Some Remarks on the Stefan Problem*

By Alan Solomon

1. Introduction. In this discussion we examine a method, motivated by M. Rose [4], for the determination of the temperature distribution in a medium undergoing a change of phase.

Consider a semi-infinite slab $x \geqq 0$ of material which has a critical temperature $T_c > 0$ at which a change of phase occurs. Let the slab be initially at a constant temperature $V > T_c$. If at the initial time, $t = 0$, the temperature at $x = 0$ is set at $T = 0$ and remains so for all time, then a phase changing process is initiated. Hence at a later time there is a region, $0 \leqq x \leqq x^*$, consisting of material in Phase "I" separated from the material in the original Phase "II" by a front $x^*(t)$ moving to the right (see Figure 1). Let H be the latent heat of the material, which is lost during the change from Phase II into Phase I. We will for simplicity suppose that the density ρ of the material is the same for each phase. Let c_1, K_1 and c_2, K_2 be the specific heat and the conductivity of Phase I material and Phase II material respectively, and set $\kappa_i = K_i/(c_i\rho)$, $i = 1, 2$.

The problem of finding the temperature distribution in this situation was solved explicitly by F. Neumann (see [1, Chapter XI]).

We wish to consider a related problem for a function which up to an additive constant can be identified with the specific internal energy, and show that the above problem is equivalent to this related one, by obtaining from it, Neumann's explicit solution.

Let $T(x, t)$ be the temperature of the slab at time t and position x, and define T to be a function of the "internal energy" e by the relation

$$(1) \qquad T(e) = \begin{cases} \dfrac{e - H}{c_1} + T_c, & e < H, \\ T_c, & H \leqq e \leqq 2H, \\ T_c + \dfrac{e - 2H}{c_2}, & e \geqq 2H. \end{cases}$$

(See Figure 2.) For any small $\epsilon, \delta > 0$ define the function $\kappa(e)$ by:

$$(2) \qquad \kappa(e) = \begin{cases} \kappa_1, & \text{for } e \leqq H, \\ \phi_1(e), & H \leqq e \leqq H + \epsilon, \\ \delta, & H + \epsilon \leqq e \leqq 2H - \epsilon, \\ \phi_2(e), & 2H - \epsilon \leqq e \leqq 2H, \\ \kappa_2, & 2H \leqq e \end{cases}$$

where ϕ_1, ϕ_2 are any smooth monotonic functions so defined that $\kappa(e)$ together with its first derivative $\kappa'(e)$, is continuous (see Figure 3). In Section 2 we find a solution

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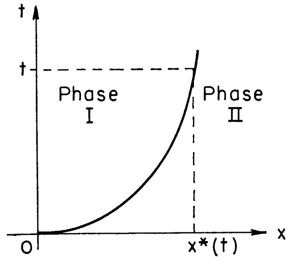

Figure 1.

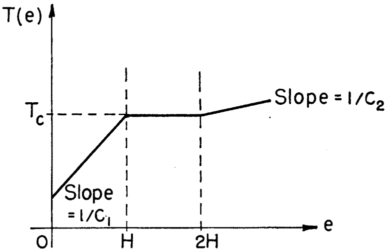

Figure 2. T = T(e)

$e(x, t)$ of the equation

$$e_t = (\kappa(e)e_x)_x, \quad \text{for } t, x > 0, \tag{3a}$$

such that

$$e(x, 0) = e_2, \quad e(0, t) = e_1, \tag{3b}$$

with

$$e_1 = H - c_1T_c, \qquad e_2 = 2H + c_2(V - T_c) \tag{3c}$$

and show that for $\epsilon \to 0$, $\delta \to 0$, it yields Neumann's solution. This proof justifies some confidence in the numerical method based on the specific interval energy formulation proposed by Rose [4] for solving the Stefan problem. In Section 4, we investigate a numerical example which reveals certain unanswered questions related to the accuracy of the numerical scheme as a function of the parameters introduced in Section 2 to study the specific internal energy formulation. The scheme proposed by Rose [4] corresponds to a special choice of these parameters.

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2. Solution of the Problem. Using Boltzmann's transformation $z = x/(4t)^{1/2}$, problem (3a, b) is transformed into the following boundary value problem for a function $E(z) = e(x, t)$.

Find $E(z)$ such that:

$$\frac{d}{dz}\left(\kappa(E)\frac{dE}{dz}\right) + 2z\frac{dE}{dz} = 0, \tag{4a}$$

$$E(0) = e_1, \qquad E(\infty) = e_2, \tag{4b}$$

where by (3c),

$$e_1 < H < 2H < e_2. \tag{4c}$$

This problem is dealt with in the following manner.

For any number $A > 0$ there exists a unique function $E(z)$ satisfying (4a) and the initial conditions

$$E(0) = e_1, \qquad \kappa_1E'(0) = A, \tag{5}$$

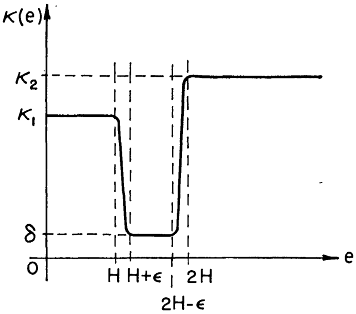

Figure 3. κ = κ(e)

or equivalently, the integral equation

$$E(z) = e_1 + A \int_0^z \frac{1}{\kappa(E(s))} \exp\left\{ -\int_0^s \frac{2t\,dt}{\kappa(E(t))} \right\} ds \tag{6}$$

(see [2]), and defined for all values of z. Moreover, since $\kappa(E(s)) \geqq \delta > 0$ for all s, the integral on the right-hand side of (6) converges as z tends to infinity, to a well defined limit; thus $E(z)$ converges as well to a definite limit, which we denote by ϕ.

Conversely, for any $\phi > e_1$ we can find a constant $A > 0$ and thus a corresponding $E(z)$ for which

$$\phi = e_1 + A \int_0^\infty \frac{1}{\kappa(E(s))} \exp\left\{ -\int_0^s \frac{2t}{\kappa(E(t))}\,dt \right\} ds; \tag{7}$$

for if $\kappa^* = \max(\kappa_1, \kappa_2)$, with any $A > 0$,

$$(\pi\delta)^{1/2}/2\kappa^* \leqq \int_0^\infty \frac{\exp\left\{ -\int_0^s \frac{2t}{\kappa(E(t))}\,dt \right\}}{\kappa(E(s))}\,ds \leqq (\pi\kappa^*)^{1/2}/2\delta, \tag{8}$$

and since E depends continuously on A, as A ranges through all positive values, the integral in (8) will as well.

Now for a given ϕ, both A and $E(z)$ depend on the choice of ϵ in (2). From (6), $E'(z) > 0$ for all z, so that, if $\phi > 2H$ there are points $z_{H+\epsilon} > z_H$, and $z_{2H} > z_{2H-\epsilon}$ for which

$$E(z_H) = H, \qquad E(z_{H+\epsilon}) = H + \epsilon, \qquad E(z_{2H-\epsilon}) = 2H - \epsilon, \qquad E(z_{2H}) = 2H. \tag{9}$$

From (7), (8),

$$0 < 2\delta(\phi - e_1)/(\pi\kappa^*)^{1/2} \leqq A \leqq 2\kappa^*(\phi - e_1)/(\pi\delta)^{1/2}, \tag{10}$$

and A is bounded independently of ϵ. Since by (6), (9), and (2),

$$H = (A/\kappa_1) \int_0^{z_H} \exp(-s^2/\kappa_1)\,ds + e_1 = e_1 + (A\pi^{1/2}/(4\kappa_1)^{1/2})\,\mathrm{Erf}\,(z_H/\kappa_1^{1/2}) \tag{11}$$

with Erf the error function, while by (4c), (10),

$$\text{Erf}\,(z_H/\kappa_1^{1/2}) \geqq \frac{(\delta\kappa_1)^{1/2}(H - e_1)}{\kappa^*(\phi - e_1)} > 0,$$

we find that z_H is bounded from below by a positive constant independent of ϵ. On the other hand, from (6), (7), (10a)

$$(12)\qquad \begin{aligned} 0 < \phi - (H + \epsilon) &= A \int_{z_{H+\epsilon}}^{\infty} \frac{1}{\kappa(E(s))} \exp\left\{ -\int_0^s \frac{2t\,dt}{\kappa(E(t))} \right\} ds \\ &\leqq \frac{2\kappa^*(\phi - e_1)}{\delta(\pi\delta)^{1/2}} \int_{z_{H+\epsilon}}^{\infty} \exp\,(-s^2/\kappa_2)\,ds \end{aligned}$$

so that $z_{H+\epsilon}$ (and thus z_H) is bounded from above by a constant independent of ϵ. Now by (6),

$$(13)\qquad \begin{aligned} \epsilon &= A \int_{z_H}^{z_{H+\epsilon}} \frac{1}{\kappa(E(s))} \exp\left\{ -\int_0^s \frac{2t\,dt}{\kappa(E(t))} \right\} ds \\ &\geqq \frac{A}{\kappa^*} \int_{z_H}^{z_{H+\epsilon}} \exp\left\{ -\frac{z_H^2}{\kappa_1} - \int_{z_H}^s \frac{2t\,dt}{\kappa(E(t))} \right\} ds \\ &\geqq (A/\kappa^*) \exp\,(-z_H^2/\kappa_1 + z_H^2/\delta - z_{H+\epsilon}^2/\delta)(z_{H+\epsilon} - z_H), \end{aligned}$$

so that as $\epsilon \to 0$, $z_{H+\epsilon} - z_H \to 0$. Similarly, we can easily show that $z_{2H-\epsilon}$, z_{2H} are bounded by positive constants independent of ϵ, and $z_{2H} - z_{2H-\epsilon} \to 0$. Let now $\epsilon \to 0$ and $\phi > 2H$ be fixed. Then for each ϵ we can find a value A and a function $E(z)$ obeying (6). Choose a sequence $\epsilon_n \to 0$ such that the corresponding sequences of points z_H, $z_{H+\epsilon}$, and $z_{2H-\epsilon}$, z_{2H} converge to values denoted by z_H, z_{2H}, while the A-values converge to a value A. The corresponding functions $E(z)$ are uniformly bounded (by ϕ), and equicontinuous in every z interval, since the derivatives:

$$E'(z) = \frac{A \exp\left\{ -\int_0^z \frac{2t\,dt}{\kappa(E(t))} \right\}}{\kappa(E(z))} < \frac{2\kappa^*(\phi - e_1)}{\pi^{1/2}\delta^{3/2}}$$

are uniformly bounded independently of ϵ. Thus by the Arzela-Ascoli lemma, we can extract a uniformly convergent subsequence converging to a continuous function $E(z)$, satisfying Eq. (6), where $\kappa(E)$ is now a piecewise constant function:

$$(14)\qquad \kappa(E) = \begin{cases} \kappa_1, & E < H \\ \delta, & H < E < 2H \\ \kappa_2, & 2H < E \end{cases}$$

and $E(\infty) = \phi$.

We now claim that for a given $\phi > 2H$ there is only one such function $E(z)$ determined by a unique A, which is equal to ϕ at $z = \infty$.

To see this we need only to show that ϕ increases monotonically as A increases, for any solution of (6). But as A increases, (11) implies that z_H decreases, while by (6), (14),

$$(15)\qquad \begin{aligned} H &= \frac{A}{\delta} \int_{z_H}^{z_{2H}} \exp\left\{ -\int_0^s \frac{2t\,dt}{\kappa(E(t))} \right\} ds \\ &= \frac{A}{\delta} \exp\left(z_H^2 \left[\frac{1}{\delta} - \frac{1}{\kappa_1} \right] \right) \int_{z_H}^{z_{2H}} \exp\,(-s^2/\delta)\,ds. \end{aligned}$$

Letting $t = s - z_H$ in this integral, we find that

$$H = \frac{A}{\delta \exp(z_H^2/\kappa_1)} \int_0^{z_{2H}-z_H} \exp(-t^2/\delta - 2z_H t/\delta)\, dt, \tag{15a}$$

so that as A increases, the integral in (15a) must decrease; since z_H decreases with increasing A, $z_{2H} - z_H$ must decrease and so z_{2H} must decrease as well. However, by (6), (14),

$$\phi - 2H = \frac{A}{\kappa_2} \exp\left\{z_H^2\left(\frac{1}{\delta} - \frac{1}{\kappa_1}\right) - z_{2H}^2\left(\frac{1}{\delta} - \frac{1}{\kappa_2}\right)\right\} \cdot \int_{z_{2H}}^{\infty} \exp(-s^2/\kappa_2)\, ds \tag{16}$$

$$\begin{aligned} &= \frac{A}{\kappa_2} \exp\left\{-(z_{2H} + z_H)(z_{2H} - z_H)\left(\frac{1}{\delta} - \frac{1}{\kappa_1}\right)\right\} \\ &\qquad \cdot \exp\left\{-z_{2H}^2\left(\frac{1}{\kappa_1} - \frac{1}{\kappa_2}\right)\right\} \cdot \int_{z_{2H}}^{\infty} \exp(-s^2/\kappa_2)\, ds; \end{aligned} \tag{16a}$$

supposing without loss of generality that $\kappa_1 \leqq \kappa_2$, we see that as A increases, ϕ will also increase.

Thus for each ϕ we can find a unique A and a solution $E(z)$ of (6), (14). Choose that solution $E(z)$ for which $\phi = E(\infty) = e_2$. $E(z)$ is continuous, and on the intervals $[0, z_H]$, $[z_H, z_{2H}]$, $[z_{2H}, \infty]$ has a derivative

$$E'(z) = \frac{1}{\kappa(E(z))} A \exp\left\{-\int_0^z \frac{2t\, dt}{\kappa(E(t))}\right\}, \tag{17}$$

having jump discontinuities at z_H, z_{2H}. For $z \leqq z_H$,

$$E(z) = e_1 + \frac{A}{\kappa_1} \int_0^z \exp\left\{-\frac{s^2}{\kappa_1}\right\} ds, \tag{18a}$$

$$E'(z) = \frac{A}{\kappa_1} \exp(-z^2/\kappa_1); \tag{18b}$$

for $z_H \leqq z \leqq z_{2H}$,

$$E(z) = e_1 + A \exp(-z_H^2/\kappa_1) \int_0^z \frac{\exp\{-(s^2 - z_H^2)/\delta\}}{\kappa(E(z))}\, ds, \tag{19a}$$

$$E'(z) = \frac{A}{\delta} \exp(-z_H^2/\kappa_1) \exp((z_H^2 - z^2)/\delta), \tag{19b}$$

and for $z_{2H} \leqq z$,

$$\begin{aligned} E(z) &= e_1 + A \exp\left\{-\frac{z_H^2}{\kappa_1}\right\} \exp\left\{-\frac{(z_{2H}^2 - z_H^2)}{\delta}\right\} \\ &\qquad \cdot \int_0^z \frac{1}{\kappa(E(s))} \exp\left\{-\frac{(s^2 - z_{2H}^2)}{\kappa_2}\right\} ds, \end{aligned} \tag{20a}$$

$$E'(z) = \frac{A}{\kappa_2} \exp\left\{-\frac{z_H^2}{\kappa_1}\right\} \exp\left\{\frac{z_{2H}^2 - z^2}{\kappa_2}\right\} \exp\left\{\frac{z_H^2 - z_{2H}^2}{\delta}\right\}. \tag{20b}$$

We claim now that as $\delta \to 0$, $E(z)$ tends to the internal energy function corresponding by (1), to Neumann's solution. To see this, we show that as $\delta \to 0$,

$z_{2H} - z_H \to 0$ and z_{2H}, z_H tend to some common finite number z^*. We will again assume, without loss of generality that $\kappa_1 \leqq \kappa_2$, and $\delta \ll \kappa_1$. By using (10) with $\phi = e_2$ and $\kappa^* = \kappa_2$ and (16a), we find that

$$e_2 - 2H \leqq \frac{(e_2 - e_1)\kappa_2^{3/2}}{\delta^{1/2}} \exp\left\{-\left(\frac{1}{\delta} - \frac{1}{\kappa_2}\right)(z_{2H}^2 - z_H^2)\right\}; \tag{21}$$

or

$$\exp\left\{\left(\frac{1}{\delta} - \frac{1}{\kappa_2}\right)(z_{2H}^2 - z_H^2)\right\} \leqq \left(\frac{e_2 - e_1}{e_2 - 2H}\right)\frac{\kappa_2^{3/2}}{\delta^{1/2}}, \tag{21a}$$

whence

$$z_{2H}^2 - z_H^2 \leqq \frac{\delta\kappa_2}{\kappa_2 - \delta} \ln\left\{\frac{\left(\dfrac{e_2 - e_1}{e_2 - 2H}\right)\kappa_2^{3/2}}{(\delta)^{1/2}}\right\}; \tag{21b}$$

thus

$$z_{2H}^2 - z_H^2 \to 0 \quad \text{as} \quad \delta \to 0. \tag{21c}$$

We next claim that there exists a bound M_1 independent of δ, such that

$$z_H,\, z_{2H} \leqq M_1. \tag{22}$$

However, noting that for $\kappa_1 < \kappa_2$, and since $z_{2H} > z_H$, the first two exponentials in (16a), with $\phi = e_2$, are bounded by 1, we substitute the value of A obtained by writing $z = z_H$ in (18a), and find

$$0 < e_2 - 2H \leqq \frac{(H - e_1)\kappa_1}{\kappa_2} \frac{\displaystyle\int_{z_{2H}}^{\infty} \exp(-s^2/\kappa_2)\, ds}{\displaystyle\int_0^{z_H} \exp(-s^2/\kappa_1)\, ds} \tag{23}$$

for all small $\delta > 0$. If for some null sequence of δ values, we had $z_{2H} \to \infty$, then by (21c) we must have z_H bounded away from 0, in which case the right hand side would tend to zero, which is impossible. Thus (22) is proved.

Using again (18a) with $z = z_H$, we see that

$$A \geqq 2(H - e_1)(\kappa_1/\pi)^{1/2} > 0 \tag{24}$$

for all $\delta > 0$, so that the A values are bounded away from zero. Now by (16) with $\phi = e_2$

$$A = \frac{\kappa_2(e_2 - 2H)\exp\{(z_{2H}^2 - z_H^2)/\delta\}}{\exp\left\{\dfrac{z_{2H}^2}{\kappa_2} - \dfrac{z_H^2}{\kappa_1}\right\}\displaystyle\int_{z_{2H}}^{\infty} \exp(-s^2/\kappa_2)\, ds}, \tag{25}$$

thus implying, by (15), that

$$\begin{aligned} H &= \left[\frac{\exp(-z_H^2/\kappa_1)\kappa_2(e_2 - 2H)}{\exp(z_{2H}^2/\kappa_2 - z_H^2/\kappa_1)\displaystyle\int_{z_{2H}}^{\infty}\exp(-s^2/\kappa_2)\, ds}\right]\frac{\exp(z_{2H}^2/\delta)}{\delta} \\ &\qquad \cdot \int_{z_H}^{z_{2H}} \exp(-s^2/\delta)\, ds \\ &\geqq \left[\frac{\kappa_2(e_2 - 2H)\exp(z_H^2/\kappa_1)}{\exp\left\{\dfrac{z_{2H}^2}{\kappa_2} - \dfrac{z_H^2}{\kappa_1}\right\}\displaystyle\int_{z_{2H}}^{\infty}\exp(-s^2/\kappa_2)\, ds}\right]\frac{(z_{2H} - z_H)}{\delta}, \end{aligned} \tag{26}$$

where we have used the inequality

$$\int_{z_H}^{z_{2H}} \exp(-s^2/\delta)\, ds \geqq (z_{2H} - z_H) \exp(-z_{2H}^2/\delta).$$

Thus

$$(27) \qquad z_{2H} - z_H \leqq \frac{\delta H \exp\left\{\dfrac{z_{2H}^2}{\kappa_2} - \dfrac{z_H^2}{\kappa_1}\right\} \displaystyle\int_{z_{2H}}^{\infty} \exp(-s^2/\kappa_2)\, ds}{\kappa_2(e_2 - 2H)\exp(-z_H^2/\kappa_1)} \leqq \delta M_2,$$

where M_2 is independent of δ.

We claim now that A is bounded from above independently of δ; however, by (25), since z_{2H} is bounded from above, and since (27) implies that,

$$\frac{z_{2H}^2 - z_H^2}{\delta} \leqq (z_{2H} + z_H)M_2$$

this assertion is immediate. This implies by (18a) for $z = z_H$ that z_H and therefore z_{2H}, are bounded away from 0, independently of δ.

Thus for all $\delta < \kappa_1$, there are constants c_0, c_1, c_2, such that

$$(28) \qquad 0 < c_0 \leqq z_H, z_{2H}, A \leqq c_1 < \infty, \qquad z_{2H} - z_H \leqq c_2\delta.$$

Now let $\delta \to 0$, and choose the corresponding sequence $E(z)$ of solutions of (6) with $\kappa(E)$ defined by (14), such that the points z_H, z_{2H} converge to one finite value z^*, while the A values converge to a number denoted again by A. This can clearly be done by (28). Then $E(z)$ as defined by (18a) for any closed subinterval of $[0, z^*]$ converges to a function, denoted again by $E(z)$, and defined by

$$(29) \qquad E(z) = e_1 + (A/\kappa_1)\int_0^z \exp(-s^2/\kappa_1)\, ds,$$

which can then be defined by continuity on $[0, z^*]$, with $\lim E(z) = H$ as z tends to z^*.

Moreover, by using the fundamental theorem of the calculus, the mean-value theorem for integrals, (18a) and (19a), we find for any $\delta > 0$, that

$$\begin{aligned} \exp(-(z_{2H}^2 - z_H^2)/\delta) &= 1 + \int_{z_H}^{z_{2H}} \frac{d}{ds}\exp(-(s^2 - z_H^2)/\delta)\, ds \\ &= 1 - \int_{z_H}^{z_{2H}} \frac{2s}{\delta}\exp(z_H^2/\delta)\exp(-s^2/\delta)\, ds \\ &= 1 - 2s^*\exp(z_H^2/\kappa_1)\int_{z_H}^{z_{2H}} \frac{\exp\left(-\displaystyle\int_0^s \frac{2t}{\kappa(E(t))}\, dt\right)}{\kappa(E(s))}\, ds \\ &= 1 - 2s^*\exp(z_H^2/\kappa_1)H/A, \end{aligned}$$

where $z_H \leqq s^* \leqq z_{2H}$. Thus, by (20a), for $z \geqq z_{2H}$,

$$(30) \qquad \begin{aligned} E(z) = e_1 + A\exp(-z_H^2/\kappa_1)&\left(1 - \frac{2s^* H \exp(z_H^2/\kappa_1)}{A}\right) \\ &\cdot \int_0^z \frac{\exp(-(s^2 - z_{2H}^2)/\kappa_2)}{\kappa(E(s))}\, ds \end{aligned}$$

which converges to the function

$$(30\text{a})\qquad E(z) = e_1 + A \exp(-(z^*)^2/\kappa_1)\left(1 - \frac{2z^*H \exp((z^*)^2/\kappa_1)}{A} \cdot \int_0^z \frac{\exp(-(s^2 - (z^*)^2)/\kappa_2)}{\kappa(E(s))}\, ds\right)$$

as δ tends to 0, where in (30a), $\kappa(E) = \kappa_1$, for $z \leqq z^*$, and κ_2 for $z \geqq z^*$. The two functions, of (29) and (30a), differ in magnitude by H at $z = z^*$.

We now wish to obtain the values of A and z^*, and thus the values of the solution, and to identify the results with those of Neumann.

For this reason, let $\lambda = z^*/\kappa_1^{1/2}$. Since for $E(z)$ as defined in (30a) we have

$$e_2 - 2H = E(\infty) - E(z^*),$$

we have from (30a), with A obtained from (29) by setting $z = z_H$,

$$(31)\qquad \frac{\kappa_2^{1/2}(e_2 - 2H)}{(\pi\kappa_1)^{1/2}\,\mathrm{Erfc}\,(\lambda\kappa_1^{1/2}\kappa_2^{-1/2})} = \frac{\exp(\lambda^2\kappa_1/\kappa_2)\exp(-\lambda^2)(H - e_1)}{\pi^{1/2}\,\mathrm{Erf}\,\lambda} - \lambda H \exp(\lambda^2\kappa_1/\kappa_2),$$

where Erfc $= 1 -$ Erf. Now by (1),

$$(1\text{c})\qquad e_2 - 2H = c_2(V - T_c), \qquad H - e_1 = c_1 T_c$$

so that (31) becomes

$$(32)\qquad -\frac{K_2\kappa_1^{1/2}(V - T_c)\exp(-\lambda^2\kappa_1/\kappa_2)}{K_1\kappa_2^{1/2}T_c\,\mathrm{Erfc}\,(\lambda(\kappa_1/\kappa_2)^{1/2})} = -\frac{\exp(-\lambda^2)}{\mathrm{Erf}\,\lambda} + \frac{\lambda H\pi^{1/2}}{c_1 T_c}.$$

Now again using (29) with $z = z_H$, we find

$$(33)\qquad A = \frac{2(H - e_1)\kappa_1^{1/2}}{\pi^{1/2}\,\mathrm{Erf}\,\lambda} = \frac{2c_1 T_c \kappa_1^{1/2}}{\pi^{1/2}\,\mathrm{Erf}\,\lambda},$$

where λ is found from (32), and so (29) takes the form

$$(34)\qquad E(z) = e_1 + c_1 T_c\,\mathrm{Erf}\,(z/\kappa_1^{1/2})/\mathrm{Erf}\,\lambda,$$

for $z \leqq z^* = \lambda\kappa_1^{1/2}$. From (30a) for $z \geqq z^*$, we have

$$(35)\qquad \begin{aligned} E(z) &= e_2 - (E(\infty) - E(z)) \\ &= e_2 - \frac{\pi^{1/2}\exp(\lambda^2\kappa_1/\kappa_2)}{2\kappa_2^{1/2}}[A\exp(-\lambda^2) - 2\lambda H\kappa_1^{1/2}]\cdot\mathrm{Erfc}\,(z/\kappa_2^{1/2}). \end{aligned}$$

But by using (33), (32) and (3c),

$$A\exp(-\lambda^2) - 2\lambda H\kappa_1^{1/2} = \frac{2c_1\kappa_1^{1/2}}{\pi^{1/2}}\cdot\frac{K_2\kappa_1^{1/2}}{K_1\kappa_2^{1/2}}\cdot\frac{(V - T_c)\exp(-\lambda^2\kappa_1/\kappa_2)}{\mathrm{Erfc}\,(\lambda(\kappa_1/\kappa_2)^{1/2})}$$

so that finally, for $z \geqq z^* = \lambda\kappa_1^{1/2}$,

$$(35\text{a})\qquad E(z) = e_2 - \frac{c_2(V - T_c)\,\mathrm{Erfc}\,(z/\kappa_2^{1/2})}{\mathrm{Erfc}\,(\lambda(\kappa_1/\kappa_2)^{1/2})}.$$

By using the transformation (1) and (1c), as well as the definition $z = x/(4t)^{1/2}$

we obtain as the solution, two temperature distributions in the Phase I and Phase II media, separated by the curve

$$x(t) = 2z^* t^{1/2} = 2\lambda(\kappa_1 t)^{1/2},$$

where λ is the root of (32); in I the solution $T(x, t)$ is given by

$$T(x, t) = \frac{T_c}{\operatorname{Erf} \lambda} \operatorname{Erf} (x/(4\kappa_1 t)^{1/2}), \tag{36}$$

while in II,

$$T(x, t) = V - \frac{(V - T_c)(\operatorname{Erfc} (x/(4\kappa_2 t)^{1/2})}{\operatorname{Erfc} (\lambda(\kappa_1/\kappa_2)^{1/2})} \tag{37}$$

which is the solution of F. Neumann. (See [1, p. 285].) The fact that any other null sequence of values δ will lead to the same solution follows from the fact that any other such sequence would lead again to the transcendental equation (32) which has exactly one root. (See [3, p. 121].) Our proof is now complete.

3. Remarks on the Derivation of the Equation. We have been led to considering a function κ as defined by (2) by the following heuristic argument. In any change of phase involving some latent heat H, the internal energy at a point undergoing such a change of phase (i.e. melting) reaches a critical value H. Then all additional heat will merely contribute to the mechanism of phase change (i.e. change from a crystalline to liquid structure), until the internal energy locally reaches the value $2H$, at which time the new phase is attained. Thus heat should not be conducted "in" the region of the interface between the two phases but will be used merely to change the phase.

4. Numerical Computations for a One-Dimensional Slab. The usefulness of the result of Section 2 rests on the possibility of its extension to more general phase change problems for which no explicit solution is known. For by applying numerical procedures to problem (3a, b) or to its analog arising from other phase change problems, and then obtaining the temperature distribution from (1), one could hope to solve such problems numerically, without the costly necessity of paying explicit attention to the location and behavior of the phase change curve or surface. (See [4, p. 249].)

In this section we describe the results of some numerical experiments made for a problem of freezing a one-dimensional semi-infinite slab. Our computations are for the case in which, in the notation of Section 1, $V = T_c$; this is a common situation which is not dealt with by the work of Section 2. Nevertheless, if in (31), $e_2 \rightarrow 2H$, we obtain in (34) a solution $e(x, t)$ to our original problem, for $\delta = 0$, again yielding Neumann's temperature distribution given by (32), (36), (37) for this case; it is reasonable to conjecture that this solution is also obtainable from the limit of the solution of (3a, b, c) for $V = T_c$ as $\epsilon, \delta \rightarrow 0$.

We consider the case where $V = T_c = 170$, $H = 30$, c_i, ρ, $K_i = 1$, $i = 1, 2$. Defining T as a function of e by (1), and choosing for $\kappa(e)$ the step function

$$\kappa(e) = \begin{cases} 1, & e \leqq 30, \\ \delta, & 30 < e < 60, \\ 1, & e \geqq 60, \end{cases} \tag{38}$$

TABLE I
Location of interface

t	$x^*(t)$	$x^*_{i,j}$
0	0	0
20	9.79905	9.19076
40	13.85795	13.10134
60	16.97245	16.24252
80	19.59810	18.73658
100	21.91134	21.37472
120	24.00268	23.66167
140	25.92585	25.52550
160	27.71590	26.99391
180	29.39716	28.29732
200	30.98732	30.07765
220	32.49978	31.92538
240	33.94491	33.66367
260	35.33099	34.20495
280	36.66470	36.11142
300	37.95157	37.83937

TABLE II
True solution values

x	T
0	0
2	12.589754
4	25.095902
6	37.436500
8	49.532872
10	61.311111
12	72.703425
14	83.649283
16	94.096340
18	104.001112
20	113.329385
22	122.056374
24	130.166616
26	137.653646
28	144.519453
30	150.773771
32	156.433226
34	161.520389
36	166.062763
38	170.000000

we seek a solution to the equation

$$(3a') \qquad e_t = (\kappa(e)e_x)_x, \qquad x, t > 0,$$

for which $e(0, t) = e_1 = -140$, $e(x, 0) = e_2 = 60$. For Δx, $\Delta t > 0$ and natural numbers i, j, define $e_i^j = e(i\Delta x, j\Delta t)$. Equation (3a′) is formally replaced by the

TABLE III
Error = computed solution − true solution

x	$\Delta x = 2$	$\Delta x = 1$	$\Delta x = .5$	$\Delta x = .25$	$\Delta x = .125$
0	0	0	0	0	0
2	.02006	.01582	.01675	.00873	.00476
4	.00318	.03165	.03338	.01733	.00946
6	.05984	.04750	.04974	.02570	.01406
8	.01090	.06341	.06570	.03385	.01851
10	.09776	.07947	.08109	.04136	.02276
12	.02832	.09577	.09575	.04846	.02676
14	.12883	.11240	.10949	.05498	.03049
16	.05654	.12935	.12209	.06086	.03389
18	.13880	.14652	.13335	.06607	.03695
20	.09171	.16363	.14313	.07057	.03964
22	.10239	.18026	.15129	.07438	.04195
24	.15842	.19586	.15771	.07750	.04383
26	.07321	.21007	.16220	.08003	.04530
28	.38241	.22530	.16464	.08205	.04631
30	.27324	.25031	.16471	.08381	.04681
32	.71507	.27405	.16188	.08564	.04678
34	.35301	.20271	.16155	.08431	.04590
36	−.18386	.43959	.24106	.08048	.04622
38	0	0	0	0	0

difference equation

$$\frac{e_i^{j+1} - e_i^j}{\Delta t} = \frac{1}{\Delta x^2}\left[\kappa(e_{i+1/2}^j)(e_{i+1}^j - e_i^j) - \kappa(e_{i-1/2}^j)(e_i^j - e_{i-1}^j)\right] \tag{39}$$

with $e_i^0 = e_2$, $e_0^j = e_1$, and

$$\kappa(e_{i\pm 1/2}^j) = \tfrac{1}{2}(\kappa(e_i^j) + \kappa(e_{i\pm 1}^j)). \tag{40}$$

We require that $2\Delta t/\Delta x^2 \leqq 1$, a condition which probably guarantees the stability of (39).

In Section 2 the interface between the two phases was seen to be the limit, for $\delta \to 0$, of those points (x, t) for which $H < e(x, t) < 2H$. In our computations, we choose as an approximation to the location of the interface curve for $t = j\Delta t$, the point $i\Delta x$ where i is the greatest integer for which

$$e_i^j \leqq H < e_{i+1}^j. \tag{41}$$

This is practical, since as indicated in [4], when $\delta = 0$ the width of the interval at fixed j, for which $H < e_i^j < 2H$ cannot exceed $2\Delta x$, while for sufficiently small $\delta > 0$, the width of the interval does not increase significantly beyond $2\Delta x$. (Which is intuitively clear since for small δ, little heat can be conducted across the interval.)

To explain our numerical results, we denote by $T_i^j(\delta, \Delta x, w)$, $e_i^j(\delta, \Delta x, w)$ for $w = 2\Delta t/\Delta x^2$, the temperature and energy obtained by (39) at $(i\Delta x, j\Delta t)$ for the choice of δ in (38), and given values of Δx and w.

Using (38), (39), (1), the temperature $T_i^j(\delta, \Delta x, w)$ was computed at time $t = 300$ for various choices of δ, Δx and w, and compared with the actual solution.

TABLE IV

x	Error	Relative error = error/true value
0	0	0
2	.00435	$.0345 \times 10^{-2}$
4	.00860	$.0343 \times 10^{-2}$
6	.01274	$.0340 \times 10^{-2}$
8	.01668	$.0337 \times 10^{-2}$
10	.02039	$.0332 \times 10^{-2}$
12	.02379	$.0327 \times 10^{-2}$
14	.02687	$.0321 \times 10^{-2}$
16	.02958	$.0314 \times 10^{-2}$
18	.03190	$.0307 \times 10^{-2}$
20	.03382	$.0298 \times 10^{-2}$
22	.03535	$.0290 \times 10^{-2}$
24	.03646	$.0280 \times 10^{-2}$
26	.03719	$.0270 \times 10^{-2}$
28	.03755	$.0260 \times 10^{-2}$
30	.03755	$.0249 \times 10^{-2}$
32	.03716	$.0238 \times 10^{-2}$
34	.03702	$.0229 \times 10^{-2}$
36	.03047	$.0188 \times 10^{-2}$
38	0	0

In Table I is listed the actual location of the interface curve $x^*(t) = 2\lambda t^{1/2}$ at intervals of 20 time units for the root $\lambda = 1.0955674986099$ of (32); also shown are the results of interpolating for the point $x^*_{i,j}$ where $e = H$ from the values e_i^j, e_{i+1}^j of (41), for $\delta = 0$, $\Delta x = 2$, $w = 1$. It is seen that the error in each of these values is less than $\Delta x = 2$. This same degree of accuracy, with an error smaller than Δx, was obtained in all the experiments performed.

In Table II are listed the true temperature values at time 300, and at intervals of length 2 from $x = 0$ to $x = 38$; from Table I we know the interface is at $x = 37.95$ for $t = 300$.

We began by computing the values of $T_i^j(0, \Delta x, 1)$, for $\Delta x = 2, 1, .5, .25, .125$ and comparing them with the true solution of Table II. In Table III is listed the error $= T_i^j(0, \Delta x, 1) - T(i\Delta x, j\Delta t)$ for each of these cases. The errors for $\Delta x = 1$ are seen to be linear in x. In halving Δx to .5, the error is reduced near the interface. In again halving Δx to .25, the error is seen to be halved, implying that extrapolation from these values to $\Delta x = 0$, by letting $\bar{T}_i^j = 2T_i^j(0, .25, 1) - T_i^j(0, .5, 1)$ will reduce the error $\bar{T}_i^j - T(i\Delta x, j\Delta t)$ by one additional decimal place except at $x = 36$. Halving Δx again, to .125, no longer halves the error, raising doubts as to whether the solution of (39) actually will converge to the true solution as $\Delta x, \Delta t \rightarrow 0$.

The choice $w = 2\Delta t/\Delta x^2 = 1$ in (39) does not yield the most accurate results. In Table IV are listed the errors and relative errors for $T_i^j(0, .125, .5)$, when $w = .5$. These results are somewhat more accurate than those found for $T_i^j(0, .125, 1)$ of Table III, as was indicated in [4].

Our last experiments were made for small $\delta \neq 0$. The values of $T_i^j(\delta, \Delta x, .5)$ were found for $\Delta x = .25, .125$, and $\delta = .001, .0001$. For each value of δ, the two values T_i^j for $\Delta x = .25, .125$ were extrapolated to $\Delta x = 0$, yielding

TABLE V

Errors in extrapolation for $\delta \neq 0$

x	$T_i^j(.001)$	$T_i^j(.0001)$
0	0	0
2	.00022	−.00017
4	.00041	−.00038
6	.00052	−.00066
8	.00053	−.00106
10	.00040	−.00569
12	.00012	−.00226
14	−.00033	−.00312
16	−.00096	−.00414
18	−.00178	−.00534
20	−.00276	−.00671
22	−.00390	−.00820
24	−.00518	−.00981
26	−.00659	−.01148
28	−.00814	−.01319
30	−.00998	−.01504
32	−.01232	−.01719
34	−.00942	−.01400
36	−.01546	−.02295
38	0	0

$$T_i^j(\delta) = 2T_i^j(\delta, .125, .5) - T_i^j(\delta, .25, .5).$$

The errors of the resulting values are listed in Table V. For $\delta = .001$, the values $T_i^j(\delta)$ are the most accurate of any calculations performed. When δ is decreased to .0001 the error grows, due we believe to the growth of the derivative of the solution at some points.

For $\delta = 0$ the function $\kappa(e)$ of (38) could be considered replaced by the smooth function $\kappa(e)$ of (2) with no change in the numerical results, when

$$\epsilon < \Delta x \cdot \min_{H \leq e \leq 2H} | e_x |. \tag{42}$$

This relation raises questions about the convergence of the solution to (38), (39) to the true solution $e(x, t)$ as $\Delta x, \Delta t \to 0$, since we would then have $\epsilon \to 0$, causing $\kappa'(e)$ to grow of the order $1/\epsilon$ over certain intervals of small length. (See Figure 3.) Indeed, as indicated by our numerical results, further study of the ideal relations between δ, ϵ, Δx and Δt for computing the solution of our problem, would be of both theoretical and practical value.

In all of our experiments the true interface location never differed by more than Δx from the location given by (41). However, an attempt to better locate the curve by interpolating for the point at which $e = H$ did not result in greater accuracy, and a deeper examination of the roles played by ϵ, δ, Δx, Δt might also be of help in this regard.

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