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SUMMARY

The purpose of the work to be described was to develop an accurate and efficient numerical method to model melting-attack on reactor structures following a hypothetical accident. To this end, the isotherm migration method (IMM) has been investigated.

In the IMM the change in location of a set of isotherms is followed with time; mathematically this is equivalent to a change of dependent variable. The method has advantages over classical numerical techniques for problems involving the passage, with possible broadening, of a thermal front through a medium and in the treatment of melting and freezing problems, since the phase change temperature may be chosen as one of the set of isotherms. The method also provides a way of handling temperature dependent thermal properties simply and efficiently.

The IMM is generalised for multidimensional problems in this paper using a complete co-ordinate transformation; one spatial variable is chosen as the new dependent variable and the independent variables are the remaining spatial co-ordinates and temperature (T). Orthogonal curvilinear co-ordinates (u,v,w) are used to derive a general equation of the form

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

where ψ is a function of the new dependent variable u(v,w,T,t), and the flux functions (Φ^T etc) are functions of u and its first derivatives. This equation is used to derive a conservative numerical scheme using standard finite difference techniques. The present formulation has the advantage that the calculation may be carried out on a uniform mesh in (v,w,T) space with no interpolations necessary. The conservative formulation is particularly useful when propagation into an ambient medium is being considered.

Explicit discretisation leads to a similar timestep constraint as that found for the usual explicit treatment of the diffusion equation. Implicit discretisation has been investigated and produces notable run-time savings for medium-sized meshes.

Results for test problems in one dimension and specimen calculations for the growth of a melt-pool using a two dimensional code are discussed.

1. INTRODUCTION

In the highly unlikely event of a core meltdown in a reactor, debris may collect on reactor structures. If insufficient cooling is available decay heat produced within the debris may lead to melting of these structures. There is a small possibility that debris will penetrate the reactor tank and that a molten pool will form within the reactor substrate. This pool will grow by engulfing the material of the substrate, be it concrete, bed-rock or a specially chosen 'sacrificial' material such as alumina. The growth of the pool is controlled, firstly, by the rate of decay heat generation and heat transfer within the pool, and, secondly, by the heat balance at the pool boundary. Some of the thermal flux originating in the pool is conducted into the substrate whilst the rest provides the latent heat necessary for further melting and pool growth.

In modelling such an accident sequence it is necessary to calculate the rates of melting of both internal structures and the substrate; it may be necessary to perform calculations in one, two or even three dimensions. Standard heat diffusion packages require considerable modification to handle the movement of a melt-front satisfactorily, and it is appropriate to investigate other methods of modelling these situations. Fox [1] and Meyer [2] provide useful reviews of the available techniques.

The problems encountered fall roughly 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). Modifications of standard finite difference schemes (e.g. Crank - Nicolson [3]) work well for this group, at least if the problems are essentially one-dimensional [4], and these problems will not be discussed further in the present paper. The second group is characterised by the propagation of a thermal front, associated with the melt-front, into an essentially ambient medium. The growth of a melt-pool in the reactor substrate is a good example of this type of problem; here the scale-length of the thermal front may be less than one centimetre initially in a medium that occupies many cubic metres.

Dix and Cizek [5] proposed the isotherm migration method (IMM) for one-dimensional forms of this group of problems. In the IMM the governing equations (heat diffusion and heat balance at the melt-front) are transformed so that they give the velocities with which isotherms move through the medium; the positions of the isotherms may then be found by integrating the equations numerically. The advantages of this approach are that by tracking isotherms, rather than following the temperatures at a fixed set of spatial points, a good representation of the temperature profile is obtained irrespective of the width and position of the thermal front, and no re-meshing is required to follow the broadening of the front. The IMM is particularly suited to melting and freezing problems as, provided the phase change occurs at a constant temperature, the phase boundary is itself an isotherm. As the governing equations are discretised for a set of isotherms, temperature dependent properties can be handled simply and efficiently, without recourse to interpolation.

The original form of the IMM as proposed by Dix and Cizek [5] and tested satisfactorily by Crank and Phahle [6] is non-conservative being a direct second-order discretisation of a non-linear equation. This is not very satisfactory for problems involving propagation into an ambient medium, for which Dix and Cizek had to invoke a penetration distance, as the numerical scheme does not exhibit an overall heat balance. In this paper the IMM is rederived in a conservative form, so that heat can be exactly conserved by the numerical scheme. The IMM is also expressed in a general multidimensional formulation based on orthogonal curvilinear co-ordinates. Previous generalisations to two dimensions have either relied on interpolation to evaluate derivatives in one of the spatial directions (Crank and Gupta [7]; Durack and Wendroff [8]) or tracked isotherms along normal flow lines (Crank and Crowley [9]); neither approach generalises readily to three dimensions. The method described in this paper (section 2) uses a full transformation of the governing equations, resulting in a conservative formulation, which may be discretised without interpolation on a uniform mesh in the computational space.

One dimensional calculations are discussed in section 3, whilst specimen calculations for the growth of an axisymmetric melt-pool are discussed in section 4.

2. DERIVATION OF GOVERNING EQUATIONS

We consider the heat diffusion equation in a homogeneous medium:

$$\rho c \frac{\partial T}{\partial t} = \underset{\sim}{\nabla}.(k\underset{\sim}{\nabla}T) \tag{1}$$

where the thermal conductivity k and the specific heat c may be functions of the temperature T, and ρ is the density. Choosing a general set of orthogonal curvilinear co-ordinates (u, v, w) where the metric is defined by

$$ds^2 = h_1{}^2\, du^2 + h_2{}^2\, dv^2 + h_3{}^2\, dw^2 \tag{2}$$

(see e.g. [10]), equation (1) becomes

$$\rho c \frac{\partial T}{\partial t} = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial u}\left(\frac{h_2 h_3}{h_1} k \frac{\partial T}{\partial u}\right) + \frac{\partial}{\partial v}\left(\frac{h_1 h_3}{h_2} k \frac{\partial T}{\partial v}\right) + \frac{\partial}{\partial w}\left(\frac{h_1 h_2}{h_3} k \frac{\partial T}{\partial w}\right)\right] \tag{3}$$

Here $T \equiv T(u, v, w, t)$ is the dependent variable.

To obtain an equation describing the motion of the isotherms we must effect a change of dependent variable as we wish to evaluate partial derivatives either with respect to temperature or at constant temperature surfaces. The new dependent variable is u and standard rules for partial derivatives are applied [e.g. $\partial T/\partial t \equiv -u_t/u_T$; $\partial T/\partial u \equiv 1/u_T$; and $(\partial/\partial v)|_u \equiv (\partial/\partial v)|_T - (u_v/u_T)(\partial/\partial T)|_u$ - where sufficies of u denote partial derivatives of u(v,w,T,t) and $|_x$ denotes that x is held constant when the derivative is taken].

When terms are collected together the following equation results

$$\frac{\partial \psi}{\partial t} = -\left(\frac{\partial \Phi^T}{\partial T} + \frac{\partial \Phi^v}{\partial v} + \frac{\partial \Phi^w}{\partial w}\right) \tag{4}$$

where the independent variables are v, w, T and t, and

$$\psi(v,w,T,t) = \rho c(T) \int_0^u h_1 h_2 h_3 \, du' \tag{5}$$

for $h_1 \equiv h_1(u',v,w)$ etc;

$$\Phi^T = \frac{h_2 h_3}{h_1} \cdot \frac{k}{u_T} \cdot \left[1 + \frac{h_1^2}{h_2^2} u_v^2 + \frac{h_1^2}{h_3^2} u_w^2\right] \tag{6a}$$

$$\Phi^V = -\frac{h_1 h_3}{h_2} k\, u_v \quad \text{and} \quad \Phi^W = -\frac{h_1 h_2}{h_3} k\, u_w \tag{6b}$$

The divergence form of (4) may also be obtained directly from first principles by considering the fluxes into and out of the volume bounded by the planes in which v, v+dv, w, w+dw, T and T+dT are constants. The time derivative in (4) is taken at constant temperature whilst ψ is dependent on the dependent spatial co-ordinate u (equation (5)) and so (4) may be used to track the movement of isotherms along the u co-ordinate.

It is noted that u_T occurs in a denominator in equation (6a), so it should not pass through zero in the region of interest; thus u should be a monotonic function of temperature.

The form of equation (4) permits construction of a conservative numerical scheme (see e.g.[11]) for $\iiint \psi dV$. In a conservative scheme the numerical value of this integral, which is related to the heat content of the system, can only be changed by fluxes across the boundaries of the calculational domain. [$dV \equiv h_2 h_3 dv dw$]

For melting problems the boundary (Stefan) condition must also be transformed. Heat balance at the melt-front implies

$$\rho L \frac{d\underset{\sim}{n}}{dt} = \underset{\sim}{\phi} + k\underset{\sim}{\nabla} T \tag{7}$$

where L is the latent heat, $\underset{\sim}{\phi}$ is the normal heat flux density in the liquid phase and $\underset{\sim}{n}$, which denotes the position of the interface is taken in the direction normal to the melt-front. It may be shown that

$$\frac{d\underset{\sim}{n}}{dt} = h_1 u_t \left(1 + \frac{h_1^2}{h_2^2} u_v^2 + \frac{h_1^2}{h_3^2} u_w^2\right)^{-\frac{1}{2}} \tag{8}$$

from which it follows that (7) may be written in the form

$$\frac{L}{C}\frac{\partial\psi}{\partial t} = \phi h_2 h_3 \left(1 + \frac{h_1^2}{h_2^2} u_v^2 + \frac{h_1^2}{h_3^2} u_w^2\right)^{\frac{1}{2}} - \Phi^T\Big|_{T = T_m} \tag{9}$$

where T_m is the melting temperature.

3. ONE DIMENSIONAL APPLICATIONS

3.1 Discretisation

The governing equations for one dimensional applications may be found from equations (4), (5), (6) and (9) by suppressing v and w. Writing $r \equiv u$ and taking the appropriate values of h_1, h_2, h_3 it is found that

$$\psi = \rho c r^N / N \quad \text{and} \quad \Phi^T = k r^{N-1} / r_T \tag{10, 11}$$

where N=1 (plane), N=2 (cylinder) or N=3 (sphere). Thus a standard finite difference approximation to equation (4) for the plane case is

$$\frac{r_i(t+\Delta t) - r_i(t)}{\Delta t} = \frac{1}{\rho c_i}\left[\frac{k_{i-\frac{1}{2}}}{r_i - r_{i-1}} - \frac{k_{i+\frac{1}{2}}}{r_{i+1} - r_i}\right] \qquad (12)$$

where r_i is the position of isotherm T_i; there are equal temperature intervals between the isotherms that are followed in the calculation. The conservative form of (12) provides the additional constraint sought in [2] for problems involving propagation into an ambient medium as heat balance may be applied rigorously; details will be given elsewhere [12].

Results are now presented for two test problems; for comparison with analytic solutions temperature independent properties are used.

3.2 Test Problems

TEST PROBLEM 1: Propagation of a plane thermal front into an ambient medium induced by a step change in temperature at the origin.

Scaling the variables gives the system of equations:

$$T=0 \;;\quad r>0,\quad t=0 \qquad (13a)$$

$$T=1 \;;\quad r=0,\quad t>0 \qquad (13b)$$

$$T=0 \;;\quad r\to\infty,\quad t>0 \qquad (13c)$$

$$\text{and}\quad \partial T/\partial t = \partial^2 T/\partial r^2 \qquad (13d)$$

There is no melting in this problem which has the well-known analytic solution $T=\text{erfc}\,(r/(2t^{\frac{1}{2}}))$ (e.g. Carslaw and Jaeger [13]). This temperature profile was discretised at t=0.005 to give the positions of a set of isotherms between T=0 and T=1. These positions were then followed numerically using the new version of the IMM based on the discretisation shown in equation (12). Results for t=10 and isotherm spacing ΔT = 0.2, 0.1 and 0.05 are given in Table I. These results demonstrate that accurate results are obtainable from the new method using only a limited number of isotherms and that convergence is good. Comparison calculations were also performed with the discretisation of the IMM given in [2]; acceptable results were obtained but the accuracy was not as good as that shown in Table I.

TEST PROBLEM 2: Steady propagation of a plane melting front into an ambient medium.

The problem is specified in scaled form by

$$\partial T/\partial t = \partial^2 T/\partial r^2 \; ; \quad t \geq 0; \quad r \geq r_m \tag{14a}$$

$$L\frac{dr_m}{dt} = \Phi + \frac{\partial T}{\partial r} \text{ at } T=1 \text{ (i.e. } r=r_m; \text{ the melt front), } t>0 \tag{14b}$$

where L = 1 and Φ = 2,

$$T = 0, \; r \to \infty, \; t > 0 \tag{14c}$$

$$\text{and } T = \exp\,[-r]; \quad t = 0 \tag{14d}$$

The analytic solution is $r_m = t$ and $T = \exp[-(r-r_m)]$ for $r \geq r_m$ [13]. Equation (14d) was discretised at t=0 to give the positions of a set of isotherms and the IMM used to solve the diffusion problem. Positions of the melt-front at t=0.1, t=1 and t=10 using ΔT = 0.2, 0.1 and 0.05 are shown in Table II; in all cases the temperature profile obtained was a good approximation to the analytic solution. Again the method has good accuracy for few mesh points and convergence to the analytic solution is good; using the discretisation given in [2] rather then equation (12) does not produce such good results particularly at later times.

Further details of both calculations are given in [12].

The results of these test calculations auger well for the accuracy of the method when applied to realistic problems, which will in general show a combination of the feature of problem 1 (broadening profile) with that of problem 2 (profile transition because of moving melt-front).

3.3 Timestep Constraints and Implicit Methods

The test calculations used an explicit discretization of (4) (i.e. the RHS of (12) is evaluated using $r_i(t)$). For an explicit discretisation the maximum timestep is limited; Dix and Cizek [2] gave an heuristic argument to show that $\Delta t \leq \rho c(r_{i+1} - r_{i-1})^2/8k$ for all i; which is equivalent to the usual timestep constraint for an explicit diffusion scheme. Thus for a given problem computer time would go roughly as M^3 where M is the number of isotherms that are used. To improve running times for large meshes (and particularly to study the implications for multidimensional applications) equation (12) was written in the time-centred form

$$\frac{r_i^+ - r_i}{\Delta t} = \frac{1}{2} \cdot \frac{1}{\rho c_i}\left[\left(\frac{k_{i-\frac{1}{2}}}{r_i - r_{i-1}} - \frac{k_{i+\frac{1}{2}}}{r_{i+1} - r_i}\right) + \frac{k_{i-\frac{1}{2}}(r_{i+1}^+ - r_i^+) - k_{i+\frac{1}{2}}(r_i^+ - r_{i-1}^+)}{(r_i^* - r_{i-1}^*)\;(r_{i+1}^* - r_i^*)}\right] \tag{15}$$

where no superscript denotes values at t, + denotes values to be calculated at t+Δt (which are found by inverting a tridiagonal matrix) and * denotes values at t+Δt which must be either predicted from past data or derived from a previous iteration for r^+. This linearisation removes exact conservation from the scheme but in practice results from implicit and explicit calculations agree very well, with shorter running times for the implicit schemes usually found if M=10 (depending on the problem and accuracy parameter specified). Running time for the implicit scheme is found to scale as M^y where $1 < y < 1.5$ for specific problems.

4. A TWO-DIMENSIONAL APPLICATION: GROWTH OF AN AXISYMMETRIC MELT-POOL

The motive for this study of the isotherm migration method was to develop a method for melt-pool growth in the reactor substrate and in this section an idealisation of this problem is considered. In order to concentrate on melting and heat diffusion in the substrate a heat flux density distribution from the pool is assumed and the boundary conditions are simplified so that there is no heat loss from the solid to the overlying coolant.

The simplest co-ordinate system to use is spherical polars with origin at the pool surface; so $u \equiv r$, $v \equiv \theta$ and w is ignorable. Thus $h_1 = 1$, $h_2 = r$ and $h_3 = r \sin\theta$, so

$$\psi = r^3 \sin\theta/3 \; ; \tag{16}$$

$$\Phi^T = \frac{kr^2 \sin\theta}{r_T}\left(1 + \frac{r_\theta^2}{r^2}\right); \quad \text{and } \Phi^\theta = -k \sin\theta . r_\theta \tag{17,18}$$

To make use of the 'divergence' form of equation (4) the computational (θ, T) space is divided up into equal elements with sides $\Delta\theta$ and ΔT (see fig. 1); the mesh points lie at the centres of the elements. Extra mesh points are introduced along the melt-front ($T=T_m$) so that the boundary condition given by equation (9) can be discretised. The other boundary conditions are that (i) $\Phi^T = 0$ when $T=T_a$ (no heat loss from the solid); (ii) $\Phi^\theta=0$ when $\theta=0$ (symmetry) and (iii) $\Phi^\theta=0$ when $\theta = \pi/2$ (simplifying assumption - see above). For the general mesh point designated by '0' in fig. 1 discretisation of equation (4) gives

$$\frac{\psi_0(t+\Delta t) - \psi_0(t)}{\Delta t} = -\left[\frac{\Phi_N^T - \Phi_S^T}{\Delta T} + \frac{\Phi_E^\theta - \Phi_W^\theta}{\Delta\theta}\right] \tag{19}$$

where subscripts here denote the place of evaluation. Values of r_0 may be found directly from values of ψ_0 using (16). The first order derivatives required to evaluate Φ^T and Φ^θ may be calculated to $O((\Delta T)^2)+O((\Delta\theta)^2)$ from the values at the mesh points.

For the idealised problem it is assumed that decay heat from a 1000 MWe reactor is generated in the pool. Two thirds of the heat is carried upwards to the overlying coolant, whilst the remaining third appears as a heat flux around the lower pool boundary with a distribution that would maintain a hemispheroidal pool with an axial ratio of four were conduction into the bed negligible. (These assumptions are consistent with the present understanding of heat transfer in a growing internally heated pool). The properties assumed for the bed are typical of basalt (ρ = 2200 kg m^{-3}, c = 1580 J kg^{-1} K^{-1}, L = 38800 J kg^{-1}, k = 2W m^{-1} K^{-1}, T_m = 1100 C) and T_a = 20 C. At times up to a few days after pool formation (and neutronic shutdown) the pool grows rapidly, and, apart from a thin thermal front causing preheating of material before melting, little heat is conducted into the bed. Thus at these times there is no need for a detailed solution for the bed, and so the calculation is not started until 3×10^5s after pool formation, at which time a hemispheroidal shape with an axial ratio of four is assumed (see fig. 2). The subsequent pool growth and the diffusion of heat into the solid (consequently restricting pool growth as less heat is available for melting) are shown in fig.2. These computations, for which $\Delta T = 0.2\ (T_m - T_a)$ and $\Delta\theta = \pi/20$, took 4 minutes CPU time on the ICL 4-70 at Culham. The relatively small mesh produces errors in maximum pool dimensions and volume of around 10%, where the estimate is obtained by considering the trend from results on smaller meshes. Substantially larger meshes are practical if an implicit discretisation in time is used (fully implicit or time-centred); this has been demonstrated for test problems in two dimensions using a generalisation of the iterative scheme discussed in section 3.3. [12].

The IMM provides the capability of describing the growth of arbitrarily shaped melt-pools; to take advantage of this, more detailed models of convective processes in the pool are required to determine the form of the heat flux distribution function.

5. CONCLUSIONS

A generalised form of the isotherm migration method has been derived. The governing equations may be discretised conservatively, which is particularly important for problems involving the propagation of a thermal front into am ambient medium. The method may be applied to practical problems by choosing the most suitable set of orthogonal curvilinear co-ordinates, recognising that the new dependent variable should be a monotonic function of temperature. Excellent results have been obtained for test problems in one dimension, and it has been indicated how further accuracy may be obtained without large running times by using time-centred discretisation in conjunction with a larger mesh. The two-dimensional application considered in section 4 demonstrated the use of the method, and, although larger meshes appear necessary for high accuracy, indicated that useful results can be obtained with the method and a limited amount of computer time.

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TABLE I

Results for test problem 1 at t=10 calculation started at t=0.005.

ISOTHERM T =	ANALYTIC SOLUTION	NUMERICAL SOLUTION		
		ΔT = 0.2	ΔT = 0.1	ΔT = 0.05
1.0*	0.	0.	0.	0.
0.8	1.133	1.138	1.134	1.133
0.6	2.345	2.353	2.348	2.346
0.4	3.764	3.768	3.766	3.765
0.2	5.731	5.693	5.720	5.728

*T=1.0 isotherm fixed at origin.

TABLE II

Result for test problem 2 : position of melt front (r_m)
Calculation started at t=0, r_m=0.

TIME t=	ANALYTIC SOLUTION	NUMERICAL SOLUTION		
		ΔT=0.2	ΔT=0.1	ΔT=0.05
0.1	0.1	0.1004	0.1001	0.1000
1.0	1.0	1.004	1.001	1.000
10.0	10.0	10.006	10.003	10.001

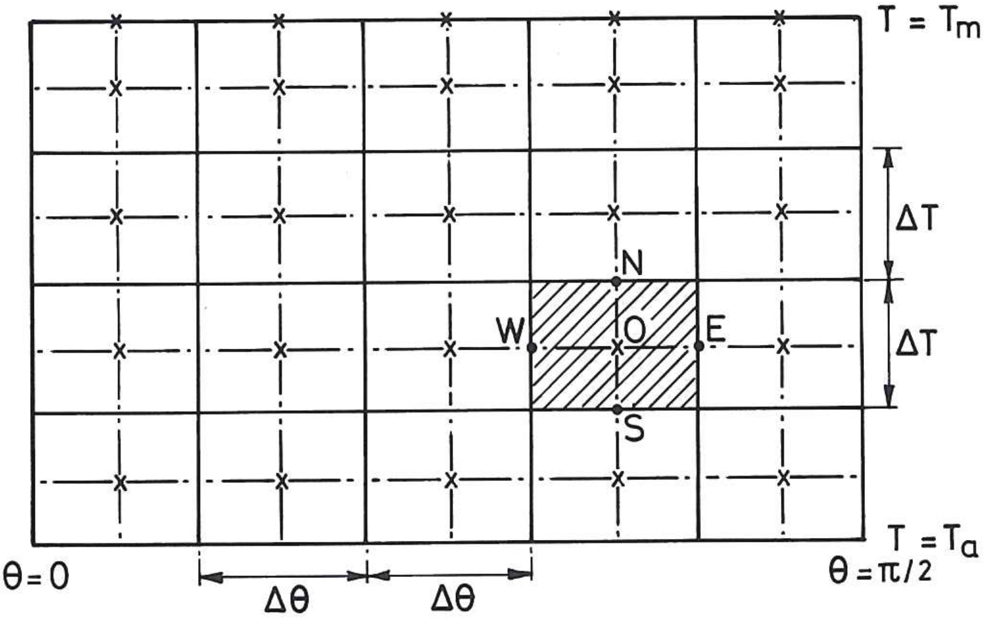

Fig.1 Mesh in (θ,T) space for multi-dimensional IMM. Mesh points are indicated by crosses. A typical cell is shown hatched. In the calculation Φ^T is evaluated at points N and S to construct $\partial\Phi^T/\partial T$ and Φ^θ is evaluated at points E and W to construct $\partial\Phi^\theta/\partial\theta$. ψ is evaluated at the mesh point 0.

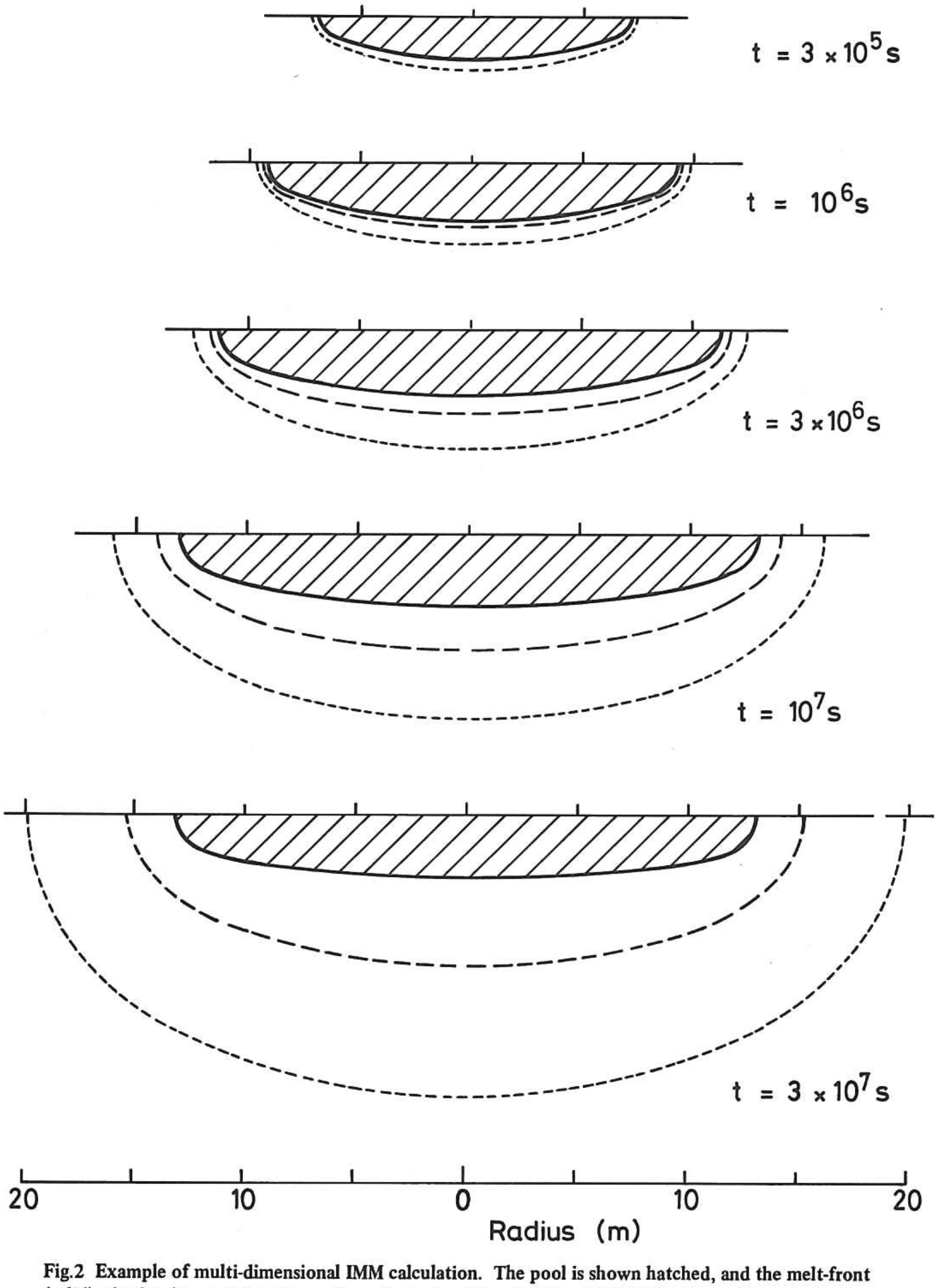

Fig.2 Example of multi-dimensional IMM calculation. The pool is shown hatched, and the melt-front (solid), the 0·5 ($T_m + T_a$) isotherm (long dashes) and the (0·1 T_m + 0·9 T_a) isotherm (short dashes) are shown for various times after pool formation. The calculation was started at t = 3 x 10^5 s.