Int. J. Heat Mass Transfer. Vol. 22, pp. 941–947
Pergamon Press Ltd. 1979. Printed in Great Britain

ON THE NUMERICAL SOLUTION OF AN ALLOY SOLIDIFICATION PROBLEM

A. B. CROWLEY and J. R. OCKENDON
Oxford University Computing Laboratory, 19 Parks Road, Oxford OX1 3PL, U.K.

(*Received* 21 *June* 1978 *and in revised form* 11 *November* 1978)

Abstract—A model is described for the solidification of a dilute alloy, in which the equations of heat and mass transfer are coupled through the conditions at the moving phase boundary. The equations are rewritten in conservation form, and this suggests a method for finding numerical solutions without explicitly tracking the phase boundary. Although the method cannot be rigorously justified, it gives results which compare well with known analytical solutions in a situation where good agreement might not have been expected.

NOMENCLATURE

b,	slope of phase boundary in (u, v) plane;
c,	concentration of impurity;
D,	diffusion coefficient;
H,	enthalpy;
k_1, k_2,	slope of solidus and liquidus lines in (u, c) plane;
L,	latent heat;
$s(t)$,	position of phase boundary;
t,	time;
u,	temperature;
v,	chemical activity;
x,	spatial variable.

Greek symbols

κ,	thermal conductivity;
σ,	specific heat.

Subscripts

L,	liquidus;
s,	solidus.

1. INTRODUCTION

IN THIS paper we discuss the numerical solution of a model for the solidification of a dilute alloy. This is a moving boundary problem in which the equations of heat and mass transfer are coupled through the conditions at the phase boundary. Across this boundary there exist discontinuities in both heat content and concentration of impurity, the boundary temperature being related to the local impurity concentration.

This physical situation is more complicated than that of the classical Stefan problem for phase changes in a pure substance [1, 2]. There, numerical solutions can be obtained by the "fixed domain" or "enthalpy" method suggested by Rose [3], in which explicit tracking of the phase boundary is avoided. The crucial step is to write the equation of heat transfer in conservation form before discretization and it can then be proved [1, 4] that suitable discretizations will converge to the unique weak solution associated with the conservation form.

For the problem of a general dilute alloy, we do not even know of a weak formulation of the solidification problem, let alone any results about the convergence of fixed domain numerical methods. The only numerical analysis we have seen used a variational formulation [5].

This paper has two objectives, namely to suggest a fixed domain discretization of the problem and then to test this discretization on a class of problems where analytical solutions are available. First, in Section 2, we describe the physical problem in more detail and reformulate the equations in conservation form through the introduction of the chemical activity. Although this reformulation does not in general suggest a suitable definition of a weak solution to the problem, it does suggest the discretization described in Section 3. In Section 4, we present the results of some numerical experimentation on this discretization.

There is only one very special situation, namely when the diffusivity and the conductivity are functions of the activity and temperature respectively, when we have any right to hope that our discretization will converge to a sensible physical limit. Fortunately, however, in a broader class of situations, analytical similarity solutions have been given [6], with which we can compare our numerical results. The agreement is good enough to give some confidence in the applicability of our method to more general situations where similarity solutions do not exist.

2. THE PHYSICAL PROBLEM

We need to model the solidification of a metal containing a small concentration of impurity. For several metals and impurities this phenomenon may be described in terms of the equilibrium diagram in Fig. 1, where u denotes the temperature and c the concentration of the impurity. In a more general alloy solidification problem, where c may be larger, the solidus and liquidus may no longer be straight lines, but we will take them as straight in this paper.

If the local values of c, u at some point in the

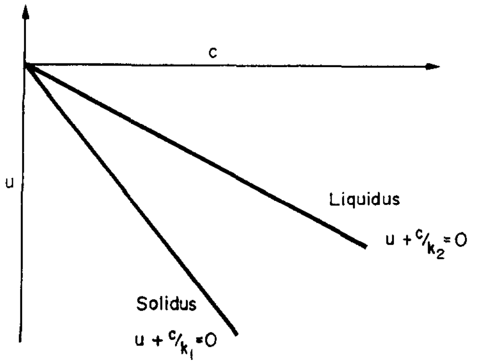

FIG. 1. Typical equilibrium diagram for a dilute alloy.

material are such that $c+k_2u > 0$ then the material is in the stable liquid phase, while if $c+k_1u < 0$, then the material is in the stable solid phase. Chemical equilibrium is not possible at values of c such that $-k_1u < c < -k_2u$.

Throughout this paper we shall make the assumption that the material on either side of the phase boundary is in chemical equilibrium. Thus, assuming further that the temperature is continuous at the phase boundary, there is a concentration discontinuity there with

$$c_s = (k_1/k_2)c_L, \tag{2.1}$$

the constant k_1/k_2 being known as the distribution coefficient.

We consider a solidification process in which the impurity diffuses in both phases $i = 1,2$, $i = 1$ being the solid, and in which density changes are negligible. In one space dimension the governing equations are then

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial x}\left(D_i \frac{\partial c_i}{\partial x}\right), \quad i = 1,2 \tag{2.2}$$

$$\sigma \frac{\partial u_i}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_i \frac{\partial u_i}{\partial x}\right), \quad i = 1,2 \tag{2.3}$$

where D denotes the mass diffusion coefficient, κ the thermal conductivity of the bulk material, and σ the specific heat of this material. For simplicity, we shall take $\sigma \equiv 1$.

At the phase change interface $x = s(t)$ the equilibrium conditions give

$$u_1 = u_2, \; c_1 = -k_1u_1, \; c_2 = -k_2u_2 \tag{2.4}$$

and the conservation of heat and mass yields

$$L\frac{\mathrm{d}s}{\mathrm{d}t} = -[\kappa\partial u/\partial x]_1^2, \tag{2.5a}$$

$$[c]_1^2 \frac{\mathrm{d}s}{\mathrm{d}t} = -[D\partial c/\partial x]_1^2. \tag{2.5b}$$

Here $[f]_1^2 = f_2 - f_1$ denotes the discontinuity in f between phases, and L is the latent heat of fusion of the bulk material, assumed constant. To complete the specification of the boundary value problem we require appropriate data initially and at the fixed boundaries.

Motivated by the derivation of the weak formulation of the classical Stefan problem, we write the equations in conservation form (see Rose [3]). The liquid phase is defined by $u+c/k_2 > 0$, and the solid by $u+c/k_1 < 0$. Thus, in view of (2.5a), we define the enthalpy H as

$$H = \begin{cases} u & u+c/k_1 < 0, \\ u+L & u+c/k_2 > 0. \end{cases} \tag{2.6}$$

The condition of chemical equilibrium at the interface, $c_1 = (k_1/k_2)c_2$, is simply a statement that the chemical potential, or equivalently the chemical activity, is continuous across the phase change surface. For dilute solutions where the temperature range is not too large, the concentration of the impurity may be taken as proportional to its chemical activity v (see Guggenheim [7]), and so we have

$$c_i = bk_iv_i \tag{2.7}$$

for some constant b. The interface condition $c_1/k_1 = c_2/k_2$ then reduces to $v_1 = v_2$, and thus v, as well as u, is continuous across the phase boundary $u+bv = 0$. Although (2.7) in general only defines v at the phase boundary for the dilute alloys we are considering in which $k_i = \text{const.}$, we can define v globally by (2.7). Then the chemical activity and the concentration play the same roles in the mass-transfer problem as the temperature and enthalpy in the heat-transfer problem. (2.2) may now be written as

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial x}\left(D_i' \frac{\partial v_i}{\partial x}\right), \quad D_i' = D_ibk_i$$

with

$$[v]_1^2 = 0, \; [c]_1^2 \frac{\mathrm{d}s}{\mathrm{d}t} = -\left[D' \frac{\partial v}{\partial x}\right]_1^2, \; u+bv = 0$$

at $x = s(t)$.

Thus we have obtained the conservation forms

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_i' \frac{\partial v}{\partial x}\right), \; \frac{\partial H}{\partial t} = \frac{\partial}{\partial x}\left(\kappa_i \frac{\partial u}{\partial x}\right), \tag{2.8}$$

with the relations

$$c = \begin{cases} bk_1v & u+bv < 0, \\ \in[bk_1v, bk_2v] & u+bv = 0, \\ bk_2v & u+bv > 0, \end{cases}$$
$$H = \begin{cases} u & u+bv < 0, \\ \in[u, u+L] & u+bv = 0, \\ u+L & u+bv > 0. \end{cases} \tag{2.9}$$

Before discussing the numerical solution of (2.8), (2.9) let us make some remarks about a possible discretization in a very special case. If $\kappa_i = \kappa_i(u)$ and $D_i' = D_i'(v)$, we can use Kirchoff transformations to define

$$\hat{u} = \int^u \kappa(u')\,\mathrm{d}u', \quad \hat{v} = \int^v D'(v')\,\mathrm{d}v'.$$

Then (2.8) becomes

$$\frac{\partial H}{\partial t} = \frac{\partial^2 \hat{u}}{\partial x^2}, \quad \frac{\partial c}{\partial t} = \frac{\partial^2 \hat{v}}{\partial x^2}, \tag{2.8a}$$

and (2.9) may be rewritten in terms of $\hat{u}$, $\hat{v}$. Following Oleinik [8] we can now multiply these equations by test functions ϕ_i and integrate twice by parts to motivate the definition of a weak solution of (2.8a), (2.9) with say, u, v prescribed on $x = 0, 1$, as a set of bounded measurable functions $\{H, c, \hat{u}, \hat{v}\}$ satisfying (2.9) rewritten, and such that both

$$\int_0^T \int_0^1 \frac{H\partial\phi_1}{\partial t} + \hat{u}\frac{\partial^2\phi_1}{\partial x^2}\,\mathrm{d}x\,\mathrm{d}t = \int_0^T \hat{u}\frac{\partial\phi_1}{\partial x}\bigg|_{x=1}\mathrm{d}t - \int_0^T \hat{u}\frac{\partial\phi_1}{\partial x}\bigg|_{x=0}\mathrm{d}t - \int_0^1 H\phi_1\bigg|_{t=0}\mathrm{d}x, \tag{2.10}$$

and a similar integral equation involving c, $\hat{v}$ and ϕ_2 are satisfied for all suitable ϕ_i. Such ϕ_i would be smooth functions for which $\partial\phi_i/\partial x$, $\partial^2\phi_i/\partial x^2$, $\partial\phi_i/\partial t$ exist and are continuous, and which satisfy $\phi_i(x,t) = 0$ on $x = 0, 1$ and $\phi_i(x, T) = 0$.

Now in the case of a pure metal $c \equiv v \equiv 0$, it can be shown that the weak solution exists, is unique, and can be computed by implicit or explicit discretization of (2.8a), (2.9). Moreover it is classical away from the phase boundary, but across this boundary, the so-called "Rankine-Hugoniot" conditions can be obtained by local application of (2.10). These turn out to be simply (2.5a) and the condition that $\hat{u}$ is continuous. For the case (2.10) with $c \not\equiv 0$, however, we have been unable to prove either existence or uniqueness* for the weak solution, although we can similarly derive both (2.5a,b) and

$$[\hat{u}]_1^2 = [\hat{v}]_1^2 = 0, \tag{2.11a}$$

i.e.

$$[u]_1^2 = [v]_1^2 = 0. \tag{2.11b}$$

The situation is worse still in the general coupled problem where $\kappa = \kappa_i(u,v)$, $D_i' = D_i'(u,v)$ are functions with possible discontinuities at the phase boundary. The Kirchoff transformation leading to (2.8a) is no longer available and then, after multiplying (2.8) by test functions ϕ_i, it is only convenient to integrate once by parts, so that the equation analogous to (2.10) has as left-hand side

$$\int_0^T \int_0^1 H\frac{\partial\phi_1}{\partial t} - \frac{\partial\phi_1}{\partial x}\kappa\frac{\partial u}{\partial x}\,\mathrm{d}x\,\mathrm{d}t.$$

Although we could still attempt to define a weak solution on this basis, only jumps of the form (2.5) would be assured, and there would be no guarantee that (2.11b) would be satisfied.

While a rigorous justification of a numerical solution of (2.8), (2.9) based on the idea of a weak solution seems impossible, it is nonetheless of interest to test the performance of a naive discretization of (2.8), (2.9) in a case where (2.8a) does not apply. We can fortunately carry out such a test using Rubinstein's [6] class of explicit similarity solutions where κ, D' are constant save for jump discontinuities at the phase boundary. We will in fact find that (2.11b) holds at the phase boundary, although, as explained above, we have found no satisfactory explanation for this result.

In order to describe our numerical discretization of (2.8), (2.9) as simply as possible, we will henceforth assume that κ_i and D_i' are constant in each phase, although they may have jump discontinuities at the phase boundary.

3. THE NUMERICAL PROCEDURE

In order to solve (2.8) and (2.9) by the type of "fixed domain" method discussed in [1, 3], it is necessary to invert (2.9) to give u, v in terms of H, c. This yields

$$u = \begin{cases} H & H + c/k_1 < 0, \\ H - L & H + c/k_2 > L, \end{cases} \qquad v = \begin{cases} c/bk_1 & H + c/k_1 < 0, \\ c/bk_2 & H + c/k_2 > L, \end{cases} \tag{3.1}$$

but gives no obvious information if $H + c/k_1 > 0$, and $H + c/k_2 < L$. This interval corresponds to points between the liquidus and solidus lines in Fig. 1.

We now describe two equivalent ways of determining $u(H,c)$ if $H + c/k_1 > 0$, $H + c/k_2 < L$. [As $u + bv = 0$ in this region, $v(H,c)$ is immediately found if $u(H,c)$ is known]. The first is based on physical arguments suggested by Chalmers [9]. Since the material cannot exist in equilibrium at these values of H, c, these are taken as "partitioned" values of H, c which represent an element of material of which a fraction f is solid and $(1-f)$ liquid. The values of u, c_s, c_L for the element are compatible with local equilibrium. Thus we write

$$c = c_s f + c_L(1-f)$$

$$H = u + (1-f)L$$

where $c_s = -k_1 u$, $c_L = -k_2 u$. Eliminating c_s, c_L, f yields

$$\frac{k_1 - k_2}{L}u^2 + \left[k_1 - \left(\frac{k_1 - k_2}{L}\right)H\right]u + c = 0 \tag{3.2}$$

---

* An alternative approach based on the use of variational inequalities and monotone operators may be more successful in this respect (J. D. P. Donnelly, private communication).

and hence

$$u = u^* = \frac{-\left[k_1 - \left(\frac{k_1-k_2}{L}\right)H\right] + \left\{\left[k_1 - \left(\frac{k_1-k_2}{L}\right)H\right]^2 - 4\left(\frac{k_1-k_2}{L}\right)c\right\}^{1/2}}{2\left(\frac{k_1-k_2}{L}\right)} \tag{3.3}$$

where we take the positive square root so that u is H on the solidus, and $H-L$ on the liquidus.

An alternative argument relies on the assumption that u is continuous across the moving boundary. Thus $u = u(H, c) =$ constant for each material particle in the region between the solidus and the liquidus. Therefore the changes in H and c which result from the phase boundary moving a distance δs through this material particle are related by

$$\frac{\partial u}{\partial H}\delta H + \frac{\partial u}{\partial c}\delta c = 0, \tag{3.4}$$

where, from conservation of heat and mass,

$$\delta H = L\delta s, \quad \delta c = [c]_1^2 \delta s = (k_1 - k_2)u\delta s.$$

Hence

$$L\frac{\partial u}{\partial H} + (k_1 - k_2)u\frac{\partial u}{\partial c} = 0,$$

yielding

$$u = F[(k_1 - k_2)uH - Lc],$$

for an arbitrary function F, and using the condition that both the solidus and the liquidus curves lie on this surface in u, H, c space, we again obtain (3.3).

Hence the inversion of (2.9) is taken to be (3.1) together with

$$u = u^*, \quad v = -u^*/b \text{ in } H + c/k_2 - L < 0 < H + c/k_1, \tag{3.5}$$

where u^* is given by (3.3).

An explicit finite difference scheme may be used for the solution of (2.8) with u, v defined in terms of H, c by (3.1) and (3.5), provided care is taken to ensure the scheme conserves heat and mass. If the mesh points $(n-1)\delta x$, $n\delta x$, $(n+1)\delta x$ lie in the same phase the difference equations are

$$H_n^{m+1} = H_n^m + (\delta t/\delta x^2)\,\kappa_n^m(u_{n+1}^m - 2u_n^m + u_{n-1}^m) \tag{3.6}$$

and

$$c_n^{m+1} = c_n^m + (\delta t/\delta x^2)D_n'^m(v_{n+1}^m - 2v_n^m + v_{n-1}^m) \tag{3.7}$$

where $H_n^m = H(n\delta x, m\delta t) m = 0, \ldots M$, $n = 1, \ldots N$, u_n^m, c_n^m, v_n^m are defined similarly, and κ_n^m, $D_n'^m$ take the values appropriate to that phase.

We require that the finite difference equations conserve heat and mass across the phase boundary. If (3.6) is used at all mesh points in the interior of the fixed domain, we see that on integrating (3.6), the change of heat content in an interval δt is given by

$$\begin{aligned}\delta x \sum_1^{N-1} (H_n^{m+1} - H_n^m) &= \delta t/\delta x \sum_1^{N-1} \kappa_n^m(u_{n+1}^m - u_n^m) - \kappa_n^m(u_n^m - u_{n-1}^m) \\ &= \delta t/\delta x \sum_1^{N-1} (\kappa_n^m - \kappa_{n+1}^m)(u_{n+1}^m - u_n^m) + \kappa_N^m(u_N^m - u_{N-1}^m) - \kappa_1^m(u_1^m - u_0^m).\end{aligned}$$

Thus, unless $\kappa_n^m = \kappa_{n+1}^m$ for $n = 1 \ldots N-1$, which is only possible if $\kappa_1 = \kappa_2$, there will be a heat loss (or gain) at the phase boundary. Hence a modification of (3.6), and similarly (3.7), is necessary near the moving boundary. Near this boundary, the position of which may be determined by linear extrapolation on the values of $u + bv$ at the mesh points, a modified form of κ, D' is needed. If $s(m\delta t) = n\delta x + h_1$, where $0 < h_1 < \delta x$, with the solid phase in $x < s(t)$, the expressions for $(\partial/\partial x)(\kappa \partial u/\partial x)$ at $n\delta x$ and $(n+1)\delta x$ are replaced by

$$\frac{\partial}{\partial x}\left(\kappa\frac{\partial u}{\partial x}\right)_n^m = (1/\delta x^2)[\kappa^*(u_{n+1}^m - u_n^m) - \kappa_1(u_n^m - u_{n-1}^m)] \tag{3.8}$$

and

$$\frac{\partial}{\partial x}\left(\kappa\frac{\partial u}{\partial x}\right)_{n+1}^m = (1/\delta x^2)[\kappa_2(u_{n+2}^m - u_{n+1}^m) - \kappa^*(u_{n+1}^m - u_n^m)] \tag{3.9}$$

where κ^* is the modified thermal conductivity, with similar expressions for $(\partial/\partial x)(D'\partial v/\partial x)$. Best agreement with the analytical solution, described in the next section, is obtained using

$$\kappa^* = (h_1/\delta x)\kappa_1 + (1 - h_1/\delta x)\kappa_2$$

rather than κ_1, κ_2 or $(\kappa_1 + \kappa_2)/2$, together with a similar expression for D'^*.

At a mesh point where $u_n^m + bv_n^m = 0$, the equation

$$\frac{\partial}{\partial x}(\kappa \partial u/\partial x)_n^m = (1/\delta x^2)[\kappa_2(u_{n+1}^m - u_n^m) - \kappa_1(u_n^m - u_{n-1}^m)] \tag{3.10}$$

is used. These finite difference replacements together yield a conservative scheme for the solution of (2.8) with (3.1) and (3.5). They form a "fixed domain" discretization, requiring no explicit application of the conditions (2.5a,b) at the phase boundary.

4. RESULTS AND DISCUSSION

We now consider the numerical solution of the one-dimensional solidification of a block of molten alloy, with uniform initial temperature and concentration distributions $u_0 = 1$, $c_o = 0.1$, occupying the region $x > 0$. At the initial instant the temperature at the face $x = 0$ is lowered to $u = -1$, and we assume there is no mass flux out of the material.

This problem was chosen because the analytical solution is known [6]. For our choice of initial and boundary conditions the solution is

$$\left.\begin{aligned} c_1 &= -k_1 u_s, \\ c_2 &= 0.1 - (k_2 u_s + 0.1)\frac{\operatorname{erfc}[x/2(D_2 t)^{1/2}]}{\operatorname{erfc}[\beta/(D_2)^{1/2}]} \\ u_1 &= -1 + (u_s + 1)\frac{\operatorname{erf}[x/2(\kappa_1 t)^{1/2}]}{\operatorname{erf}[\beta/(\kappa_1)^{1/2}]} \\ u_2 &= 1 + (u_s - 1)\frac{\operatorname{erfc}[x/2(\kappa_2 t)^{1/2}]}{\operatorname{erfc}[\beta/(\kappa_2)^{1/2}]}\cdot \\ s(t) &= 2\beta(t)^{1/2} \end{aligned}\right\} \tag{4.1}$$

where β is the root of

$$\begin{aligned} &L\beta(\pi)^{1/2}\operatorname{erf}[\beta/(\kappa_1)^{1/2}]\operatorname{erfc}[\beta/(\kappa_2)^{1/2}]\exp(\beta^2/\kappa_1 + \beta^2/\kappa_2) \\ &\qquad -(\kappa_1)^{1/2}\operatorname{erfc}[\beta/(\kappa_2)^{1/2}]\exp(\beta^2/\kappa_2) + (\kappa_2)^{1/2}\operatorname{erf}[\beta/(\kappa_1)^{1/2}]\exp(\beta^2/\kappa_1) \\ &\quad = \{(\kappa_1)^{1/2}\operatorname{erfc}[\beta/(\kappa_2)^{1/2}]\exp(\beta^2/\kappa_2) + (\kappa_2)^{1/2}\operatorname{erf}[\beta/(\kappa_1)^{1/2}]\exp(\beta^2/\kappa_1)\} \\ &\qquad\qquad \times\left[\frac{-0.1(D_2)^{1/2}}{k_2(D_2)^{1/2} + \beta(\pi)^{1/2}(k_1 - k_2)\operatorname{erfc}[\beta/(D_2)^{1/2}]\exp(\beta^2/D_2)}\right], \end{aligned} \tag{4.2}$$

and the constant phase change temperature u_s is given by

$$u_s = \frac{-0.1(D_2)^{1/2}}{k_2(D_2)^{1/2} + \beta(\pi)^{1/2}(k_1 - k_2)\operatorname{erfc}[\beta/(D_2)^{1/2}]\exp(\beta^2/D_2)}. \tag{4.3}$$

In the first example we choose $D_1' = D_2' = \kappa_1 = \kappa_2 = 1$, $k_1 = 1$, $k_2 = 2$, $b = 1$, $L = 1$. Thus, using $D_i = D_i'/bk_i$, $D_1 = 1$, $D_2 = \frac{1}{2}$. The resulting value of β is found from (4.2) to be 0.353. The solution was computed using the scheme described in Section 3, with $\delta t = 5 \times 10^{-5}$, $\delta x = 1/80$. In Fig. 2(a),(b) the temperature and concentration history at the point $x = 0.1$ obtained from the numerical results is compared with the analytical solution, and it is seen that the agreement is reasonable.

From (4.1)–(4.3) we see that the solution is independent of D_1. The above calculation was therefore repeated with the choice $D_1' = \frac{1}{4}$, $D_2' = 1$, with results indistinguishable from those in Fig. 2.

A further example, with a discontinuity in thermal conductivity at the phase boundary was also solved. With $\kappa_1 = 1$, $\kappa_2 = 4/5$, we find $\beta = 0.363$, and the results obtained are shown in Fig. 3.

The position of the moving boundary at any time may be estimated by extrapolation using the values of $u + bv$ (which is zero at the boundary) from one phase or the other. With linear extrapolation from the liquid phase, the error in the calculated position of the boundary compared with (4.1) is less than 5%, and less than half a mesh spacing.

The slight oscillations of the numerical results seen in Fig. 2, and less clearly in Fig. 3, are caused by neighbouring mesh points passing through the region $u + bv = 0$. Comparison with calculations with $\delta x = 1/20$, $\delta x = 1/40$ suggests that these oscillations

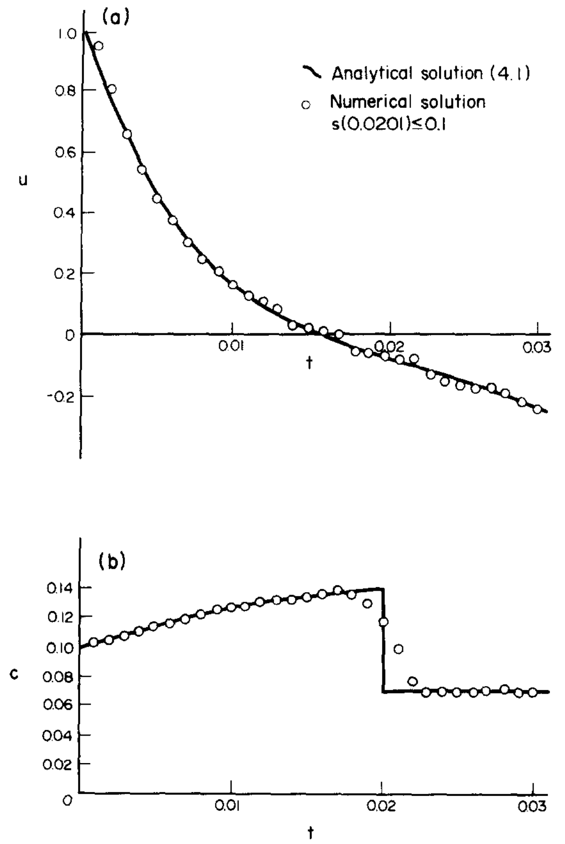

FIG. 2. Temperature and concentration history at $x = 0.1$, showing the analytical solution (4.1) and numerical results, for $\kappa_1 = \kappa_2 = 1, D'_1 = D'_2 = 1$.

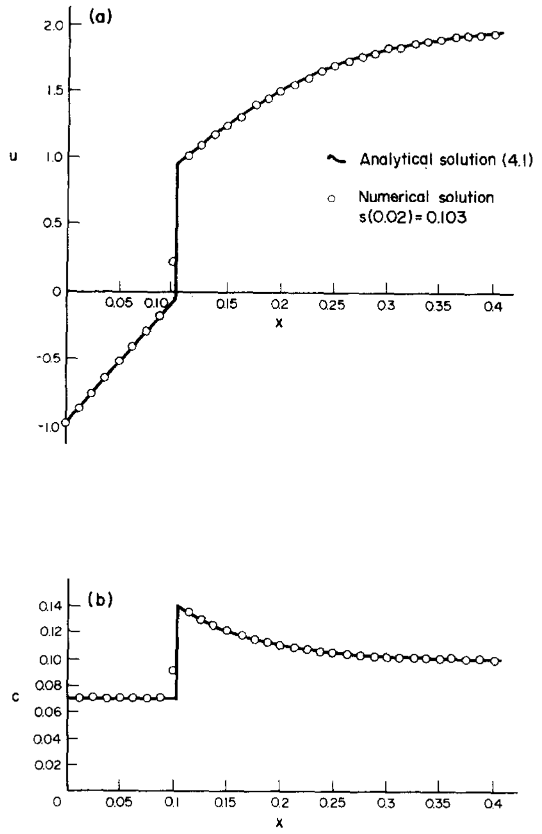

FIG. 3. Enthalpy and concentration profiles at $t = 0.02$, showing the analytical solution (4.1) and numerical results, for $\kappa_1 = 1, \kappa_2 = 4/5, D'_1 = \frac{1}{4}, D'_2 = 1$.

decrease in amplitude as the number of mesh points increases. The results shown in Figs. 2 and 3 were obtained in 43 s computing time on an ICL 1906A.

Acknowledgement—One author (A.B.C.) wishes to thank the Royal Commission for the Exhibition of 1851 for the award of a research fellowship.

REFERENCES

1. S. L. Kamenomostskaja, On the Stefan problem, *Mat. Sb.* **53**(95), 489–514 (1961).
2. A. Friedman, The Stefan problem in several space variables, *Trans. Am. Math. Soc.* **133**, 51–87 (1968).
3. M. E. Rose, A method for calculating solutions of parabolic equations with a free boundary, *Math. Comp.* **14**, 249–256 (1960).
4. D. R. Atthey, A finite difference scheme for melting problems, *J. Inst. Math. Applics.* **13**, 353–366 (1974).
5. G. J. Fix, Numerical methods for alloy solidification problems, in *Moving Boundary Problems*, Edited by D. G. Wilson, A. D. Solomon and P. J. Boggs. Academic Press, New York (1978).
6. L. I. Rubinstein, *The Stefan Problem*, Chapter I, Section 3, Translations of Mathematical Monographs, Vol. 27. American Mathematical Society (1971).
7. E. A. Guggenheim, *Thermodynamics*, pp. 223–224. North-Holland, Amsterdam (1967).
8. O. A. Oleinik, A method of solution of the general Stefan problem, *Soviet Math. Dokl.* **1**(2), 1350–1354 (1960).
9. B. Chalmers, *Principles of Solidification*, pp. 4–6. John Wiley, New York (1964).

SUR LA SOLUTION NUMERIQUE DU PROBLEME DE LA SOLIDIFICATION D'UN ALLIAGE

Résumé—On donne un modèle de la solidification d'un alliage dilué et pour lequel les équations des transferts de chaleur et de masse sont couplées par les conditions à la frontière mobile des phases. Les équations sont écrites sous une forme de conservation qui suggère une méthode pour trouver les solutions numériques sans suivre explicitement la limite des phases. Bien que la méthode ne puisse être justifiée rigoureusement, elle donne des résultats qui se comparent favorablement aux solutions analytiques connues, dans des cas où un bon accord peut ne pas être attendu.

ZUR NUMERISCHEN LÖSUNG DES PROBLEMS EINER ERSTARRENDEN LEGIERUNG

Zusammenfassung—Es wird ein Modell für die Erstarrung einer verdünnten Legierung beschrieben, in welchem die Gleichungen des Wärme- und Stofftransports durch die Bedingungen der wandernden Phasengrenzfläche gekoppelt sind. Die Gleichungen werden entsprechend den Erhaltungssätzen umgeschrieben, und das führt auf eine Methode zur numerischen Lösung ohne ausdrückliche Verfolgung der Phasengrenzfläche. Obwohl diese Methode nicht streng begründet werden kann, liefert sie Ergebnisse, welche mit bekannten analytischen Lösungen gut vergleichbar sind, auch für Fälle, in denen gute Übereinstimmung nicht zu erwarten wäre.

ЧИСЛЕННОЕ РЕШЕНИЕ ЗАДАЧИ О ЗАТВЕРДЕВАНИИ СПЛАВА

Аннотация — Предложена модель затвердевания жидкого сплава, в которой уравнения тепло- и массопереноса связаны через условия на подвижной границе раздела фаз. Уравнения, записанные в форме уравнений сохранения, позволили разработать метод нахождения численного решения без явного учёта перемещения границы раздела фаз. Несмотря на отсутствие строго обоснованной формулировки, данный метод позволяет получать результаты, которые хорошо согласуются с известными аналитическими решениями задач.