Now consider the region $\mu_{0.5} < \mu$, i.e. $J_{0.5} < J \leqslant J(2\mu_{0.5}, \sigma)$. $J < J_{0.5}$ is described above. $J \geqslant J(2\mu_{0.5}, \sigma)$ implies $Y_{ox} = 0$. Figure 3's odd symmetry suggests the image variables $Y^*_{ox}/Y_{ox,\infty} \equiv 1 - Y_{ox}/Y_{ox,\infty}$ and $\mu^*/\mu_{0.5}$. Since equation (10) is only valid for $J \leqslant J_{0.5}$, an image J^* is required for any $J > J_{0.5}$. This J^* in equation (10) yields a $Y^*_{ox}/Y_{ox,\infty}$ and the desired $Y_{ox}/Y_{ox,\infty} = 1 - Y^*_{ox}/Y_{ox,\infty}$. To find J^*, first convert the known J to a μ using Fig. 2, then μ to μ^* from the above definition and finally μ^* to J^* again from Fig. 2. Since $r \lesssim 1$, $\mu_{0.5} \lesssim 0.3$ and $J(2\mu_{0.5}, \sigma) \lesssim 0.6$ from Fig. 2 which also shows that for $0.4 \lesssim J \lesssim 0.6$, $\mu = J$. For $J_{0.5} \leqslant J \lesssim 0.4$, i.e. $0 \lesssim \mu \lesssim 0.4$ in Fig. 2, a second order fit $\mu(J)$ is used

$$\mu = [(0.4\mu_{0.5} - 0.4\mu_{0.5}\sigma^2 - J^2_{0.5} + 0.1\sigma^2)(J - 0.4\sigma) + (J_{0.5} - 0.4\sigma - \mu_{0.5} + \sigma\mu_{0.5}) \times (J^2 - 0.16\sigma^2)]/[(J_{0.5} + 0.4\sigma^2)(0.4 - J_{0.5}) + \sigma(J^2_{0.5} - 0.16)]. \quad (13)$$

This μ gives a μ^* in the range 0–$\mu_{0.5}$. Writing equation (13) in terms of μ^* and J^* and inverting gives $J^*(\mu^*)$ which, with the μ^* found above, gives the required $0 \leqslant J^* \leqslant J_{0.5}$.

In summary, turbulent transport equations are used to obtain J and g at each point in the flow field. Equation (9) gives $\mu_{0.5}$ in terms of the parameter r and equations (10)–(12) yield $Y_{ox}(Y_{ox,\infty}, r, J, g)$. The remaining species and temperature time-mean variables are then given explicitly by equations (6)–(8) as functions of Y_{ox}, J, g, r and D_3. Systems which can not be approximated with a clipped Gaussian pdf [10] require more general expressions than equations (10–(12).

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TIME DEPENDENT SOLIDIFICATION OF BINARY MIXTURES*

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NOMENCLATURE

- A, parameter characterizing the liquidus line [equation (18)];
- B, $= (\kappa/D)^{1/2}$ [equation (13)];
- c, specific heat;
- C, mass-fraction of solute;
- D, diffusion coefficient;
- f, function;
- k, partition coefficient;
- K, thermal conductivity;
- l, latent heat of fusion;
- L, thickness;
- m, slope of liquidus line;
- M, principal fusion parameter [equation (18)];
- Q, heat flux;
- s, position of solid–liquid interface [ξ, equation (10a)];
- t, time [y, equation (10a)];
- T, temperature [V, equations (16)];
- x, distance from exposed surface [X, equation (13)].

Greek symbols

- δ, $(\kappa_S/\kappa_L)^{1/2}$ [equation (13)];
- η, ratio of liquid to solid diffusivities [equation (18)];
- κ, diffusivity;
- λ, similarity coefficient in constant surface temperature solution;
- ρ, density.

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INTRODUCTION

THE PROBLEM of solidification (or melting) of mixtures has received attention for a number of years both from fundamental and practical points of view (cf. [1]). Analytical solutions of the corresponding coupled heat- and mass-transfer boundary-value problem have been discussed for semi-infinite bodies under sudden changes of surface temperature (e.g. [2–4]). The response to these special conditions has been found to be characterized by similarity, and by constancy of concentration in the solid, and in both phases at the interface. The present work examines a slab, solidifying under arbitrarily time-dependent cooling conditions at the surface, and derives a solution in series form. Neither similarity nor the special behavior alluded to earlier prevails in this solution.

FORMULATION OF THE PROBLEM

Consider a slab $(0 < x < L)$, initially $(t = 0)$ liquid with temperature T_{L0} and with solute concentration C_{L0}, under prescribed cooling conditions at $x = 0$ and (to fix ideas) insulated and with no mass transfer at $x = L$. Solidification will start at $x = 0$ at a time t_m, i.e. when the temperature reaches the value

$$T_m(t_m) = T_0 - mC_{L0} \tag{1}$$

where [2] $T = T_0 - mC_L$ is the equation of the liquidus curve in the (linearized) phase diagram of the binary mixture in question. The pre-solidification solution is easily obtained by standard methods [5], since it does not involve any coupling between heat and mass flow, and in fact corresponds to

$$C_L(x,t) = C_{L0} \quad t \leqslant t_m. \tag{2}$$

For $t > t_m$, the solid phase will occupy the space $0 < x < s(t)$, and the problem is then described by the following equations (for properties constant but not necessarily equal in the solid and the liquid):

Field equations:

$$K_L T_L'' - \rho c_L \dot{T}_L = 0;$$
$$DC_L'' - \dot{C}_L = 0 \quad \text{in} \quad s(t) < x < L; \tag{3}$$

$$K_S T_S'' - \rho c_S \dot{T}_S = 0;$$
$$DC_S'' - \dot{C}_S = 0 \quad \text{in} \quad 0 < x < s(t). \tag{4}$$

Boundary conditions (for example):

$$-K_S T_S'(0,t) = Q_0(t) \quad \text{or} \quad T_S(0,t) = T_{S0}(t);$$
$$C_S'(0,t) = 0; \tag{5}$$

$$-K_L T_L'(L,t) = Q_L(t) \quad \text{or} \quad T_L(L,t) = T_{LL}(t);$$
$$C_L'(L,t) = 0. \tag{6}$$

Interface conditions:

$$T_L(s,t) = T_S(s,t) = T_m(t) \equiv T_0 - mC_L(s,t);$$
$$C_S(s,t) = kC_L(s,t); \tag{7}$$

$$K_S T_S' - K_L T_L' = \rho l \dot{s};$$
$$D_S C_S' - D_L C_L' = (1-k) C_L \dot{s} \quad \text{at} \quad x = s(t). \tag{8}$$

To these, initial ($t = t_m$) conditions must be added, stipulating that temperature and concentration are continuous at $t = t_m$ and that

$$s(t_m) = 0. \tag{9}$$

In the above equation k is the partition coefficient, and the other symbols have obvious meanings (c.f. [2]).

BASIC CONSIDERATIONS

It is convenient, in order to construct a solution to equations (3)–(9), to begin with some general considerations based on experience with the analogous uncoupled heat-conduction problem. This eliminates the necessity of employing a direct method of solution (e.g. the embedding technique [6]) which, although applicable to the coupled problem, is likely to be rather cumbersome. What will then be used will be an inverse method, that is one in which the form of the solution is assumed at the outset, and it is then shown that all conditions of the problem can be satisfied on the basis. To complete the solution it is then necessary to show that the solution thus found is the only possible one. The appropriate uniqueness theorem will be presented in a subsequent publication and is not considered here.

We first note that, in the uncoupled problem, a distinction must be made [7] depending on whether

$$\lim_{y \to 0} \xi(y)/(y)^{1/2} = 0 \quad \text{or} \quad \lim_{y \to 0} \xi(y)/(y)^{1/2} \neq 0 \tag{10a}$$

where

$$\xi(y) = \frac{s(t)}{2(\kappa_S t_m)^{1/2}}; \quad y = (t/t_m) - 1. \tag{10b}$$

The second of (10) is satisfied by the similarity solution earlier mentioned, which is a direct extension of the classical Neumann solution [5] of Stefan's problem. We note that, in both uncoupled and coupled solutions of this type, the form of ξ is the same, i.e. $\xi = 2\lambda(y)^{1/2}$ for $y \ll 1$, where λ is a constant. We will return to that problem later; our present aim is the discussion of problems characterized by the first of (10), and we shall assume that there too the form of $\xi(y)$ is unchanged by coupling.

The form of the function $\xi(y)$ is known in a number of cases. The starting solution (i.e. the first term of series expansion) is known for any arbitrary cooling history [7]. For the general class of problem in which the surface heat flux is expressible in a series of a half-integral powers of y, it is found [7] that $\xi(y)$ is also so expressible, while for the companion problem in which the surface temperature is so expressible, $\xi(y)$ requires [8] a series in powers of $y^{1/4}$. Let us consider the former of these classes of problems, and assume that the heat flux is continuous; then [7] gives

$$\xi(y) = \sum_{n=0}^{\infty} \xi_n y^{(n+3)/2}. \tag{11}$$

Inspection of the second of equation (8) can now be used to guess the first term of a series representation for the concentration. The RHS of that equation is proportional to $\dot{s}$, or, with (11), initially proportional to $(y)^{1/2}$. Hence it is reasonable to expect that the concentration be distributed, for short times, in the manner corresponding to a surface flux also proportional to $(y)^{1/2}$, or

$$\frac{C_L(X,y)}{C_{L0}} = 1 + C_{L2}\, y\, i^2 \operatorname{erfc}[XB_L\delta/(y)^{1/2}] \quad \text{for} \quad y \ll 1 \tag{12}$$

where

$$X = \frac{x}{2(\kappa_S t_m)^{1/2}}; \quad B_{L,S} = (\kappa_{L,S}/D_{L,S})^{1/2};$$
$$\delta = (\kappa_S/\kappa_L)^{1/2}. \tag{13}$$

For C_S we write a similar expression, but imaged about $X = 0$ so as to satisfy (5), or, still for $y \ll 1$,

$$\frac{C_S(X,y)}{C_{L0}} = C_{S0} + \frac{kC_{S2}}{2} \times y\{i^2 \operatorname{erfc}[XB_S/(y)^{1/2}] + i^2 \operatorname{erfc}[-XB_S/(y)^{1/2}]\} \tag{14}$$

where the last of (7) requires that $C_{S0} = kC_{L0}$, and where the factor $k/2$ has been introduced for future convenience.

To extend the solution, it is again conjectured that a series in half-integral powers of y is appropriate, or

$$\frac{C_L(X,y)}{C_{L0}} = 1 + \sum_{n=2}^{\infty} C_{Ln} y^{n/2} i^n \operatorname{erfc}[XB_L\delta/(y)^{1/2}] \tag{15a}$$

$$\frac{C_S(X,y)}{C_{L0}} = k\Big(1 + \tfrac{1}{2}\sum_{n=2}^{\infty} C_{Sn} y^{n/2} \times \{i^n \operatorname{erfc}[XB_s/(y)^{1/2}] + i^n \operatorname{erfc}[-XB_s/(y)]\}\Big). \tag{15b}$$

Similar arguments may now be applied to the first of equations (8) to obtain the form of the temperature functions. In this case, one must be careful however to add particular solutions of (3) and (4) which will insure satisfaction of the non-homogeneous boundary conditions (5). The simplest way of achieving this is to employ [6, 9] the analytic continuation $T^*(X,y)$, into the post-solidification period, of the pre-solidification solution. Thus

$$V_L(X,y) \equiv \frac{T_L(X,y)}{T_{L0} - T_m(t_m)} = \frac{T^*(X,y)}{T_{L0} - T_m(t_m)} + \sum_{n=2}^{\infty} T_{Ln} y^{n/2} i^n \operatorname{erfc}[X\delta/(y)^{1/2}] \tag{16a}$$

$$V_S(X,y) \equiv \frac{T_S(X,y)}{T_{L0} - T_m(t_m)} = \frac{T^*(X,y)}{T_{L0} - T_m(t_m)} + \tfrac{1}{2}\sum_{n=2}^{\infty} T_{Sn} y^{n/2}\{i^n \operatorname{erfc}[X/(y)] + i^n \operatorname{erfc} \times [-X/(y)^{1/2}]\}. \tag{16b}$$

Equations (15) and (16) satisfy all conditions of the problem, with the exception of the conditions to be satisfied at the solid–liquid interface, namely (7) and (8). In dimensionless form, these take the following form (the arguments ξ, y being understood throughout):

$$V_L = V_S = V_0\left(1 - A\frac{C_L}{C_{L0}}\right) \qquad (17a, b)$$

$$(C_S/C_{L0}) = k(C_L/C_{L0}) \qquad (17c)$$

$$\frac{\partial V_S}{\partial X} - \eta\frac{\partial V_L}{\partial X} = \frac{2(\pi)^{1/2}}{M}\frac{d\xi}{dy} \qquad (17d)$$

$$\frac{\partial(C_S/C_{L0})}{\partial X} - \left(\frac{B_S}{\delta B_L}\right)^2\frac{\partial(C_L/C_{L0})}{\partial X} = 4B_S^2(1-k)\frac{C_L}{C_{L0}}\frac{d\xi}{dy} \qquad (17e)$$

with the dimensionless notation:

$$M = \frac{(\pi)^{1/2}}{2}\frac{c[T_{L0} - T_m(t_m)]}{l}; \quad A = \frac{mC_{L0}}{T_0};$$

$$V_0 = \frac{T_0}{T_{L0} - T_m(t_m)};$$

$$\eta = \frac{K_L}{K_S}; \quad \left(\frac{B_S}{\delta B_L}\right)^2 = \frac{D_L}{D_S}. \qquad (18)$$

The five sets of coefficients ξ_n, C_{Ln}, C_{Sn}, T_{Ln}, T_{Sn} must be adjusted so as to satisfy the five equations (17a–e).

SOLUTION AND DISCUSSION

The solution now requires the substitution of (11), (15) and (16) into (17a–e); separation of the resulting equations into terms of like powers of y, then gives sets of equations from which the unknown coefficients can be derived. The process is straight forward but rather laborious, since it requires expansion in powers of y of the several integrated error functions, whose arguments themselves are power series. The details of the process will be omitted, but it may be noted that the calculations fall in a distinct pattern. It is convenient to consider first the lowest-order terms in equations (17a, d, e); these yield three simultaneous equations for (ξ_0, C_{L2}, T_{L2}), and the coefficients (T_{S2}, C_{S2}) are then found from (17b, c) respectively. The pattern repeats for further coefficients: a set of three simultaneous equations for (ξ_1, C_{L3}, T_{L3}) results from the next-order terms in (17a, d, e), with (T_{S3}, C_{S3}) obtained again from (17b, c), and so forth.

As an example, the case of a constant flux Q_0 at $x = 0$ was considered in detail. Here

$$\frac{T^*(X,y)}{T_{L0} - T_m(t_m)} = \frac{T_{L0}}{T_0 - T_m(t_m)} - [\pi(1+y)]^{1/2} i\,\mathrm{erfc}\frac{X}{(1+y)^{1/2}} \qquad (19)$$

and the following results are obtained (for simplicity we take $\delta = \eta = 1$ and $B_L = B_S$):

First-order terms:

$$\xi_0 = \frac{1}{\dfrac{3\pi}{2M} + 3(\pi)^{1/2}B(1-k)AV_0}$$

$$C_{L2} = C_{S2} = 6(\pi)^{1/2}B(1-k)\xi_0; \quad T_{L2} = T_{S2} = 3\pi\xi_0/M. \qquad (20a)$$

Second-order terms:

$$\xi_1 = \frac{-3\pi\xi_0}{\dfrac{8(\pi)^{1/2}}{M} + 16(1-k)BAV_0}$$

$$C_{L3} = C_{S3} = 32(1-k)B\xi_1; \quad T_{L3} = T_{S3} = 16(\pi)^{1/2}\xi_1/M. \qquad (20b)$$

Third-order terms:

$$\xi_2 = \frac{48(\pi)^{1/2}\xi_0^2 + 2M[3(\pi)^{1/2}\xi_0 - 1] + 3\pi^{3/2}\xi_0\left(\dfrac{2M^2}{(\pi)^{1/2} + 2(1-k)BAV_0M} - 3\xi_0\right) + 3B^2AV_0M(1-k)\xi_0^2[32 - 15\pi(1-k)]}{15\pi + 30(\pi)^{1/2}AV_0BM(1-k)};$$

$$C_{L4} = 30(\pi)^{1/2}(1-k)B[2\xi_2 + 3(\pi)^{1/2}B(1-k)\xi_0^2]; \quad C_{S4} = C_{L4} - 192B^2\xi_0^2(1-k); \qquad (20c)$$

$$T_{L4} = \frac{6\pi}{M}\left\{5\xi_2 + \left[3(\pi)^{1/2}\xi_0 - \frac{2M}{(\pi)^{1/2}}\right]\xi_0\right\}; \quad T_{S4} = T_{L4} - 96(\pi)^{1/2}\xi_0^2/M$$

and so forth. Some comments on the above solution may be useful.

The method employed for the solution makes it clear why a distinction must be made depending on which of equations (10) holds. In fact, when (as at present) the first of (10) is valid, the various error-function integrals tend, as $y \to 0$ and on $X = \xi(y)$, to constants independent of the problem parameters. When the second of (10) holds, in contrast, the error functions are dependent on the proportionality constant λ between ξ and $(y)^{1/2}$. This implies, for example, that $C_L(\xi, y) \to f(\lambda)$ as $y \to 0$, and therefore $T_m(t)$ is also dependent on λ. The quantity λ would appear in all equations, and the present separation of the several equations would no longer be possible. The procedure followed here could of course still be employed, but it would be much more cumbersome. It is rather more convenient to solve the problem separately in these cases, as indeed was done in [2–4].

The present solution reduces to the uncoupled one [9] if either $A = 0$ or $k = 1$; in all other cases the form of ξ is the same but the coefficients differ. The concentration at the interface, given by

$$\frac{C_L(\xi,y)}{C_{L0}} = \frac{1}{k}\frac{C_S(\xi,y)}{C_{L0}} = 1 + \frac{C_{L2}}{4}y + \frac{C_{L3}}{6(\pi)^{1/2}}y^{3/2} + \left(\frac{C_{L4}}{32} - \frac{B\xi_0}{(\pi)^{1/2}}C_{L2}\right)y^2 + \ldots \qquad (21)$$

exhibits (Fig. 1) a gradual increase from its initial value. Note that the concentration in the solid is not uniform.

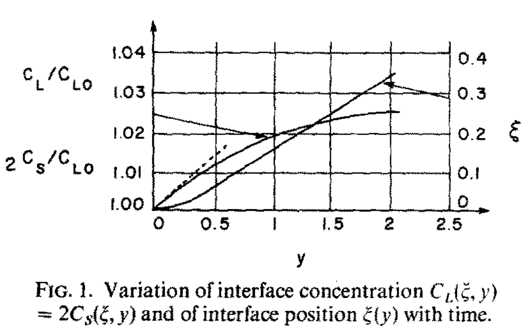

FIG. 1. Variation of interface concentration $C_L(\xi, y) = 2C_S(\xi, y)$ and of interface position $\xi(y)$ with time. $M = 0.1$; $k = A = 0.5$; $\eta = \delta = B_S = B_L = V_0 = 1$.

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A NUMERICAL METHOD FOR HEAT TRANSFER IN AN EXPANDING ROD

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NOMENCLATURE

- c, heat capacity of the rod;
- $f(x,t)$, distributed source or sink;
- $g[u, u_x, L(t)]$, boundary value defined by equation (3b);
- k, thermal conductivity of the rod;
- $L(t)$, free end-coordinate of the rod;
- t, time variable;
- $u(x,t)$, temperature;
- $u_n(x)$, approximate temperature at time $t_n = n\Delta t$;
- $v_n(x)$, $ku_n'(x)$;
- $w_i(x)$, solution of the equation (10);
- x, length coordinate;
- z_n, auxiliary function derived from equation (7).

Greek symbols

- α, coefficient of linear expansion of the rod;
- $\alpha(t)$, $\beta(t)$, end temperatures;
- $\gamma\delta$, heat-transfer coefficients;
- Δt, time step;
- Δx, space step;
- Δu, temperature drop;
- ρ, density of the rod;
- ϕ_n, auxiliary function defined by equation (11).

Subscripts

- i, 1, 2;
- n, 0, 1, ... ; indicates time level $t_n = n\Delta t$;
- x, denotes partial derivative with respect to x.

Superscript

- $'$ d/dx.

INTRODUCTION

IT IS the purpose of this note to describe a simple and reasonably fast numerical technique for computing conductive heat transfer in an expanding rod. An algorithm which specifically accounts for changes in length has several possible uses. It can be employed for the determination of the temperature in a rod or slab where an initially perfect thermal contact is lost because of shrinkage so that the heat flow across the regressing face and the subsequent cooling of the rod are retarded. It can be used to compute transient thermal stresses in rods with significant axial temperature variations, and it may allow a computer matching of thermal expansion data obtained from the heating and cooling periods of push rod dilatometer measurements which currently use only equilibrium temperatures [2].

THE MODEL

The interdependence between the length of the rod and its temperature can be modeled by a free boundary problem. Let us suppose a rod of initial length $L(0)$ is heated (or cooled). If its length at a future time t is $L(t)$ then the temperature distribution in the rod is given by the conduction equation

$$(ku_x)_x - c\rho u_t = f(x,t), \quad 0 < x < L(t), \quad t > 0 \tag{1}$$

where $f(x,t)$ accounts for possible sources and sinks, and where k, c and ρ may be space and time dependent. We shall assume that the rod has a known initial temperature distribution

$$u(x,0) = u_0(x), \quad 0 \leqslant x \leqslant L(0). \tag{2}$$

and that at the fixed end the temperature is given as

$$u(0,t) = \alpha(t), \quad t > 0. \tag{3a}$$

The boundary condition on the free end will be written as

$$g[u, u_x, L(t)] = 0. \tag{3b}$$

For example, if the temperature is specified at $L(t)$ we have $g[u, u_x, L(t)] \equiv u[L(t), t] - \beta(t) = 0$ where $\beta(t)$ is a given function. If radiation between a fixed boundary at $L(0)$ with temperature $\beta(t)$ and the regressing boundary at $L(t)$ across the gap $L(0)$–$L(t)$ occurs, we can write, under certain assumptions ([5], p. 324),

$$u_x[L(t), t] = \gamma\{\beta^4(t) - u^4[L(t), t]\}/\{\tfrac{3}{4}[L(0) - L(t)] + \delta\}.$$

As we shall see the specific form of g in equation (3b) does not greatly influence the algorithm.

In order to find the length $L(t)$ we suppose that over a time span of length Δt a small rod segment of length $\Delta x(t)$ is transformed into an expanded (or contracted) segment $\Delta x(t + \Delta t)$ according to the usual linear law

$$\Delta x(t + \Delta t) = (1 + \alpha\Delta u)\Delta x(t)$$

where α is the coefficient of expansion and Δu the average