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A SURVEY OF THE FORMULATION AND SOLUTION OF FREE AND MOVING BOUNDARY (STEFAN) PROBLEMS.

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Introduction

Following Cryer (FB, 1976)[†], a FREE BOUNDARY PROBLEM (FBP; plural FBPs) may be defined as a steady-state boundary value problem, typically an elliptic partial differential equati on with associated boundary conditions, which has to be solved in a domain, parts of whose boundaries, the FREE BOUNDARIES (FB; plural FBs) are unknown and must be determined as part of the solution. Correspondingly, a MOVING BOUNDARY PROBLEM (MBP; plural MBPs) or STEFAN PROBLEM may be defined as a non-stationary or time-dependent boundary value problem, namely a parabolic partial differential equation with associated initial and boundary conditions, which has to be solved in a time-dependent space domain with MOVING BOUNDARIES (MB; plural MBs). Since the FB or MB has to be determined as part of the solution it can readily be shown that such problems are inherently non-linear.

Heat conduction or diffusion problems with phase changes from solid, liquid or vapour states constitute a large class of MBPs. A simple example is the melting and freezing of ice/water which was first studied by Stefan (1889) and after whom this class of problems is named. FB and MBPs occur in many areas of practical interest such as the metal, glass, plastics and oil industries, space vehicle design, preservation of foodstuffs; chemical and diffusion processes, statistical decision theory, semiconductors, astrophysics, metereology, geophysics and plasmaphysics (references and details are given in section 6).

† The references are split into two sections, one for moving and one for free boundary problems. References in sections 1-6 are for the former unless prefixed FB.

The main part of this survey is concerned with the numerical solution of MBPs. The need for an up-to-date survey is apparent from the large amount of research effort expended on these problems in recent years, especially with regard to the multi-dimensional case. Earlier surveys have mainly concentrated on the one (space)-dimensional problem, see Muehlbauer and Sunderland (1965), Bankoff (1964), Rubinstein (1971), Boley (1972), Crank (1975). More recent surveys have included multi-dimensional applications, see Furzeland (1974), Crank and Fox in Ockendon (1975), Meyer (1975a,1976), Hoffmann (1977, I-III); the references in Ockendon and Hoffmann being the most comprehensive and containing many practical applications.

In the following sections the formulations of MBPs and their approximate analytical and numerical solutions are discussed. The terminology used in the heat conduction context is employed in order to fix ideas. For completeness, a brief section on the formulation and numerical solution of FBPs is included in order to bring the literature on the subject up-to-date. The references are split into two parts, one for MBPs and one for FBPs.

1. Classical formulations of MBPs

A simple example of a MB (Stefan) problem is the one-phase, one-dimensional melting ice problem. The classical formulation of the problem is to find the pair of unknowns (u(x,t),s(t)), where u(x,t) denotes the temperature distribution in space x and time t, and s(t) the position of the ice/melted water interface (MB), subject to the equations (in their simplest, non-dimensional form):

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad , \quad 0 < x < s(t), \;\; t > 0 \; , \qquad (1.1)$$

(the governing partial differential, heat conduction equation)

$$u = 1 \;\; \text{on} \;\; x = 0 \;\; , t > 0 \;\; , \qquad (1.2)$$

(the fixed boundary condition, constant temperature)

$$\left.\begin{matrix} u = 0 \\ s = 0 \end{matrix}\right\} \;\; \text{at } t = 0 \;\; \text{(initial conditions)} \; , \qquad (1.3)$$

(1.4)

$$\left.\begin{matrix} u = 0 \\ \dfrac{\partial u}{\partial x} = -\dfrac{ds}{dt} \end{matrix}\right\} \;\; \text{on the MB } \; x = s(t), \;\; t > 0. \qquad \begin{matrix}(1.5)\\(1.6)\end{matrix}$$

Equation (1.5) denotes the phase change temperature on the isotherm x = s(t) which is moving away from the heat input boundary x = 0. Equation (1.6) is known as the 'Stefan condition' and is derived from heat balance arguments at the MB.This condition explicitly relates the velocity of the MB, ds/dt, with the heat flux, $\partial u/\partial x$, on x = s (t). The problem is one-phase if it is assumed that the semi-infinite block of ice x > s(t) is, and remains, at u = 0.

The corresponding two-phase problem is to find the triple $(u_1(x,t),u_2(x,t),s(t))$ where u_1 and u_2 denote the temperatures in each phase, e.g. liquid and solid respectively. An example of this would be the finite block of ice, $0 \le s(t) \le x \le 1$, where $u_2(x, t)$ is not constant. In this case there is one governing equation (1.1) for each phase and the MB conditions are

$$\left.\begin{array}{l} u_1 = u_2 = 0, \\ \left[\frac{\partial u}{\partial x}\right]_1^2 \equiv \beta \frac{\partial u_2}{\partial x} - \frac{\partial u_2}{\partial x} = -\frac{ds}{dt}, \end{array}\right\} \quad \text{on } x = s(t) \qquad \begin{array}{r} (1.7) \\ (1.8) \end{array}$$

This can be generalised to multi-phase, multi-MBPs with different phase change temperatures on each MB. For example, the melting and solidification of alloys involving, a mixture of two or more metals, Chuang et al. (1975), or the ablation of the alloy walls of a space vehicle which leads to a three-phase, solid-liquid-vapour, problem with two MBs, Koh et al. (1969). A piece of ice immersed in water represents a two-phase problem with two MBs, Cannon et al. (1967).

More general formulations of the classical problem are based on combinations of the following:-

(a) Non-linear governing equations, e.g. in the heat conduction problem where there are temperature-dependent thermal properties $c(u)$, $k(u)$, $\rho(u)$ and internal (body) heating function $Q(x,t)$ i.e.

$$\rho(u)c(u)\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[k(u)\frac{\partial u}{\partial t}\right] + Q(x,t) \quad , \qquad (1.9)$$

or in non-steady flow through a porous medium, - the filtration problem discussed by Fulks and Guenther (1969), Graveleau and Jamet (1971), Kamin (1976), Peletier and Gilding (1976), Cannon and Fasano (1977),

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}(u^m) \quad , \quad m > 1 , \qquad (1.10)$$

More general non-linear forms are given in Hoffmann (1977, III).

If convection effects in the liquid phase are significant then a connective term $v\partial u/\partial x$, where v is the velocity of the liquid phase, needs to be added to the governing conduction equation, Haitz and tfestwater 0-970), Kroeger and Ostrach (1974).

The heat conduction equation may also be coupled with another equation such as one describing mass transfer, e.g. moisture movement and temperature distribution in humid porous flow, Aguirre-Puente and Fremond (1975), Mikhailov (1975, 1976); heat and concentration diffusion, Mebditch, Tayler in Ockendon, (1975, pp. 112, 120); temperature and pressure distributions in multi-phase flow, Koh et al. (1969).

(b) Time-dependent or non-linear fixed boundary conditions, e.g.

$$u = \phi(t) \quad \text{or} \quad \frac{\partial u}{\partial t} = h(t) \quad \text{or} \quad \frac{\partial u}{\partial x} = g(u,t) \quad \text{on} \quad x = 0. \tag{1.11}$$

Space-dependent initial conditions, e.g.

$$u = u_0(x) \quad \text{at} \quad t = 0 \quad , \tag{1.12}$$

(c) Space and time-dependent phase change temperatures,

$$u = \mu_1(x,t) \quad \text{on} \quad x = s(t) \quad , \tag{1.13}$$

and variable thermal properties and heat source (or sink) function in the MB condition,

$$\frac{\partial u}{\partial x} = \lambda\ (x,t)\ \frac{ds}{dt} + \mu_2\ (x,t) \quad \text{on} \quad x = s(t). \tag{1.14}$$

A particular case of (1.14) is X - 0, i.e. there are Cauchy data prescribed on the MB. Such problems have been termed implicit' MBPs by Sackett (1971a) since there is no longer an explicit relationship for the position or velocity of the MB in terms of u or its derivatives. This causes difficulties in both theoretical and numerical treatments. Implicit MBPs arise in biomechanics, Crank and Gupta (1972a); statistical decision theory (see section 6);

Bingham plastic flow, Rubinstein (1971); filtration, Ventcel (1960); diffusion flames, Saitoh (1972).

Schatz (1969), has shown that the transformations

$$v = \frac{\partial u}{\partial x} \quad \text{or} \quad v = \frac{\partial u}{\partial t}\,, \tag{1.15}$$

will transform the implicit $\lambda = 0$ case into the explicit $\lambda \neq 0$ case. However, such transformations are not always possible or may introduce singularities if any of the data Q, ϕ, h, g, u_0, μ_1 or μ_2 the above equations are zero or discontinuous, see Tayler in Ockendon (1975, p.125).

In general, (1.14) may take the non-linear functional relationship

$$F(u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}, x, \frac{ds}{dt}, t) = 0 \quad \text{on} \quad x = s(t)\ , \tag{1.16}$$

see Hoffmann (1977, III), and the practical examples given by Ciment and Guenther (1974), Meyer (1975b), Chuang et al. (1975), Friedman and Jensen (1975)

Proofs of the existence and uniqueness properties of classical solution to MBPs have been mainly restricted to the one-dimensional, one-phase case. For explicit (Stefan-type) MB conditions, proofs have been given by Evans (1951), Cannon et al. (1970), Rubinstein (1971); for implicit MB conditions by Schatz (1969), Sackett (1971a), Sherman (1971). Smoothness, differentiability and monotonicity properties of the MB have been discussed by Friedman (1968), Schaeffer (1976). Two and three-phase problems have been treated by Cannon et al. (1975), Fasano and Primicerio (1977); non-linear problems are discussed in Hoffmann (1977,III). For more general, multi-dimensional problems the results need to be expressed in terms of weak solutions which are considered in the following section.

In three (space)-dimensions $\underline{x} = (x, y, z)$ the two-phase MBP is

$$\rho c \frac{\partial u}{\partial t} = \nabla(k \nabla u) + Q \ , \ \underline{x} \ \varepsilon D_i \ , \ i = 1,2, \ 0 < t < T, \tag{1.17}$$

$$\frac{\partial u}{\partial t} - hu_i = -h + g_i(\underline{x}, t) \ , \ \underline{x} \ \varepsilon \partial D_i, \ 0 < t < T \ , \tag{1.18}$$

$$\left.\begin{aligned} u(\underline{x}, 0) &= u_o(\underline{x}) \quad (1.19) \\ f(\underline{x}, 0) &= f_o(\underline{x}) \quad (1.20) \end{aligned}\right\} \text{ at } t = 0 \ ,$$

$$\left.\begin{aligned} u_1(\underline{x}, t) &= u_2(\underline{x}, t) = u_m \quad (1\ 21) \\ \left[k \frac{\partial u}{\partial n}\right]_1^2 &= -\rho L \ v_n + q \quad (1.22) \end{aligned}\right\} \text{ on the MB } f(\underline{x}, t) = 0 \ , \ 0 < t < T \ ,$$

where, in the heat conduction context, u_i denotes the temperature in each phase i =1,2, u_M the phase change temperature (constant), L the latent heat, n the outward normal to the MB f ($\underline{x}$,t)= 0, and v_n the velocity of the MB in the normal direction; $D = D_1 \cap D_2$ and $\partial D = \partial D_1 \cap \partial D_2$ denotes the interior and boundary of the region in Figure 1. The thermal properties c, ρ, k, body heating function Q and MB heat source q may be functions of u,x and t or may vary between phases.

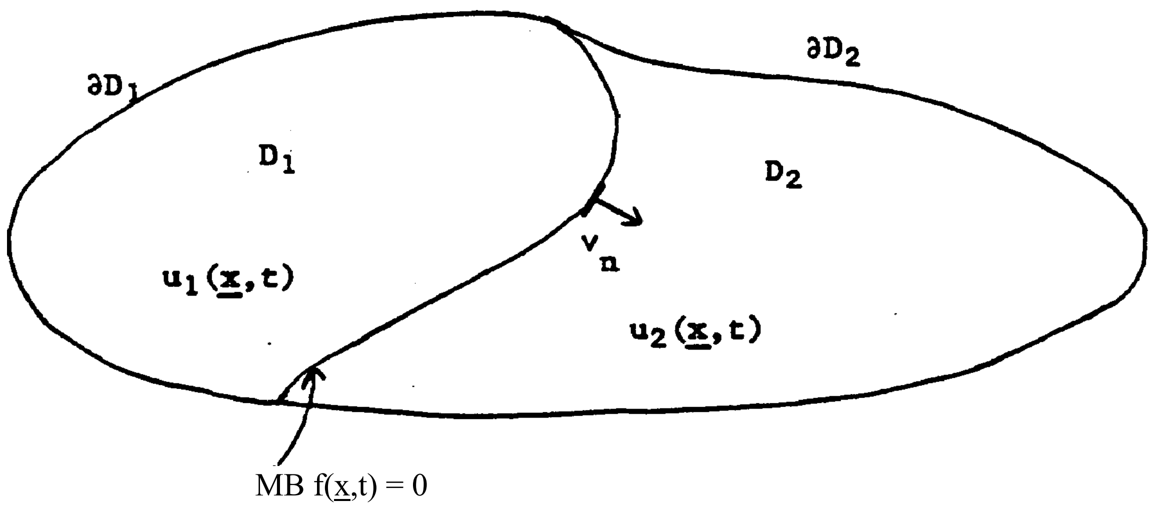


Figure 1 - Two "-phase region with a MB

Patel (1968) showed that the MB condition (1.22) can be simplified by using differential relationships on the isotherm (1.21), e.g. to

$$\left[1 + \left(\frac{\partial s}{\partial x}\right)^2 + \left(\frac{\partial s}{\partial y}\right)^2 \right] \left[k \frac{\partial u}{\partial z} \right]_1^2 = -\rho L \frac{\partial z}{\partial t} \quad \text{on} \quad z = s\,(x, y, t) \;, \tag{1.23}$$

for the case q = 0. This is an explicit relationship for the component $\partial u/\partial z$ of grad u in terms of derivatives of the MB curve $f(\underline{x},t)=0$ written as z = s(x,y,t). Similar relations hold for the other two components $\partial u/\partial x$ and $\partial u/\partial y$. This form is useful for developing approximations, typically finite-difference ones, for the components of grad u, see Sikarskie and Boley (1965), Lazaridis (1970), Rathjen and Jiji (1971), Crank and Gupta (1975), Furzeland (1977, Ch.4). The corresponding form for the two-dimensional, one-phase problem with MB y = s(x,t) is

$$k \left[1 + \left(\frac{\partial y}{\partial x}\right)^2 \right] \frac{\partial u}{\partial y} = -\rho L \frac{\partial y}{\partial t} \quad \text{on} \quad y = s(x,t)\;. \tag{1.24}$$

2. Alternative formulations - enthalpy, veak solutions and variational inequalities

Certain classes of MBPs may be formulated in such a way that the MB conditions may be absorbed into the new governing equations and the new problem may be solved without any explicit reference to the position of the MB or to the MB conditions. The position of the MB is located, a posteriori, when the solution is complete. This reformulation may also be effected for FBPs, see later.

One of the earliest such formulations was based on use of the heat enthalpy (content or internal energy) function H(u) as first used by Albasiny+(1956), Rose (1960), with theoretical justification by Kamenomoatskaj.a (1961), Oleinik (1960). Using heat balance arguments, the two-phase MBP (1.17), with MB conditions (1.21) and (1.22), can be reformulated as the single equation over the whole domain D

$$\frac{\partial H(u)}{\partial t} = \nabla(k\nabla u) + Q \quad , \underline{x}\varepsilon D \quad ,0 < t < T \quad , \qquad (2.1)$$

or in integral form over an arbitrary volume V of D

$$\int_O^T \int_V \{\frac{\partial H}{\partial t} = \nabla(k\nabla u) - Q\} \quad d\nabla dt = 0 \quad , \qquad (2.2)$$

where H(u) represents the sum of the sensible and latent heat content Szekely and Themelis (1971), Hodgkins, Longworth, Tayler in Ockendon (1975, pp.26, 54, 120),Shaxnsundar and Sparrow (1975). The MB conditions have been absorbed into (2.1) by the definition of H, Budak et al. (1965), Bonacina et al. (1973) ,

$$H(u) = \int_{U_R}^{U} \{p(\varsigma)c(\varsigma) + Lp\ (\varsigma - u_M)d\ \varsigma \quad , \qquad (2.3)$$

† Albasiny does,in fact, mention earlier use of this idea by Evres et al. in 1946.

where $u_R < u_M$ is an arbitrarily chosen, reference temperature and δ is the Dirac (impulse) function, see Figure 2.

H(u) has a jump discontinuity at $u = u_M$ of the form

$$[H(u_M)]_1^2 = pL \ , \qquad (2.4)$$

and dH/du is infinite at $u=u_M$. If equation (2.1) is integrated over a small volume V around the MB, and the limit fit $\delta t \to 0$ taken, then the Stefan condition (1.22) is obtained, Shamsundar and Sparrow (.1975) . This demonstrates the equivalence of (2.1) to the classical problem (1.17), (1.21) and (1.22).

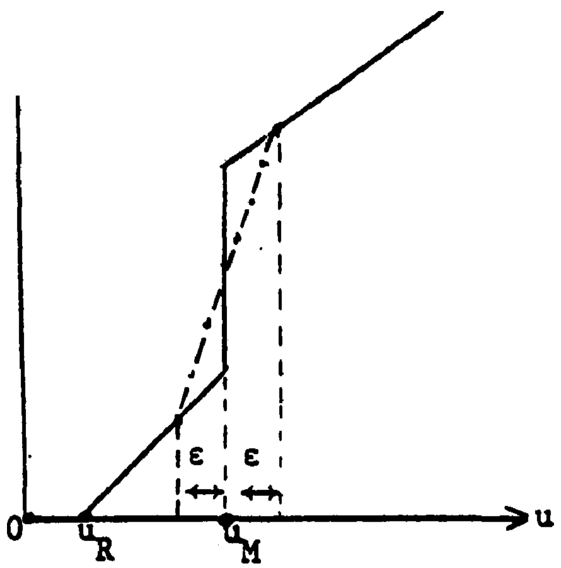


Figure 2 -Has a function of u.

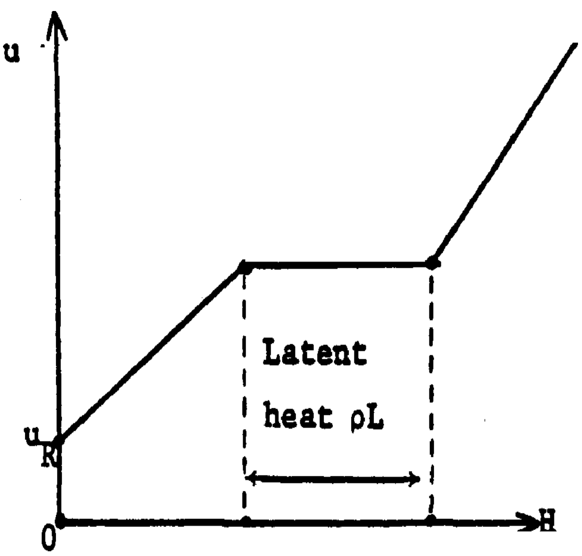


Figure 3-u as a function of H.

If H and k are known functions of u over the region of solution D, or over each small volume V of D, e.g. by standard tables or experimental data, then the numerical solution can proceed and the MB is given, a posteriori, by values of $\underline{x}$ where $u=u_M$, see Hodgkins in Ockendon (1975). If such relations are not known then the definition (2.3) is used and the discontinuous nature of H(u) is approximated by smoothing the jump at u_M, over the small interval $[u_M - \varepsilon, u_M + \varepsilon]$in Figure 2, see Budak at al. (1965), Moiseynko et al. (1965), Meyer (1973), Bonacina et al. (1973), The smoothing approach is justified in practice by the fact that most materials contain a certain amount of impurity and so the phase change occurs over a range and not at a point.

Alternatively, u may be regarded as a function of H and standard data for u(H) may be used, Albasiny (1956), Longworth in Ockendon (1975, p.54). Otherwise the definition proposed by Rose (1960) and At they (1974) is' needed

$$\left.\begin{array}{l} u = H/c, \quad H \le Cu_M \quad , \\ u = u_M \quad , \quad cu_M \le H \le cu_M + L, \\ u = (H - L)/C \quad , \quad H > Cu_M + L. \end{array}\right\} \begin{array}{c}(c \text{ constant}, \\ p \equiv 1)\end{array} \tag{2.5}$$

From a numerical point of view, this is preferable to using H(u) where small changes in u produce large changes in H near u_M if L is large. Also, Bonacina et al. (1973) have found that the magnitude e of the assumed range of phase change temperatures can appreciably effect the results, see Furzeland (1977, Ch.5).

One-phase problems can be treated in a similar way by extending the definition of u to a fixed two-phase domain in which the usual two-phase equations hold but $c(u) \equiv 0$, $p(u) \equiv 0$ in the new phase, see Budak et al. (1965). Complications arise if u_M is a function of $\underline{x}$, and, as yet, this problem has not been treated. The non-linearity, associated with k(u) can be removed by introduction of the 'flow temperature' or 'conductivity potential' function given by $\int^u k(\xi)d\xi$, see Albasiny, Longworth, and Furzeland (1977, Ch.5).

The discontinuous and non-linear nature and lack of differentiability of the enthalpy formulations suggests the use of the concept of a weak solution of the Stefan problem whereby the problem is reformulated as an integral involving no derivatives of u, rather than as a differential relation. The weak solution for (2.1) can be derived by multiplying (2.1) by an arbitrary test function ϕ, defined on D, which is twice continuously differentiable with respect to the space variables and once with respect to time and which is such that

$$\left.\begin{array}{ll} \phi(x,t). = 0 \quad , \quad \underline{x} \; \varepsilon \; \partial D \quad , \\ \phi(x,t) = 0 \quad , \quad \underline{x} \; \varepsilon \; D \quad . \end{array}\right\} \tag{2.6}$$

Integration of the resulting equation throughout D and for $0 < t < T$, followed by integration by parts and use of the conditions

$$\left.\begin{array}{ll} u = g(\underline{x},t) \quad , \quad \underline{x} \; \varepsilon \partial D \quad , \\ u = u_0(\underline{x}) \quad , \quad t = 0 \quad . \end{array}\right\} \tag{2.7}$$

gives, the integral (weak or generalised) formulation

$$\int_O^T \int \{u\nabla(k\nabla\phi) + H(u)\frac{\partial\phi}{\partial t} + Q\,\phi\}\, d\underline{x}dt \;=\; \int_0^T \oint_{\partial D} kg\,\frac{\partial\phi}{\partial n} d\underline{x}\,dt \;-\; \int_D H(u_0)\,\phi(\underline{x},0)\,d\underline{x}. \tag{2.8}$$

Existence and uniqueness theorems for weak solutions of this type in multi-dimensional, multi-phase problems have been given by kamenomostskaja (1961), Oleinik (1960), Friedman (1968) and Rubinstein (1971). Fasano and Primicerio (1975) have used the weak solution formulation to give a stability theorem for problems with sharply changing temperature-dependent coefficients. The convergence of numerical schemes to the weak solution, despite the discontinuities in u across the MB, is discussed in section 4.

Integral formulations such as (2.8) can also be developed starting from the classical problem (1.17) rather than the enthalpy form (2.1), - for an application of this to a finite-element method see Bonnerot and Jamet (1974, 1977). The theoretical properties of weak solutions are useful in cases where the existence and uniqueness of the classical solution cannot be proved e.g. for multi-dimensional problems, Friedman (1968); for 'mushy' regions, Atthey (1974), when phases disappear regenerate), Friedman (1968), Tayler in Ockendon (1975, p.120); for non-linear problems, see equation (1.10) and associated references.

The classical formulation of MBPs can also be expressed in terms of variational inequalities. Consider the one-phase MBP with implicit MB conditions:-

$$\frac{\partial U}{\partial t} = \nabla^2 u + Q \quad , \quad \underline{x}\,\varepsilon D_1 \ , \quad 0 < t < T \quad , \tag{2.9}$$

$$u = g(t) \quad , \quad x\ \varepsilon\,\partial D_1 \quad , \quad 0 < t < T \quad , \tag{2.10}$$

$$u = u_0(x) \quad , \quad t = 0 \quad , \tag{2.11}$$

$$\left.\begin{array}{l} U = 0 \\ \dfrac{\partial U}{\partial n} = 0 \end{array}\right\} \text{ on the MB } f(\ ,t) = 0, \quad 0 < t < T. \qquad (2.12)\ (2{\cdot}13)$$

If $g \geq 0$, $u_0 \geq 0$ and Q is such that $\frac{\partial u}{\partial t} - \nabla^2 u - Q \geq 0$ (a practical example of this is the oxygen diffusion problem of Crank and Gupta (1972a)), and the definition of u is extended to the whole fixed domain D by

$$u \equiv 0, \ \underline{x}\ \varepsilon\ D_2\ n \cap \partial D_2 \ , \quad 0 < t < T \quad , \tag{2.14}$$

then it is easy to show that u also satisfies the parabolic variational inequality

$$(\frac{\partial u}{\partial t}\ , \ \phi - u) \ + \ a(u, \phi - u) \ \geq \ (Q\ , \ \phi - u) \quad , \tag{2.15}$$

for all $\phi \ \varepsilon \ k(t) \equiv \{\phi \ \varepsilon \ H^1(D): \ \phi = g(t) \text{ on } \partial D_1, \phi = 0 \text{ on } \partial D_2, \ \phi \geq 0\}$, where K(t) is the space of time-dependent constraints. In (2.15) (. , .) and a(. , .) are the inner products

$$(u,\phi) = \int_D u\phi d\underline{x} \quad , \tag{2.16}$$

$$a(u,\phi) = \int_D \nabla u \nabla \phi \, d\underline{x} \quad , \tag{2.17}$$

and $H^1(D)$ is the Sobolev space for ϕ and its first space derivatives being square integrable over D. Theoretical properties of such solutions are discussed in Brezis (1972), Bensoussan, Lions and Papanicolaou (1975), Elliott (1976). Integration of (2.15) with respect to time gives the corresponding weak form, see Brezis, Elliott

$$\int_0^T \left[(\frac{\partial \phi}{\partial t}, \quad \phi - u) + a(\phi, \phi - u) \right] dt \geq \frac{1}{2} |\phi(T) - u(T)|^2 - \frac{1}{2} |\phi(0) - u_o|^2 . \tag{2.18}$$

The inequalities (2.15) or (2.18) can also be expressed in differential rather than integral variational form as

$$\left. \begin{aligned} &(\frac{\partial u}{\partial t} - \nabla^2 u - Q)u = 0, \\ &\frac{\partial u}{\partial t} - \nabla^2 u - Q \geq 0, u \geq 0, \end{aligned} \right\} \tag{2.19}$$

see Brezis, Bensoussan et al, Elliott. Inequality (2.19) is a continuous linear complementarity problem which, on suitable discretisation, leads to a quadratic programming (minimisation) problem at each time level, with simple constraints consisting of bounds on the variables, see Elliott.

A corresponding variational inequality (and complementarity problem) can be developed for problems with the classical MB condition

(1.22) as proposed by Duvaut (1973) for the one-phase problem

$$\frac{\partial u}{\partial t} = \nabla^2 u \quad , \quad t > \ell\,(x) \quad , \tag{2.20}$$

$$u \equiv 0 \qquad , \quad t \le \ell(\underline{x}) \quad , \tag{2.21}$$

$$u = g(t) > 0 \quad , \quad \underline{x}\,\varepsilon\,\partial D_1 \quad , \tag{2.22}$$

$$u = u_o(\underline{x}) > 0, \quad t = 0 \qquad , \tag{2.23}$$

$$\left.\begin{aligned} & u = 0 \\ & \nabla u \nabla\ \ell = -L \end{aligned}\right\} \text{ on } t = \ell(\underline{x}) \quad , \tag{2.24}$$

(2.25)

where the conditions t greater than or less than $\ell(x)$ are equivalent to $\underline{x}$ belonging to D_1 x or D_2 (i. e. the MB curve f ($\underline{x}$,t)=0 is the function t = $\ell(\underline{x})$, the time at which $\underline{x}$ is first in $D_1(u>0)$ given that it is initially in $D_2(u\equiv 0)$, e.g. the melting ice problem D_1 = water, D_2 = ice.

Duvaut used the Baiocchi (see FB references) type transformation of u

$$\left.\begin{aligned} & v(\underline{x},t) = \int_{\ell(\underline{x})}^{t} u(\underline{x},t)dt \quad , \ t > \ell(\underline{x}) \ , \\ & v = 0 \quad , \quad t \le \ell(\underline{x}) \ , \end{aligned}\right\} \tag{2.26}$$

to transform the explicit MB condition (2.25) into the implicit form:

$$\left.\begin{aligned} & v = 0 \\ & \frac{\partial v}{\partial n} = 0 \end{aligned}\right\} \quad t = \ell(x) \quad , \tag{2.27}$$

(2.28)

Equation (2.20) – (2.23) become

$$\frac{\partial v}{\partial t} = \nabla^2 u + u_o - L \quad , \quad t > \ell\,(x) \quad , \tag{2.29}$$

$$v = 0 \qquad , \quad t \le \ell(x) \qquad , \tag{2.30}$$

$$v = \int_0^t g\,(t)dt \equiv G(t), \qquad \underline{x}\,\varepsilon\partial D_1 \qquad . \tag{2.31}$$

The transformation (2.26) is essentially the inverse of the transformation $v = u_t$ see (1.15), given by Schatz (1969).

The two-phase problem is dealt with by a similar transformation, see Duvaut in Ockendon (1975), Aguirre - Puente and Frémond (1975) where (2.26) is termed the 'freezing index'. The variational inequality and complimentarity problems corresponding to (2.27)-(2.31) follow as before. These ideas can also be used to develop elliptic variational inequalities, see section 7.

Elliott (1976) has shown that discretisations of the parabolic inequalities derived from the transformations of Duvaut are equivalent to corresponding discretisations derived from the enthalpy formulation. This is true for both explicit and implicit time discretisations.

3. Analytical solution techniques

The need for analytical solutions arises when there is a singularity in the region of solution or on the boundary, e.g. Fox, in Ockendon (1975, p.228), discussed the need for a short-time analytical solution in the case of discontinuous agreement of initial and boundary conditions. Such solutions are also useful if only the short or long term behaviour of the solution is required, or if an independent check for a numerical solution is needed.

The complexity of the MBF means that only a few analytical solutions are available in closed form, and then only for the one-dimensional case of an infinite or semi-infinite body with relatively simple initial and boundary conditions and constant thermal properties. These exact solutions are usually in the form of error functions of the similarity variable, $x/t^{1/2}$, and are known as Neumann's solutions, see the reviews by Cho and Sunderland (1969), Crank (1975). Corresponding solutions for heat and mass transfer in a semi-infinte region are given by Mikhailov (1975, 1976), and for the non-linear filtration problem (1.10) by Kamin (1976), Peletier and Gilding (1976).

Approximate analytical solutions are needed for more general problems in finite regions. Many problems have been tackled by reducing the problem to an integral equation, or to a system of integro-differential equations, of Volterra type with kernels consisting of Green's functions.

Integral equation formulations were first given by Evans et al. (1950) who used Laplace transforms to obtain an integral form for the solution u(x,t) to a one-phase MBP. Ockendon (1975) has discussed the use of both Fourier and Laplace transforms to develop integral equations for u. Similar equations can be developed for a wide class of problems by the use of Green's functions, Rubinstein (1971), Chuang and Szekely (1971), Chuang and Ehrxch (1974), Hansen and Hougaard (1974), Chuang et al. (1975), Katz (1977). Collatz (1977) has described how these integral equations may be used to find practical error bounds. If a series solution for the MB, x= s(t), or an asymptotic expansion for small or large time, is valid then substitution of this into the integral equation completes the solution. In general, a numerical solution is needed.

Integral equations also arise in the heat-balance (Goodman's) integral method in which the governing equation is integrated with respect to x over each phase. Assumption of a temperature profile valid over the whole of each phase reduces the system of integral equations to one of ordinary differential equations in t, Goodman (1961), Cho and Sunderland (1969). The method has been extended to temperature-dependent thermal properties, Imber and Huang (1973), and to two dimensions, Foots (1962), Poots and Rodgers (.1976). Both Fox and Noble in Ockendon (1975, pp. 208, 233) suggest that the simplicity of the method merits further attention, particularly with regard to a finite-element method. Another method in the heat - balance category is based on Biot's variational principle, a Lagrangian formulation of which leads to a system of ordinary differential equations. The solution then proceeds by assuming a suitable profile for u, Agrawal in Ockendon (1975, p. 242).

Integro-differential equations arise from use of either the embedding or moving heat source methods. Boley (1961) introduced the concept of a fictitious body of constant geometry in which is 'embedded' the real body whose geometry varies with time. The fictitious body then has a fictitious flux, f(t), introduced on the boundary. The problem is then one of finding f(t) and the MB x » s(t) from two or four integro-differential equations, depending on whether the problem has one or two phases. These equations are then solved for short time by series expansions or for large time numerically. Sikarskie and Boley (1965), Boley and Yagoda (1969) extended these ideas to two—dimensional problems; the method is reviewed by Boley in Ockendon (1975, p.150). Ferriss and Hill (1974) have applied the method to the one-dimensional, oxygen consumption problem.

Rathjen and Jiji (1971) applied the idea of using a moving heat source of strength Lpds/dt on the MB to determine the temperature distribution for the two-dimensional problem of freezing in a right-angled corner x, y > 0. An integro-differential equation for the MB is derived, and an approximate solution obtained by using superhyperbolae to approximate the MB position. Budhia and Kreith (1973) extended this method to a wedge with angle between 0 and 360^0.

Asymptotic expansions (other than for integral or integro-differential equation formulations) can be developed for large or small x, t or L (latent heat). Asymptotic expansions for L are discussed by Ockendon (1975, p.143). Pertubation solutions are useful in certain cases, see Spaid et al. (1971), Pedroso and Domoto (1973), Atthey, Fox in Ockendon (1975, pp.38, 237).

4. Numerical solution techniques

The finite-difference (FD) method has been used extensively for the numerical solution of MBPs, see the reviews of Furzeland (1974), and Crank, Fox in Ockendon (1975, pp. 192, 210) and in recent years several finite-element (FE) methods have been proposed. The increased speed and storage capacity of present day computers has allowed various sophistications to be tried out with both these methods. A collection of computer programs is given in Hoffmann (1977, II).

The techniques used for the numerical solution of MBPs either belong to the class of 'front-tracking' methods, where the position of the MB is predicted along with the solution of the governing equations in each phase, or they belong to the class of enthalpy and variational inequality methods where the reformulated governing equations are solved over a fixed domain and the position of the MB is determined a posteriori. These methods are now reviewed in detail:

Front-tracking methods

The two important features of a front-tracking solution for a MBF are the ways in which approximations are developed for the new position of the MB and for the derivatives of the solution near the MB. For example, consider the one-phase, one-dimensional MBP given by equation (1.1) - (1.6) then the Euler (FD) approximation in time for (1.6) gives the explicit scheme for the new position of the MB

$$s(t^{n+1}) = s(t^n) - \delta t \ Du^{(n)} \quad , \tag{4.1}$$

where $t^n = n\delta t$ is the time at the nth level, n=0, 1, 2, ..., and $Du^{(n)}$ denotes the FD or FE approximation for $\partial u/\partial x$ at $x = s(t^n)$. In practice, the $0(\delta t)$ accuracy of this scheme is usually sufficient, as long as 6t is reasonably small.

Alternatively, an implicit scheme such as

$$s(t^{n+1}) = s(t^n) - \frac{1}{2}\delta t \ \{Du^{(n)} + Du^{(m+1)}\}\ , \qquad (4.2)$$

where an iterative scheme is used to successively approximate the unknown Du , can be employed, Bonnerot and Jamet (1974). Since this involves resolving (1.1) at each iteration, even just two iterations (a predictor-corrector scheme) would be very expensive. If necessary, an $0((\delta t)^2)$ approximation for ds/dt can be developed from the three-point, backward (implicit) difference scheme

$$3s(t^n) - 4s(t^{n-r}) + s(t^{n-2}) = 2\delta tDu^{(n)} \qquad (4.3)$$

as mentioned by Meyer (1976).

Often it is more important to approximate $Du^{(n)}$ accurately. If a fixed grid spacing $x_i = ih$, $i = 0, 1, 2, ...$, is used then, in general, the MB falls in between two grid points and this unequal spacing near the MB greatly diminishes the accuracy with which $D\acute{u}^{(\pi)}$ can be computed. It will be described later how the grid spacing can be arranged so that the MB coincides with a mesh point and thus equally spaced $u(x_i.)$ approximations can be used. Non-steady, heat flow or diffusion depends on $\partial^2 u/\partial x^2$ being appreciably different from zero and so $0(h^2)$ Taylor series (FD) approximations for $Du^{(n)}$ are preferable rather than 0(h) ones. Typically, a three-point end on (quadratic extrapolation) formula is used, Murray and Landis (1959), Lazaridis (1970). On a coarse grid, this extrapolation scheme may not always give good results and so Furzeland (1977, Ch. 4) proposed the central difference formula (centred on the MB) for $Du^{(n)}$ in conjunction with use of (1.1) at the MB to eliminate the 'fictitious' u value. This scheme is of an interpolatory nature and has a smaller truncation error. Improved accuracy for $Du^{(n)}$ can also be obtained by refining the grid near the MB, Ciment and Guenther (1974), or by the use of the 'extrapolation to the limit' method of global grid refinement, Schmidt in Hoffmann (1977, III).

An alternative formulation of the MB condition (1.6) is

$$s(t) = -\int_0^t u(0,\tau)d\tau - \int_0^{s(t)} u(x,t)dx \quad , \tag{4.4}$$

as used by Douglas and Gallie (1955), and the integrals may be evaluated using various quadrature schemes, Schmidt (ibid).

MB conditions (1.14) of the implicit (X-0) type can be dealt with by transformations (1.15) to obtain the explicit ($\lambda \neq 0$) form. Alternatively, the condition (1.13) on x = s(t) may be differentiated with respect to t (as many times as is necessary) to give an expression for ds/dt in terms of higher derivatives of u, e.g. Crank and Gupta (1972a) obtain

$$\frac{ds}{dt} = \frac{\partial^3 u}{\partial x^3} \quad , \qquad \text{on} \quad x = s(t) \quad , \tag{4.5}$$

for the oxygen consumption problem, $\lambda = \mu_1 = \mu_2 = 0$ (113) and (1.14).

In more than one dimension, the MB condition (1.22) can be written in the form of (1.23) or (1.24). Considering the two-dimensional case (1.24), then it is only necessary to form approximations for $\partial u/\partial y$ (rather than for $\partial u/\partial x$ as well) at the MB $y = s(x,t^n)$ in order to find the y ordinate of the MB at time t^{n+1} along each line x_i. In the three-dimensional case, (1.23) can be used to find the z value of the MB at t^{n+1} for each point (x,y) on $z = s(x,y,t^n)$.

For the approximation of the governing equation and the position of the MB on a fixed grid where the MB x = s(t) falls between two grid points, several special FD schemes have been proposed to deal with the unequal intervals near the MB. Crank. (1957), with recent use by Crank and Gupta (1972a), used an explicit FD method with special formulae based on Lagrangian interpolation near the MB. Ehrlich (1958), Koh et al. (1969), employed a Crank-Nicolson scheme and Taylor expansions in time and space near the MB. Murray and Landis (1959), used an explicit FD method with 3-point end-on formulae developed from the first two terms of the difference form of the Taylor's expansion for Du (they also give a variable space scheme, see later). Saitoh (1972) used both Crank-Nicolson and fully implicit schemes with unequal formulae near the MB.

The problem in two dimensions was first tackled by Allen and Severn (1962) who used a relaxation scheme with iterative adjustment of initial guesses at each time level for the MB position so as to fit the condition $u=u_M$ on the MB. The problem in both two and three dimensions has been solved by Lazaridis (1970) who used explicit FD approximations based on auxiliary equations and MB conditions such as (1.23) and (1.24) near the MB. Quadratic profiles and 3-point formulae are used to maintain $0(h^2)$ accuracy over the unequal intervals near the MB. However, the complexity of such 'irregular star' FD schemes can be avoided if the MB is chosen so that it coincides with a grid point or, in two dimensions, a grid line. To accomplish this many methods have been proposed:

(i) Douglas and Gallie (1955) chose each time step δt so that the MB always moved from one grid point to another. A fully implicit FD scheme was used and iterations for δt were calculated from the integral form (4.4). Douglas (1961) later suggested an alternative formula for δt which avoided iteration. Vasilev (1964), Nogi (1974) have extended the method to more general one-dimensional problems.

(ii) Murray and Landis (1959) reformulated the governing equations so that there was a fixed integer number, I say, of space intervals between the moving and fixed boundaries, where I is constant for all time. Their explicit FD method was extended to cover convection problems by Heitz and Westwater (1970). Bonnerot and Jamet (1974, 1975) used a similar variable space grid with finite element quadrilaterals in space and time for the non-rectangular (x,t) grid. The governing equation was expressed in weak (integral) form and solved using numerical quadrature and isoparametric finite elements. The resulting approximations were shown to be a generalisation of the Crank-Nicolson, implicit FD formula. Recently (1977), they have extended the method to two-dimensional problems (see also Furzeland (1977, Ch.4)).

(iii) Crank and Gupta (1972b) used an explicit FD scheme on a uniform grid which moved with the MB; the main benefit of this was a smoother tracking of the MB since the unequal space intervals were transferred to the fixed boundary. This moving grid method necessitated interpolation in order to calculate u values from the old grid to the new grid at the next time step. Gupta (1973) avoided these interpolations by using Taylor series expansions in time and space.

(iv) Ciment and Guenther (1974) used a fixed space grid with refinement of the grid near the MB such that the MB coincided with one of the refined grid points. A fully implicit FD scheme was used and the time step was chosen so that the MB did not pass more than one of the coarse grid points.

(v) One of the most popular methods has been that of fixing the MB at the same grid point or line for all time by a suitable co-ordinate transformation. For example, for the MBP (1.1) - (1.6), the transformation

$$\xi = x / s(t) \,, \tag{4.6}$$

fixes the MB at $\xi = 1$ for all time. Equations (1.1) and (1.6) become

$$\frac{\partial u}{\partial t} = \frac{1}{s^2} \frac{\partial^2 u}{\partial \xi^2} - \frac{\xi}{s} \frac{ds}{dt} \frac{\partial u}{\partial \xi} \quad , \; . \quad 0 < \xi < 1 \,, \; t < 0 \,, \tag{4.7}$$

$$\frac{1}{s} \frac{\partial u}{\partial \xi} = - \frac{ds}{dt} \quad \text{on } \xi = 1 \quad , \; t > 0 \; . \tag{4.8}$$

Thus fixing the MB is at the expense of transforming the essential non-linearity of the problem to the governing equation (4.7) in the form of coefficients which are functions of the MB position and velocity. This non-linearity is easily coped with in a numerical solution since s and ds/dt are already known from (4.8) before the solution of (4.7) is advanced to the next time level. If the fixed boundary is at infinity, rather than at x = 0, then (4,6) becomes

$$\xi = x - s(t) \quad . \tag{4.9}$$

Such transformations were first proposed by Landau (1950), and used in FD schemes by Crank (1957), Lotkin (1960). Their use in one-dimensional problems has been reviewed by Crank (1975, p. 314). The idea has been extended to problems with implicit MB conditions by Ferriss and Hill (1974), to non-linear problems by Mastaniah (1976). Two-dimensional problems have been treated by Spaid et al. (1971), Duda et al. (1975), Furzeland (1977, Ch.4)* who use transformations such as

$$\eta = y/s(x,t) \quad , \tag{4.10}$$

for the MB $y = s(x,t)$. Further applications of the method are discussed in Hoffmann (1977, III, pp. 4,49,91).

(vi) The above co-ordinate transformations are just simple examples of the general idea of transforming a curved-shaped region in two or more dimensions into a fixed, rectangular (say) domain. Such transformations may be carried out by a variety of body-fitted, curvilinear co-ordinate methods which are determined by the numerical solution of a set of subsidiary equations. These ideas have been applied to the solution of two dimensional MBPs by Furzeland (ibid). The use of conformal transformations for two-dimensional problems has been discussed by Goldstein and Segal (1970), Kroeger and Ostrach (1974).

(vii) A similar idea to (vi) is that of a suitable change of dependent with independent variables so that the curved MB becomes a straight line in the new plane. This concept has been ised in flow problems where the curved free streamline,

* Available as Technical Report TR/77, Department of Mathematics,

ψ = constant, in the (x,y) plane becomes a straight line in the (ϕ,ψ) plane, ϕ and ψ being harmonic conjugates† , also where the new independent variables are $p = \partial u/\partial x$, $q = \partial u / \partial y$, as in the hodograph method, Cryer (FB, 1976), or where the stream function $\psi(x,y)$ is transformed into a relationship expressing y as a function of ψ and x††.

This last idea has been applied to MB problems and is known as the isotherm migration method'(IMM) . In one dimension, the MBP (1.1) - (1.6) is rewritten so that x(u,t) becomes the dependent variable. Using (1.2), equation (1.1) and (1.6) become

$$\frac{\partial x}{\partial t} = \left(\frac{\partial x}{\partial u}\right)^{-2} \frac{\partial^2 x}{\partial u^2} \quad , \qquad 0 < u < 1 , \; t < 0 \; , \tag{4.11}$$

$$\frac{ds}{dt} = -\left(\frac{\partial x}{\partial u}\right)^{-1} \quad , \qquad u = 0, \quad t > 0 \; . \tag{4.12}$$

The non-linear equation (4.11) can be readily solved using an explicit FD scheme. Crank and Phahle (1973) , to calculate the way in which an isotherm (fixed u) moves through the medium. Crank and Gupta (1975) have extended the method to two dimensions by rewriting the problem as y = y(u,x,t). Crank and Crowley (1977) have recently proposed a novel approach for multi-dimensional MBPs by tracking the movements of the isotherms along the flow lines which, in an isotropic medium, are orthogonal to the isotherms. They use explicit F-D to solve a locally one-dimensional, IMM form of the radial heat conduction

† A. Thorn and C.J. Apelt (1961), "Field Computations in Engineering and Physics", van Nostrand.

†† J.D. Boadway (1976), Int.J.Num.Math.Engng. 10, 527 - 533.

equation and cater for the changing shape and orientation of the orthogonal system by a geometric procedure.

Front-tracking methods of different nature are required if the problem is first discretised with respect to time ('the method of lines'). In one dimension, this reduces the problem to a sequence of ordinary differential equations with free boundaries. The solution of the problem can then be expressed in an integral form and solved numerically to give the position of the boundary at each time step, Sackett (1971a,b), George and Damle (1975). Alternatively, the reduced problem can be solved by the method of invariant imbedding, Meyer (1970, 1972, 1975a, b).The method can be extended to two dimensions by working in alternating directions along each co-ordinate in turn, Meyer (1977), and is suitable for use with general, non-linear MB conditions.

Enthalpy and variational inequality (fixed domain) methods

The policy of using front-tracking methods to follow the MB explicitly is not always a good one since an a priori assumption with such methods is that the MB varies smoothly or monotonically with time. This is not always the case, particularly in more than one dimension, for the MB may have sharp peaks, or double back, or even disappear. The alternative is to essentially ignore the MB position by solving the reformulated problems given in section 2-over a fixed domain.

The enthalpy method can be applied with a smoothed enthalpy function H(u), see (.2.3) and Figure 2, or in the discontinuous form u(H), see (2.5) and Figure 3. The smoothed

H(u) approach was first applied to multi-dimensional MBPs by Budak et al. (1965), Moiseynko and Samarskii (1965), who used various order smoothings and locally one-dimensional FD methods, two dimensional,implicit FD and FE schemes with successive over-relaxation were given by Couch et al.(1970), Elliott (1976), Meyer (1973/6).Three-time level, FD and FE schemes have been used by Bonacina et al. (1973), Comini et al. (1974), Fisher and Medland (1974). Convergence results for the FD schemes to weak solutions have been given by Kamenomostskaja (1961), Oleinik (1960), Meyer (1973).

The discontinuous form u(H) was proposed by Atthey (1974) who used explicit FDs for a one-dimensional problem with a 'mushy'region. The method has been extended to two-dimensional problems using explicit and implicit FDs by Furzeland (1974,1977, Ch.5), Crowley (1976), and using FEs by Hodgkins in Ockendon (1975, p.26). Implicit FD schemes have been given by Fedorenko (1975), Longworth in Ockendon (1975, p. 54), Shamsundar and Sparrow (1975). Ciavaldini (1975) introduced the use of the u(H) enthalpy formulation analogous to (2.1)

$$\frac{\partial \phi}{\partial t} = \Delta A\phi + Q \quad , \tag{4.13}$$

where $u = A\phi = H^{-1}(\phi)$. (4.14)

Ciavaldini discretised the weak form of (4.13) by a quadrature rule and solved the resulting problem using both explicit and implicit FE schemes. Convergence proofs for the explicit FD and FE schemes were given by Atthey and Ciavaldini, and for the implicit schemes by Jerome (1976), Schafer in Hoffmann (1977, III).

Another fixed domain approach is the 'truncation method' proposed by Berger et al.(1975a) for one-phase problems with implicit MB conditions. They considered the oxygen consumption problem (see section 5) where u must be positive and equals zero on the MB. The problem is solved with either FD or FE methods over a fixed domain (0,b) with u = 0 at b. The position of the MB is then given by the nodes at which u = 0, any negative values being set (truncated) to zero†. The method has been extended to two-phase problems by alternating the use of the truncation method in each phase, Berger et al. (1975b), and has been used for solving variational inequalities such as (2.15) and (2.19) where $u \geq 0$, Berger (1976).

Elliott (1976), using FE methods, has expressed the variational inequalities of section 2 in terms of quadratic programming problems which can be solved using projected, successive over-relaxation or conjugate gradient methods. He has noted how the MB position with fixed domain methods can be located more accurately than just between two grid points' by using quadratic extrapolation based on the last two grid points in conjunction with the MB conditions.

E.g. for $u = \partial u/\partial x - 0$ at $x = s(t)$ then

$$s = (I-1)h + h/\{(u_{I-2}/u_{I-1})^{\frac{1}{2}} - 1\} \tag{4.15}$$

for the last two grid points x_{I-2}, x_{I-1}. This can also be carried over to two dimensions by working along one co-ordinate line.

† This method has also been used in two dimensions, Evans and Gourlay (1977).

5. Numerical comparisons

In one dimension, as described in section 3, there are exact analytical solutions available for comparison with numerical solutions. For the melting ice problem, Crank and Phahle (1973) have given comparisons of the exact solution with the IMM, heat-balance (Goodman), and Lagrangian interpolation methods. For non-linear problems, Hoffmann (1973, III) has given several constructed (exact) solutions for comparisons with his numerical methods.

In two dimensions, constructed solutions are usually needed to serve as exact solutions for numerical comparisons, see Ciavaldini (1975), Meyer (1976, 1977). The approximate analytical solutions described in section 3, and the experimental results of Jiji et al. (1970), Saitoh (1976), are also useful for comparisons. For the problem of the inward solidification of a square prism of liquid, Crowley (1976) has given comparisons between the experimental results of Saitoh and the numerical results of relaxation, front-tracking FD, IMM and enthalpy methods.

In recent years, the one-dimensional, oxygen diffusion with consumption problem of Crank and Gupta (1972a) has been solved by a large number of different methods and it is thus suitable for detailed numerical comparisons. Although the conclusions of such a study tend to be open-ended due to the number of variable factors involved, they do give a fair indication of the performance of each method.

In non-dimensional form, the problem is to solve for the concentration of oxygen, $c(x,t)$, and the MB, $x_o(t)$, the equations:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - 1 \quad , \quad 0 < x < x_0(t) \quad , \quad t > 0 \quad , \tag{5.1}$$

$$\frac{\partial c}{\partial x} = 0 \quad , \quad x = 0 \quad , \quad t > 0 \quad , \tag{5.2}$$

$$\left.\begin{aligned} & x_0(0) = 1 \, , && (5.3) \\ & c = \frac{1}{2}(1-x)^2 \, , \quad 0 \le x \le 1 \quad , && (5.4) \end{aligned}\right\} \quad t = 0 \, ,$$

$$\left.\begin{aligned} & c = 0 \quad , && (5.5) \\ & \frac{\partial c}{\partial x} = 0 \quad , && (5.6) \end{aligned}\right\} \quad \text{on } x = x_0(t) \, , \; t > 0 \; .$$

The problem has two interesting characteristics, first, there is a discontinuity in the initial and boundary conditions ($\partial c/\partial x = -1$, $t = 0$; $\partial c/\partial x = 0$, $t > 0$ at $x = 0$) and thus any numerical solution starting at $t = 0$ will contain 'persistent' discretisation errors for all t (see Part I, ref. [11]). Second, the MB is moving towards $x = 0$, i.e. the domain of solution is shrinking, and the MB speeds up as it approaches $x = 0$.

The concentration values at $x = 0$ and the MB position $x_0(t)$, for the given time step δt and grid length h, are shown in Tables 1 and 2. Reading from left to right, the different methods are:

(1) FD formulae based on Lagrangian interpolation for the unequal intervals near the MB and the Taylor series expansion for $x_0(t)$

$$x_0 = x_{I-1} + \sqrt{\frac{2c_{I-1}}{h}} \quad , \quad x_{I-1} \text{ the last grid point} \, , \tag{5.7}$$

Crank and Gupta (1972a). These results start at $t = 0$ and thus involve the persistent discretisation errors mentioned earlier. These results were repeated (1972a) by starting at $t = 0.0025$ and using the approximate analytical expression, see method.(12), for $t \le 0.0020$. Due to a fortuitous 'cancellation of errors' effect the earlier results seem better (when compared with the analytical ones).

Unless stated, the following methods start at t = 0.0025 and use (5.7) for the MB position:

(2) Heat balance method using a fourth-degree polynomial profile for the concentration and using the observed profile (see also (12))

$$c(x,t) = \tfrac{1}{2} - 2\sqrt{t/\pi} \qquad \text{on} \qquad x = 0\,, \tag{5.8}$$

to give a differential equation for the MB which is solved numerically using the Runge-Kutta method, Crank and Gupta (1972a).

(3) Moving grid method without interpolation, Gupta (1973). The moving grid approach gives a smoother tracking of the front since the unequal intervals are transformed to x = 0, however these unequal intervals result in less accurate values as the MB approaches x = 0.

(4) Variable space (Murray and Landis) grid using 10 intervals for all time, Gupta (1973). This gives particularly good results for large time since h decreases as the domain decreases.

(5) FE method using linear basis functions and 10 elements, Aral and Yazici (1974), no details are given so it is assumed that the solution starts at t = 0.

(6) Fixing of the boundary by using the transformation $\eta = x/x_0(t)$ solution by a Crank-Nicolson implicit FD scheme and iterations based on the method of 'false position' to locate the MB, Ferriss and Hill (1974) .

(7) Embedding method using the fictitious heat flux $\partial c / \partial x = f(t)$ at x = 1, numerical solution of the resulting integro-differential equation with $\delta t = 0.01$, Ferriss and Hill (1974).

(8) FE solution with finer mesh near the MB and $x_0(t)$ calculated from the extrapolation scheme (5.9), c.f. equation (5.7), Miller and Morton (1977).

$$x_o = x_{I-1} + \sqrt{\frac{12}{5} c_{I-1}} \qquad x_{I-1} \text{ the last grid point.} \tag{5.9}$$

(9) FE solution of the variational inequality form of (5.1) - (5.6)

$$\left.\begin{aligned} c(\partial c/\partial t - \Delta c + 1) &= 0 \\ c \geq 0 \quad , \quad \partial c/\partial t - \Delta c + 1 &\geq 0 , \end{aligned}\right\} \tag{5.10}$$

using linear basis functions with h = 0.05 and Crank-Nicolson implicit (FD) in time with $\delta t = 0.005$, Elliott (1976). The minimisation of (5.10) was carried out using projected successive over-relaxation at each time step and the position of the MB was found by the extrapolation formula (4.15).

(10) As (9) but with h =- 0.01, $\delta t = 0.001$.

(11) Hansen and Hougaard (1974) developed an integral equation for $x_o(t)$ and an integral formula for c(x,t) using Green's function techniques. The integral equation and formula were solved asymptotically for small times and numerically for all time to produce what seem to be the most consistently accurate results, particularly for large time.

(12) Crank and Gupta (1972a) developed an approximate analytical solution by assuming that the boundary does not move initially. Solving the fixed boundary value problem using Laplace transform techniques, and taking the first terms in the resulting series,

gives the approximation

$$\hat{c}(x,t) = \frac{1}{2}(1-x^2) - 2\sqrt{t/\pi}\ \exp(-x^2/4t) + x\,\mathrm{erfc}\,(x/2t^{\frac{1}{2}}), \quad (5.11)$$

valid for 'small' t.

Hansen and Hougaard's asymptotic expansion allows for the movement of the MB and can be expressed as

$$c(x,t) \sim \hat{c}(x,t) + 4\sqrt{t^3/\pi}\ \{E(2-x,t) + E(2+x,t)\}, \quad (5.12)$$

valid for $1-x \ll 1-x_0(t)$ and with a relative error of $0(t)$.

In the above

$$E(x,t) = \frac{1}{x^2}\exp(-x^2/4t). \quad (5.13)$$

The additional terms in (5.12) account for the change in c caused by the motion of the boundary, and since these terms are always ≥ 0 for x and $t > 0$, $\hat{c}$ provides a lower bound for the exact solution.

Surprisingly, expression (5.12) remains good for large time, the exponential terms E increasing extremely slowly. This can be explained on the physical grounds that the results of an instantaneous change of boundary conditions on x=0 at t=0 take a long time to diffuse through to the MB. More surprising, still is the fact that (5.11) is comparable with (5.12) up to $t = 0.15$ (to the fourth decimal place). Physically speaking, fixing $c = 0$ on $x = 1$ and fixing the MB means that the diffusion with absorption process is allowed to continue so that c becomes negative and this extra diffusion accounts for the lower values $\hat{c}$ in Table 1. The reader is referred to the works of Constable and Evans (1975/6), Murray and Taylor (1977) for a more detailed account of the physical background. Expressions (5.11) and (5.12) are also reasonable approximations for values of c away from $x = 0$, e.g. $c(0.2, 0.18) = 0.0149, 0.0156, 0.0161$ for (5.11), (5.12) and method (12) respectively, and for the time to completion $t_{end} = 0.1963$, 0.1968, 0.1976 (similarily).

Berger et al. (1975a, 1976) have solved this problem using the truncation method, and have compared their results graphically with those of Crank and Gupta (1972a). Their truncation method is based on that of solving the equation over a fixed domain $0 \leq x \leq 1$ with the negative values of c truncated to zero at each time level. The above comments on (5.11) help to explain why this apparently crude approximation works so well. Elliott also solves the problem over a fixed domain but the inequality (5.10) leads to better results since it takes into account the complementarity constraint $\partial c/\partial t - \Delta c + 1 \geq 0$ as well as the non-negativity constraint $c \geq 0$.

Finally, an enthalpy formulation of the problem has been described by Elliott (p.88) and, since discretisations of the enthalpy and variational inequality formulations are equivalent (see the comment at the end of section 2), it is expected that similar results would be obtained.

Method No.	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)
Time	Crank and Gupta		Gupta		Aral* 10 FEs	Ferriss		Miller & Morton FE with extrap. δt = .002	Elliott, FE var. inequality		Hansen* & Hougaard Integral equation	Approx. analytical upper = (5.12) lower = (5.11)
	Lagrange (i) 1972a* (ii) 1972b	Heat balance	Moving grid	Variable space, 10 intervals		Fixing* of boundary	Embedding δt = .01		h = .05 δt = .005	h = .05 δt = .005		
.005	4203 —	—	—	—	4203	4271	—	—	—	—	4202	4202 4202
.01	3875 —	—	—	—	3879	3919	—	—	—	—	3872	3872 3872
.04	2745 2742	2743	2742	2745	—	—	—	—	2744	2743	2743	2743 2743
.10	1433 1430	1432	1430	1434	1439	1446	1432	—	1433	1432	1432	1432 1432
.14	779 777	—	780	780	—	790	779	—	780	779	779	778 778
.18	218 216	213	218	218	222	228	218	—	219	218	218	216 213
.185	156 151	—	158	154	—	—	—	—	155	153	153	151 147
.19	90 —	82	—	—	—	100	—	—	—	—	90	86 82

←Most accurate→

Table 1 - Concentration values x 10^4 at the sealed surface ($x = 0$), values are for $h = .05$, $\delta t = .001$ unless stated.

* Values start from $t = .0025$ unless marked with an asterisk, then start at $t = 0$.

Method No.	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
Time	Crank and Gupta		Gupta		Aral* 10 FEs	Ferriss		Miller & Morton FE with extrap. δt = .002	Elliott, FE var. inequality		Hansen* & Hougaard Integral equation
	Lagrange (i) 1972a* (ii) 1972b	Heat balance	Moving grid	Variable space, 10 intervals		Fixing* of boundary	Embedding δt. = .01		h = .05 δt = .005	h = .01 δt = .001	
.04	— 9992	10000	9992	9988	—	—	—	9992	9990	9991	9992
.10	9352 9346	9321	9347	9309	9377	9352	9353	9354	9326	9325	9350
.14	7976 7966	7817	7979	7930	—	8005	8000	7989	7961	7986	7989
.18	4961 4942	4892	5007	4974	5000	5083	5097	4979	4991	5011	5011
.185	— 4178	—	4343	4308	—	—	—	—	4355	4333	4334
.190	3387 —	3505	—	—	—	3595	—	3402	—	—	3454
.195	1613 —	2331	—	—	1999	2352	—	—	—	—	2065

←Most accurate→

Table 2 - Moving boundary position x 10^4, values are for h = .05, δt = .001 unless stated.

* Values start from t = .0025 unless marked with an asterisk, then start at t = 0.

6. A list of practical problems involving MBPs

(1) Heat conduction

Melting and solidification (metals, glass, plastics, etc.) Cho and Sunderland (1969), Ockendon (1975); ablation and space vehicle design, Boley (1961, 1972), Koh. et al. (1969); freezing and thawing of water/ice - manufacture of ice, preservation of foodstuffs, Albasiny (1956), Bonacina and Comini (1974), Fisher and Medland (1974); humid porous media, Mikhailov (1975/6), Aguirre-Puente and Fremond (1975); moist soils (permafrost), Couch et al. (1970), Meyer et al. (1972), Meyer (1973); storage of thermal enerzv, Shamsundar and Sparrow (1974/5); heat transfer at high rates - thermal explosions, Ockendon (1975); cryosurgery, Comini and del Guidice (1976); icing of a cable, Poots and Rodgers (1976); heat conduction with convection, Heitz and Westwater (1970), Kroeger and Ostrach (1974).

(2) Chemical and diffusion processes

Corrosion, tarnishing, coating, Crank (1975), Meyer (1975a), Peel in Ockendon (1975); crystallisation, Evans et al. (1950), Chuang and Ehrich (1974); evaporation, condensation, precipitation, bubble growth, Bankoff (1966); diffusion flames, Saitoh (1972); diffusion by chemical reactions or by discontinuous diffusion coefficients, Crank (1975); diffusion of oxygen in absorbing tissue, Evans and Gourlay (1977), Constable and Evans (1975/6), Murray and Taylor (1977), see also section 5.

(3) Decision theory

Statistical decision theory - optimal stopping times (e.g. for a gambler), Breakwell and Chernoff (1964), Sackett (1971b), Kotlow (1973), Moerbeke C1974); space-ship control, inventory control, Bather and Chernoff (1967), Bather (1976).

(4) Industrial problems

Glass-melting and growth, Gelder and Guy in Ockendon (1975); thermal switching, Crowley (1975). Plastics - Bingham plastic flow, Rubinstein (1971). Metals - melting and solidification, Szekely and Themelis (1971), Boley (1972), Chuang et al. (1975); casting, Rubinstein (1971), Kroeger and Ostrach (1974); precipitation hardening, scrap melting, welding, cutting, Ockendon (1975); dip soldering, Tadjbakhsh and Liniger (1964); lightning and arc studies, Crowley (1977); oil - Rubinstein (1971), Watts (1976), see also permafrost in (1).

(5) Astrophysics/meteorology/geophysics/nuclear physics

Growth and decay of stars, Eggleton in Ockendon (1975); clouds; melting and solidification of rock, Rubinstein (1971); freezing and thawing of lakes, polar ice, Stefan (1889), Rubinstein (1971); seepage and filtration, Ventcel (1960), see also equation (1.9) and references, Ciment and Guenther (1974); geothermal power (e.g. geysers), Ockendon (1975); nuclear reactor safety, Boley (1972), Peckover (1977).

(6) Coupled or non-linear problems

Coupled heat and mass transfer - temperature and moisture content, Aguirre-Puente and Fremond (1975), Mikhailov (1975/6); heat and concentration diffusion, Mebditch, Tayler in Ockendon (1975, pp. 112, 120); temperature and pressure distributions in multi-phase flow, Koh et al. (1969); non-linear governing equations, see equation (1.9) and references; functional or non-linear MB conditions, see equation (1.16) and references.

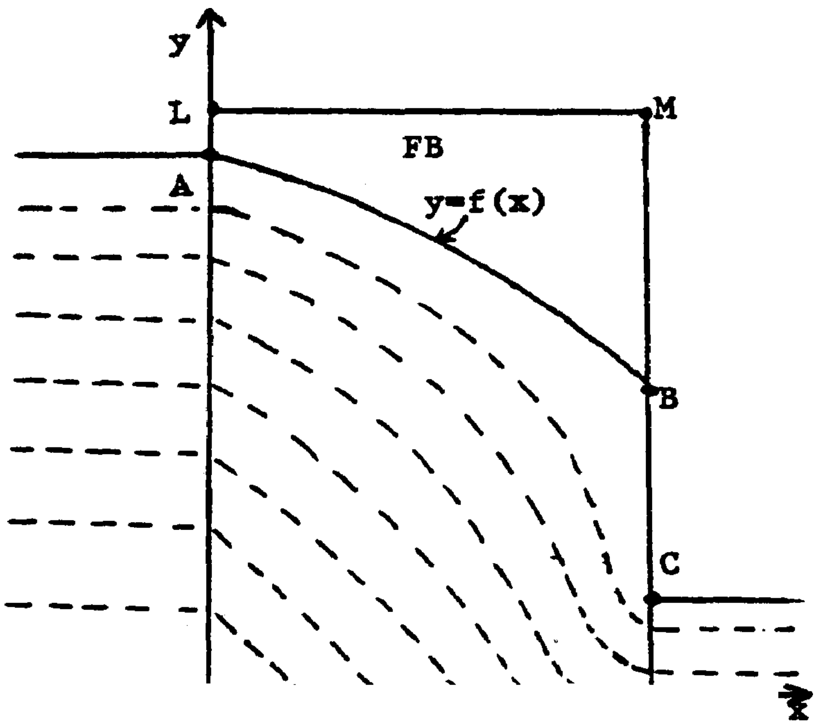
(7) Inverse Stefan problem

Applications to oil problems, Rubinstein (1971), to space vehicle design, Jochum in Hoffmann (1977, III).

7. Free boundary problems

Free boundary problems (FBPs) involve the solution of an elliptic (steady-state), partial differential equation subject to an unknown, free boundary (FB). Such problems arise in fluid mechanics (cavities, jets and waves), in porous flow, in elastic - plastic torsion and in magneto-hydrodynamics. Comprehensive reviews of porous flow problems and their solution are given in Baiocchi et al.(1973), Cryer (1976a). For a general survey of FBPs and the numerical solution, see Cryer (1976b).

The seepage of water through an earth dam (see Figure 4) has received a great deal of attention and serves as a model problem. In this problem water from a higher reservoir seeps through a rectangular earth dam to a lower reservoir. A more detailed account of the physical processes involved is given in Baiocchi et al. (1973), Cryer (1976a).



Impervious foundation

Figure 4. Seepage through a dam .

The mathematical formulation leads to the determination of the velocity potential ϕ which satisfies

$$\Delta\phi = 0 \text{ in the region R bounded by OABCD ,} \tag{7.1}$$

subject to

$$\phi = H \text{ on OA ,} \tag{7.2}$$

$$\partial\phi/\partial n = 0 \quad \text{on OD ,} \tag{7.3}$$

$$\phi = h \quad \text{on DC ,} \tag{7.4}$$

$$\phi = y \quad \text{on DC ,} \tag{7.5}$$

with the FB conditions

$$\left.\begin{array}{l} \phi = y \ , \quad (7.6) \\ \partial\phi/\partial n = 0 \ , \quad (7.7) \end{array}\right\} \text{ on AB .}$$

The problem can also be formulated in terms of the hydraulic head or pressure, see Cryer.

The numerical solution of such problems has been carried out using iterative or 'trial FB' methods where, given initial approximations $C^{(0)}$, $\phi^{(0)}$ to the FB and the potential, the sequences $\{C^{(k)}\}$, $\{\phi^{(k)}\}$ are generated by solving (7.1) to (7.6), and readjusting the FB to fit (7.7), repeatedly. Alternatively, (7.7) may be used with (7.1) - (7.5) to determine $\phi^{(k)}$ and (7.6) used to adjust the FB. These ideas were first used with relaxation methods by Southwell (1946), and then with finite-difference methods by Cryer (1968, 1970), Aitchison (1972), Fox and Sankar (1973), Doha (1977), and with finite-element methods, Taylor and Brown (1967). In the works of Cryer, a quadratically convergent algorithm is given for the determination of the $\{C^{(k)}\}$ based on an equivalent class of boundary conditions to (7.6) and (7.7).

Doha (1977) has given numerical comparisons for various finite-difference methods of iteratively computing the FB position. He notes that the $\{C^{(k)}\}$ should be determined using total derivatives of ϕ, considered as a function of x,y and $C^{(k)}$, so that both the positional change of the FB and the effect of the change in domain on the solution are taken into account.

A more recent approach, which avoids the need for iterative (trial) FB methods, is to reformulate the problem as a variational inequality over a fixed domain, typically the extension of R to the rectangle Ω (OLMD in Figure 4), based on the transformation due to Baiocchi (1972)

$$w(x,y) = -\int_0^y [\phi(x,\xi) - \xi]\, d\xi, \tag{7.8}$$

for points (x,y) on the boundary OABCD,

$$w(x,y) = \phi(x,f(x)) \text{ for } (x,y) \varepsilon\ \Omega - R. \tag{7.9}$$

Applications to other porous flow problems are discussed in Baiocchi and Magenes (1974). The resulting variational inequality has proved useful not only from a theoretical point of view, to prove existence and uniqueness of a solution, Bensoussan and Lions (1974), Stampacchia (1974), Kinderlehrer and Stampacchia (1975), but also from the point of view of numerical solutions based on finite-element methods, Baiocchi et al. (1973), Hunt and Nassif (1975), Elliott (1976), Kikuchi (1977), Aitchison (1977).

Alternative methods based on integral equations, see references in Cryer (1976b), hodograph transformations, Maria-sube (1974), Cryer (1976a), have been proposed. Difficulties occur in the numerical solution of FBPs near the singularity that arises at the 'separation' point B between fixed and free boundaries. Aitchison (1972, 1977) used complex variable analysis to obtain an expansion for the FB in the neighbourhood of B. Doha (1977) studied the singularity at the separation point in the problem of axisymmetric cavitational flow past a circular disc, Fox and Sankar (1973). An asymptotic expansion for the solution near the separation point was developed and used to improve his finite-difference results.

Practical applications of FBPs in fluid mechanics and porous flow problems are the seepage through dams, canals, ditches and wells, the reclamation of land, and the water-coning of oil wells, see Cryer (1976a). Recent applications of FBPs include the magnetohydrodynamic equilibria of a plasma subject to a magnetic field e.g. in nuclear fusion reactors, Field et al. (1977); the determination of the space charge layer in semiconductors, Hunt and Nassif (1975). McGeough and Rasmussen (1974) have given a quasi-steady model for an electrochemical machining problem where the governing equation is elliptic (steady-state), but the electrodes change shape with time. Numerical and perturbation solutions are compared in Christiansen and Rasmussen (1976), McGeough and Rasmussen (1976). A numerical solution based on a variational inequality formulation has been given by Elliott (1977).

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