways. It may be applied in other co-ordinate systems and with other conditions on the free boundary (e.g. for porous flow problems) and could be used to find solutions of free boundary (time-independent) problems by pseudo-timestepping. The computer coding requirements are relatively small, being modifications to the boundary conditions in an otherwise conventional scheme. Generalization to multiphase problems and three dimensions are also possible.

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REFERENCES.

[1] R S Peckover. The modelling of some melting problems. This volume (1981) and CLM-P

[2] D W Peaceman and H H Rachford Jr. J.soc. ind appl. Math, 3, 28 (1955).

[3] J Crank. Finite-difference methods in 'Moving Boundary Problems in Heat Flow and Diffusion' (Eds. J R Ockendon and W R Hodgkins). Oxford (1975).

[4] B D Turland and R S Peckover. European Appl. Res. Rept. - Nucl.Sci.Technol.1, 1499-1515 (1979).

[5] J E Palentine and B D Turland. The melting of horizontal stainless steel plates subjected to constant thermal loads. Proc. ICHMT conference on 'Nuclear Reactor Safety Heat Transfer (ed. S G Bankoff). Hemisphere Press (1980).

[6] R Bonnerot and P Jamet. J.Comp. Phys. 25, 163-181 (1977).

[7] R C Dix and J Cizek. The isotherm migration method for transient heat conduction analysis. Proc. 4th international heat transfer conference, Paris, volume 1. A.S.M.E.(1971).

[8] J Crank and R D Phahle. Bull. Inst. Maths Applics 9, 12-14 (1973).

[9] B D Turland. A general formulation of the isotherm migration method for reactor accident analysis. Proc. 5th international conference on Structural Mechanics in Reactor Technology, Berlin (eds. T A Jaeger and B A Boley), volume B (1979).

[10] J Crank and R S Gupta. Int. J.Heat. Mass Transfer 18, 1101-1107 (1975).

[11] J Crank and A B Crowley. Int. J.Heat Mass Transfer 21, 393-398 (1978).

[12] A B Crowley. Int. J.Heat Mass Transfer 21, 215-217 (1978).

[13] H S Carslaw and J C Jaeger. Conduction of Heat in Solids. Oxford (1959).

[14] R M Furzeland. The numerical solution of two-dimensional moving boundary problems using curvilinear co-ordinate transformations. Brunel University Mathematics Department report TR/77 (1977).