QUARTERLY OF APPLIED MATHEMATICS
JULY 1983

EXPLICIT SOLUTIONS TO PHASE CHANGE PROBLEMS*

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Abstract. We examine two heat transfer and phase change problems having explicit solutions. The first involves melting of an initially cold material and clarifies the meaning of a recent result of Tarzia [5]. The second concerns a model of binary alloy solidification which, in some cases, is seen to be incorrect.

Introduction. This paper was motivated by a recent discussion of Tarzia [5]. In it we consider the heating of a semi-infinite slab of material whose temperature is initially below the melting point, by a heat flux of the form $h_0/\sqrt{t}$ at its surface. The fact that if h_0 is too small, then no melting will occur [e.g., the Neumann solution does not exist] is derived in a complicated fashion; the actual reason for this result is that if h_0 is too small, the slab temperature is never raised up to the melting point, and hence melting is never initiated. This is the subject of Sec. 1.

The fact that problems that appear to be reasonable may not have a solution is clear in such cases as that of Sec. 1. A similar situation has been noted earlier in [6] for supercooling. However, problems of greater subtlety exist and are little recognized as possibly lacking solutions. One such problem arises in the process of binary alloy solidification. In [3] such a problem is formulated and an explicit, Neumann-like solution is provided for it. Subsequent studies (e.g., [2, 4]) have been based upon this formulation. Upon close examination, one finds that this solution in fact may not solve the original problem, in the sense that it produces a "mushy zone" in place of a sharp phase change front. This is the subject of Sec. 2.

The nomenclature used is given after Sec. 2.

1. On the paper of Tarzia. Consider a semi-infinite slab $x \geqslant 0$ of material that melts at temperature T_{cr}. Suppose that it is initially cold at the uniform temperature $T_s < T_{cr}$. If a

* Received May 20, 1982.

Research sponsored by the Applied Mathematical Sciences Research Program, Office of Energy Research, U.S. Department of Energy under contract W-7405-eng-26 with the Union Carbide Corporation.

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constant temperature $T_L > T_{cr}$ is imposed at $x = 0$, then *instantaneous* melting occurs with a melt front $x = X(t)$ emanating from $x = 0$: $X(0) = 0$. However, what happens if a heat flux q_0 is imposed at $x = 0$? If q_0 is constant, then melting is not immediately begun at $t = 0$, for the material temperature $T(0, t)$ must be raised from T_s to T_{cr} before melting begins. Recalling [1, p. 75] that

$$T(0, t) = T_s + \frac{2q_0}{K_s}\sqrt{\frac{\alpha_s t}{\pi}}$$

we find that $T(0, t)$ attains the value T_{cr} at time

$$t_0 = \frac{\pi}{\alpha_s}\left[\frac{(T_{cr} - T_s)K_s}{2q_0}\right]^2.$$

What happens if q_0 is a function of t? In the special case where $q_0 = h_0 t^{n/2}$ for $n = -1, 0, 1, \ldots$, we find

$$T(0, t) = \frac{h_0\sqrt{\alpha_s}\,\Gamma(\frac{1}{2}n + 1)}{K_s\Gamma(\frac{1}{2}n + \frac{3}{2})}t^{(n+1)/2} + T_s;$$

if $n = 0, 1, 2, \ldots$, then $T(0, t)$ will only reach T_{cr} at the time t_0 for which $T(0, t_0) = T_{cr}$ or

$$t_0 = \left[\frac{K_s\Gamma(\frac{1}{2}n + \frac{3}{2})}{h_0\sqrt{\alpha_s}\,\Gamma(\frac{1}{2}n + 1)}(T_{cr} - T_s)\right]^{1/((n+1)/2)},$$

whence $X(t_0) = 0$. However, suppose that $n = -1$. Now

$$T(0, t) = \frac{h_0\sqrt{\alpha_s}\,\Gamma(\frac{1}{2})}{K_s} + T_s = \frac{h_0\sqrt{\pi\alpha_s}}{K_s} + T_s$$

and so $T(0, t)$ is constant in time. However, if this constant temperature is less than T_{cr}, the solid can never reach its melt temperature. Thus melting will only occur if

$$\frac{h_0\sqrt{\pi\alpha_s}}{K_s} + T_s > T_{cr}$$

or

$$h_0 > \frac{K_s}{\sqrt{\pi\alpha_s}}(T_{cr} - T_s)$$

which is the condition derived in [5].

2. On a model of binary alloy solidification. Consider a semi-infinite slab of a binary alloy consisting of two components A, B. Let C be the concentration of "A". Suppose that solidification of the alloy is governed by an equilibrium phase diagram consisting of a liquidus curve $T = f_L(C)$, and a solidus curve $T = f_S(C)$, $0 < C < 1$. As in [3] we assume f_L, f_S to be monotonically increasing, $f_L(C) > f_S(C)$ and $f_L(0) = f_S(0) = T_{cr}^A$, $f_L(1) = f_S(1) = T_{cr}^B$. Material is in its solid state if $T \leqslant f_S(C)$ and liquid if $T \geqslant f_L(C)$. If $f_S(C) < T <$

$f_L(C)$, then the material state is not well defined; it is then referred to in such terms as "mushy", "heterogeneous" and "unstable".

Consider the following process. The semi-infinite alloy is initially liquid at constant temperature T_{init} and concentration C_{init}, for which $T_{\text{init}} \geqslant f_L(C_{\text{init}})$. Beginning at time $t = 0$, a cold temperature $T_{\text{wall}} < T_{cr}^A$ is imposed at $x = 0$. Freezing occurs with, in principle, a sharp phase change front $x = X(t)$ separating solid alloy ($x < X(t)$) from liquid alloy ($x > X(t)$).

A mathematical formulation of the solidification process is given in [3] as follows:

Problem: Find temperature $T(x, t)$, concentration $C(x, t)$ and phase change front $x = X(t)$, for which:

$$C_t = D_S C_{xx}, \quad 0 < x < X(t), \tag{1a}$$

$$C_t = D_L C_{xx}, \quad x > X(t), \tag{1b}$$

$$T_t = \alpha_s T_{xx}, \quad x < X(t), \tag{1c}$$

$$T_t = \alpha_L T_{xx}, \quad x > X(t), \tag{1d}$$

$$T_{cr} = T(X(t), t) = f_S[C(X(t) - , t)] = f_L[C(X(t) + , t)], \tag{1e}$$

$$\begin{aligned} X'(t)[C(X(t) - , t) - C(X(t) + , t)] \\ = -D_S C_x(X(t) - , t) + D_L C_x(X(t) + , t), \end{aligned} \tag{1f}$$

$$\rho H X'(t) = -K_L T_x(X(t) + , t) + K_S T_x(X(t) - , t), \tag{1g}$$

$$T(0, t) = T_{\text{wall}}, \quad t > 0, \tag{1h}$$

$$T(x, 0) = T_{\text{init}}, \quad x > 0, \tag{1i}$$

$$C(x, 0) = C_{\text{init}}, \quad x > 0, \tag{1j}$$

$$C_x(0, t) = 0, \quad t > 0, \tag{1k}$$

$$T_{\text{init}} > f_L(C_{\text{init}}), \tag{1l}$$

$$T_{\text{wall}} < T_{cr}^A, \tag{1m}$$

$$X(0) = 0. \tag{1n}$$

THEOREM. A solution to this problem exists for all choices of initial and boundary conditions and thermal and diffusion parameters. Moreover, for this solution the solidus and liquidus concentrations

$$C_S = C(X(t) - , t), \qquad C_L = C(X(t) + , t)$$

as well as the phase change temperature

$$T_{cr} = T(X(t), t)$$

are unchanged in time.

Proof. We note first that solutions to the heat and diffusion equations (1a)–(1b) can be expressed in the form

$$C(x, t) \equiv C_s = \text{const.}, \qquad x < X(t), \tag{2a}$$

$$T(x, t) = T_{\text{wall}} + (T_{cr} - T_{\text{wall}})\operatorname{erf}\left(x/2\sqrt{\alpha_s t}\right)/\operatorname{erf}\lambda, \qquad x < X(t), \tag{2b}$$

$$C(x,t) = C_{\text{init}} + (C_L - C_{\text{init}})\operatorname{erfc}\left(x/2\sqrt{D_L t}\right)/\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right), \quad x > X(t), \tag{2c}$$

$$T(x,t) = T_{\text{init}} + (T_{cr} - T_{\text{init}})\operatorname{erfc}\left(x/2\sqrt{\alpha_L t}\right)/\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/\alpha_L}\right), \quad x > X(t), \tag{2d}$$

where

$$T_{cr} = f_S(C_S) = f_L(C_L); \tag{3a}$$

the interface is of the form

$$X(t) = 2\lambda\sqrt{\alpha_S t} \tag{3b}$$

where λ and T_{cr} (or C_S, C_L) are yet to be determined. Substitution into the interface conditions (1f), (1g) yields the equations

$$T_{cr} = (A_1 + A_2)/(A_3 + A_4) \tag{4a}$$

where

$$A_1 = \rho H + \left[K_S T_{\text{wall}}/\sqrt{\pi}\,\alpha_S \lambda e^{\lambda^2}\operatorname{erf}\lambda\right],$$

$$A_2 = K_L T_{\text{init}}/\left[\sqrt{\pi\alpha_L\alpha_S}\,\lambda e^{\lambda^2\alpha_S/\alpha_L}\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/\alpha_L}\right)\right],$$

$$A_3 = K_S/\left[\sqrt{\pi}\,\alpha_S\lambda e^{\lambda^2}\operatorname{erf}\lambda\right],$$

$$A_4 = K_L/\left[\sqrt{\pi\alpha_L\alpha_S}\,\lambda e^{\lambda^2\alpha_S/\alpha_L}\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/\alpha_L}\right)\right],$$

and

$$(C_{\text{init}} - C_L)/(C_S - C_L) = \sqrt{\pi}\,\lambda\sqrt{\alpha_S/D_L}\,e^{\lambda^2\alpha_S/D_L}\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right). \tag{4b}$$

Let us write (4a) as

$$T_{cr} = W_1(\lambda),$$

and let us denote the functional dependence of T_{cr} on λ via (3a), (4b) by

$$T_{cr} = W_2(\lambda).$$

We claim that there exists a λ such that $W_1(\lambda) = W_2(\lambda)$, which will prove the Theorem. To see this, let us study the behavior of $W_1(\lambda)$ and $W_2(\lambda)$.

A short calculation (cf. [3, pp. 55–56]) shows that $W_1(\lambda)$ is an increasing function of λ. As $\lambda \to 0$, $W_1(\lambda) \to T_{\text{wall}}$. On the other hand, using the relation

$$\sqrt{\pi}\,z e^{z^2}\operatorname{erfc}(z) \to 1 \quad \text{as } z \to \infty, \tag{5}$$

we obtain

$$W_1(\lambda) \to \frac{\rho H + K_L T_{\text{init}}/\alpha_L}{K_L/\alpha_L} = T_{\text{init}} + \frac{H}{c_L} \quad \text{as } \lambda \to \infty.$$

As $\lambda \to 0$, (4b) implies that

$$\frac{C_{\text{init}} - C_L}{C_S - C_L} \to 0$$

or $C_L \to C_{\text{init}}$, whence $W_2(\lambda) = f_L(C_L)$ must tend to the value $T_L^* = f_L(C_{\text{init}}) > T_{cr}^A$. Similarly, as $\lambda \to \infty$,

$$\frac{C_{\text{init}} - C_L}{C_S - C_L} \to 1$$

or $C_S \to C_{\text{init}}$. Hence $W_2(\lambda) = f_S(C_S)$ must tend to the value $T_S^* = f_S(C_{\text{init}}) < T_{\text{init}}$.

Thus we see that the continuous functions $W_1(\lambda)$ and $W_2(\lambda)$ satisfy:

$$W_1(0) = T_{\text{wall}} < T_{cr}^A < T_L^* = W_2(0)$$

and

$$W_2(\infty) = T_S^* < T_{\text{init}} < T_{\text{init}} + \frac{H}{C_L} = W_1(\infty).$$

Therefore there exists at least one value of λ such that $W_1(\lambda) = W_2(\lambda)$ which provides a solution of (3), (4) and completes the proof of the Theorem.

But does this imply that our problem has a solution? We claim that the reasonable condition that $X(t)$ separate solid ($x < X(t)$) from liquid ($x > X(t)$) may not be satisfied by the solution. Let us see how this can be. Consider the behavior of our solution in the physically reasonable case in which the material diffusivity in the liquid is much smaller than the solid thermal diffusivity, $D_L/\alpha_S \to 0$.

LEMMA. λ is bounded away from zero as $\alpha_S/D_L \to \infty$.

For if not, there would be a sequence $\{\lambda_n\}$, with $\lambda_n \to 0$. But then there would be a sequence $\{T_{cr}^n\}$ of T_{cr} values for which $T_{cr}^n \to T_{\text{wall}}$, which is not possible since $T_{\text{wall}} < T_{cr}^A$.

Thus as $\alpha_S/D_L \to \infty$, $\lambda\alpha_S/D_L \to \infty$, and so $C_S(T_{cr}) \to C_{\text{init}}$. Hence $T_{cr} \to f_S(C_{\text{init}})$, and so the limiting solution for $\alpha_S/D_L \to \infty$ obeys

$$\begin{aligned} C_S &\equiv C_{\text{init}}, \\ T_{cr} &\equiv f_S(C_{\text{init}}), \end{aligned} \tag{6}$$

while λ tends to the solution λ^* for this choice of T_{cr}. Thus $X(t)$ tends to the limiting interface position $X^*(t) = 2\lambda^*\sqrt{\alpha_S t}$.

Now consider what happens to the liquid concentration for fixed $t > 0$. Let $x \geqslant X^*(t) + \delta$ for any fixed $\delta > 0$. For $D_L \to 0$, again using (5), we have

$$\sqrt{\pi}\,\frac{x}{2\sqrt{D_L t}}\,e^{x^2/4D_L t}\,\operatorname{erfc}\left(x/2\sqrt{D_L t}\right) \to 1$$

and

$$\sqrt{\pi}\,\lambda\sqrt{\alpha_S/D_L}\,e^{\lambda^2\alpha_S/D_L}\,\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right) \to 1,$$

whence

$$\left\{\frac{\operatorname{erfc}\left(x/2\sqrt{D_L t}\right)}{\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right)}\right\}\frac{x}{X(t)}\exp\left\{\frac{x^2-X(t)^2}{4tD_L}\right\}\to 1.$$

But for $x > X^*(t) + \delta$, we know that

$$\exp\left\{\frac{x^2-X(t)^2}{4tD_L}\right\}\to\infty \quad \text{as } D_L\to 0,$$

whence

$$\frac{\operatorname{erfc}\left(x/2\sqrt{D_L t}\right)}{\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right)}\to 0,$$

and so, by (2c), $C(x, t) \to C_{\text{init}}$ uniformly for $x > X^*(t) + \delta$. Meanwhile,

$$C_x(x,t) = -\frac{(C_L - C_{\text{init}})e^{-x^2/4D_L t}}{\sqrt{D_L t\pi}\,\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right)}$$

whence at $x = X(t)$,

$$\begin{aligned} C_x(X(t),t) &= -\frac{(C_L - C_{\text{init}})e^{-\lambda^2\alpha_S/D_L}}{\sqrt{D_L t\pi}\,\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right)} \\ &= \frac{-(C_L - C_{\text{init}})\lambda\sqrt{\alpha_S}}{D_L\sqrt{t\pi}\,e^{\lambda^2\alpha_S/D_L}\operatorname{erfc}\left(\lambda\sqrt{\alpha_S/D_L}\right)\lambda\sqrt{\alpha_S/D_L}} \\ &\to \pm\infty \end{aligned}$$

as $D_L \to 0$, accordingly as $C_L < C_{\text{init}}$ or $C_L > C_{\text{init}}$. We have shown the following.

PROPOSITION. As $D_L \to 0$, the explicit solution (2)–(4) has a limit. The concentration tends to C_{init} everywhere except at the front, while the temperature and phase front tend to those of the classical two-phase Stefan problem with $T_{cr} = f_S(C_{\text{init}})$. The phase diagram is no longer relevant.

A consequence of this convergence result is that the explicit solution may lose its physical meaning for very small D_L, as is shown in the following.

COROLLARY. For sufficiently small D_L and points x close to the front $X(t)$ on the liquid side ($x > X(t)$), the state (C, T) of the material at (x, t), $t > 0$, is between the liquids and solidus curves.

Indeed, as $D_L \to 0$, $T_{cr} \to f_S(C_{\text{init}})$, while the interfaces converge to some $X(t)$. For $x > X(t)$ sufficiently close to $X(t)$, $T(x, t) \geqslant T_{cr}$ and $C(x, t) < C_{\text{init}}$ when D_L is sufficiently small. Then the monotonicity of $f_S(C)$ and $f_L(C)$ implies

$$f_S(C) < f_S(C_{\text{init}}) = T_{cr} \leqslant T < f_L(C),$$

which says that (x, t) lies neither in the liquid nor in the solid.

Nomenclature

x	position (m)
t	time (s)
X	interface (m)
T	temperature $(°C)$
q	heat flux $(KJ/M^2 - S)$
T_{cr}	melting temperature $(°C)$
C	concentration
K	thermal conductivity $(KJ/m - s - °C)$
c	specific heat $(KJ/Kg - °C)$
ρ	density (KG/m^3)
$\alpha = K/(c\rho)$	thermal diffusivity (m^2/S)
H	latent heat (KJ/Kg)
D	material diffusion coefficient (m^2/s)
T_{cr}^A	melt temperature of pure A $(°C)$
T_{cr}^B	melt temperature of pure B $(°C)$
f_L	liquidus curve
f_S	solidus curve
Subscripts	
L	liquid
S	solid

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