ON THE SOLUTE DISTRIBUTION AT A MOVING PHASE BOUNDARY*

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1. Introduction. Consider an infinite rod of homogeneous binary alloy with a planar solid-liquid interface advancing at constant velocity R. Let D_i, $v^i(x, t)$ denote respectively the diffusion coefficient and solute concentration in the solid ($i = 1$) and liquid ($i = 2$) regions. For $t = 0$ we locate the interface at $x = 0$ and describe the initial solute compositions by $f_i(x)$ for $(-1)^i x \geq 0$. In order to obtain equilibrium at the interface, we require

$$V^1(Rt, t) = kV^2(Rt, t),$$

$$D_1 V_x^1(Rt, t) - D_2 V_x^2(Rt, t) = R[V^1(Rt, t) - V^2(Rt, t)],$$

where k is a constant equilibrium distribution coefficient. Assuming no convection in the liquid, the diffusion equations are $D_i V_{xx}^i = V_t^i$ in their respective regions. By putting $C^i(z, t) = V^i(z + Rt, t)$ we fix the interface at $z = 0$ and move the rod into the solid region ($z < 0$). Consequently, this one-dimensional liquid-solid transformation (solidification) can be described as

Problem S: For $i = 1, 2$ let D_i, k, R be positive constants and let $f_i(z)$ be continuous real functions defined for $(-1)^i z \geq 0$ with $f_1(0) = kf_2(0)$. Find functions $C^i(z, t)$ for $t \geq 0$, $(-1)^i z \geq 0$ satisfying

(S₁) $\quad D_i C_{zz}^i + RC_z^i = C_t^i$;

(S₂) $\quad C^i(z, 0) = f_i(z)$;

(S₃) $\quad C^1(0, t) = kC^2(0, t), \qquad -R(1 - k)C^2(0, t) = D_2 C_z^2(0, t) - D_1 C_z^1(0, t).$

The corresponding solid-liqiud transformation (Problem M for melting) is the same as Problem S except that R is replaced by $-R$ in (S_1) and (S_3). Problem S has been solved for cases $D_1 = D_2$ and $D_1 = 0$ with particular initial conditions in [1] and [2].

In this paper we give sufficient conditions that both the above problems have unique solutions and explicit solutions are obtained by Laplace transforms methods. Both problems reduce to solving an integral-differential for the function $g(t) = C^1(0, t) = kC^2(0, t)$ which describes the time behavior of solutions at the interface.

2. The reduced problem. We first show that problems M and S are equivalent to

Problem A: Given positive constants K, λ and real functions $g_i(x)$ for $x \geq 0$ with $g_1(0) = g_2(0)$, find $u^i(x, y)$ for $x \geq 0$, $y \geq 0$ so that

(A_1) $\quad u_{xx}^i = u_y^i$;

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(A_2) $u^i(x, 0) = g_i(x)$;

(A_3) $e^{-y}u^2(0, y) = e^{-\lambda y}u^1(0, \lambda y)$, $\quad (1 - K)e^{-y}u^2(0, y) = e^{-y}u_x^2(0, y) + Ke^{-\lambda y}u_x^1(0, \lambda y)$.

Functions $u^i(x, y)$ will be called solutions to problem A when (i) for $x \geq 0$, $y \geq 0$ they are continuous, satisfy (A_2) and estimates of the form $|u(x, y)| < Me^{mx^2}$ on compact y intervals; (ii) for $x > 0$, $y > 0$ u_{xx}^i and u_y^i are continuous and satisfy (A_1); (iii) for $x \geq 0$, $y > 0$ u_x^i is continuous and (A_3) holds.

Straightforward calculations verify

Lemma 1. Let u^1, u^2 solve problem A with $K = k$, $\lambda = D_2/D_1$ and $g_1(\lambda x) = e^{\lambda z}f_1(-z)$, $g_2(x) = Ke^{-z}f_2(z)$ where $x = Rz/2D_2$, $y = R^2t/4D_2$. Then

$$C^1(z, t) = e^{\lambda(z-y)}u^1(-\lambda x, \lambda y)$$
$$C^2(z, t) = \frac{1}{K}e^{z-y}u^2(x, y) \tag{1}$$

solve problem M. Similarly, if u^1, u^2 solve problem A for $K = 1/k$, $\lambda = D_1/D_2$ and $g_1(\lambda x) = e^{\lambda z}f_2(-z)$, $g_2(x) = Ke^{-z}f_1(z)$ where $x = -Rz/2D_1$, $y = R^2t/4D_1$, then

$$C^1(z, t) = \frac{1}{K}e^{z-y}u^2(x, y) \tag{2}$$
$$C^2(z, t) = e^{\lambda(z-y)}u^1(-\lambda x, \lambda y)$$

solve problem S.

Lemma 2. For $p, q \in C[0, \infty)$, solutions to $u_{xx} = u_y$ for $x > 0, y > 0$ with $u(x, 0) = p(x)$, $u(0, y) = q(y)$ are unique.

Proof: This is a standard application of the maximum principle for the heat equation. Details are similar to those given on p. 48 of [3].

Define the functions

$$S(x, y) = (4\pi y)^{-1/2} \exp(-x^2/4y)$$
$$U^i(x, y) = g_i(x), \qquad y = 0,$$
$$= \int_0^\infty [S(x - r, y) + S(x + r, y)]g_i(r)\, dr, \qquad y > 0. \tag{3}$$

Then the U^i solve (A_1), (A_2) with $U_x^i(0, y) = 0$ and

$$U^i(0, y) = 2\int_0^\infty S(r, y)g_i(r)\, dr = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-u^2}g_i(2u\sqrt{y})\, du \tag{4}$$

(see p. 53 of [3]).

Suppose that u^1, u^2 solve Problem A with g_1, g_2, $g \in C[0, \infty) \cap C'(0, \infty)$ where $g(y) = e^{-y}u^2(0, y) = e^{-\lambda y}u^1(0, \lambda y)$ is the interface function. It then follows from Lemma 2 that

$$u^1(x, y) = U^1(x, y) + \int_0^y \left(\operatorname{erfc}\frac{x}{2(y - r)^{1/2}}\right)\frac{d}{dr}[e^r g(\mu r) - U^1(0, r)]\, dr$$
$$u^2(x, y) = U^2(x, y) + \int_0^y \left(\operatorname{erfc}\frac{x}{2(y - r)^{1/2}}\right)\frac{d}{dr}[e^r g(r) - U^2(0, r)]\, dr \tag{5}$$

where $\mu = 1/\lambda$. That is, the right-hand sides in (5) solve (A_1) and agree with $u^i(0, y)$ and $u^i(x, 0)$. Substituting (5) in the last equation of condition (A_3), we see that $g(y)$ solves

$$(1 - K)g(y) = e^{-y} \int_0^y [\pi(y - r)]^{-1/2} \frac{d}{dr} [U^2(0, r) - e^r g(r)]\, dr$$
$$+ Ke^{-\lambda y} \int_0^{\lambda y} [\pi(\lambda y - r)]^{-1/2} \frac{d}{dr} [U^1(0, r) - e^r g(\mu r)]\, dr. \qquad (6)$$

These steps are reversible, giving

LEMMA 3. Let $W = C[0, \infty) \cap C'(0, \infty)$. For initial conditions $g_i \in W$, Problem A has solutions u^i with $u^i(0, y) \in W$ if and only if there exists a function $g \in W$ solving (6) with $g(0) = g_i(0)$.

For the trivial case $K = \lambda = 1$ we see that $g(y) = (e^{-y}/2)[U^1(0, y) + U^2(0, y)]$.

Denote the transform of a function by a superscript *. All the formulas used below may be found in [4].

From (4) we have $U^{i*}(0, s) = g_i^*(\sqrt{s})/\sqrt{s}$. Transforming (6) and solving for g^*, we obtain

$$g^*(s) = D^*(s)\{K\mu g_1^*((\mu s + 1)^{1/2}) + g_2^*((s + 1)^{1/2})\}, \qquad (7)$$

where $D^*(s) = [((s + 1)^{1/2} + 1) + K((\mu s + 1)^{1/2} - 1)]^{-1}$ and $\mu = 1/\lambda$. Except for the easy case $K = \lambda = 1$ we can write

$$D^*(s) = \frac{((s + 1)^{1/2} + 1) - K((\mu s + 1)^{1/2} + 1)}{((s + 1)^{1/2} + 1)(A(s + 1)^{1/2} + B)}, \qquad (8)$$

where $A = 1 - K^2\mu$ and $B = 1 - 2K + K^2\mu$. Given specific initial conditions g_1, g_2, one would now simplify (7) using (8) prior to inversion. In general we get the convolution

$$g(y) = \frac{2}{\sqrt{\pi}} \int_0^y dt \int_0^\infty r\sqrt{t}\, e^{-r^2 t}\, D(y - t)[e^{-t} g_2(2rt) + K\sqrt{\mu}\, e^{-\lambda t} g_1(2\sqrt{\lambda}\, rt)]\, dr, \qquad (9)$$

where

$$D(y) = \frac{G(y)}{1 + K\sqrt{\mu}} + \frac{(\sqrt{\mu} - 1)}{2(K\mu - 1)} [F(y) - G(y)] + \frac{\sqrt{\mu}}{2(K\mu - 1)} \int_0^y [F(t) - G(t)]E(y - t)\, dt,$$

$$E(y) = [e^{-\lambda y} - e^{-y}]/(4\pi y^3)^{1/2}, \qquad F(y) = (e^{-y}/(\pi y)^{1/2}) - \operatorname{erfc} \sqrt{y}, \qquad (10)$$

$$G(y) = 0 \qquad K^2 = \lambda$$

$$= (e^{-y}/(\pi y)^{1/2}) - Q \exp((Q^2 - 1)y) \operatorname{erfc} Q\sqrt{y} \qquad K^2 \neq \lambda,\ Q = B/A.$$

When $K\mu = 1$ we have $Q = 1$ and $F = G$ so the correct formula for D is obtained by computing $\lim_{K\mu \to 1} [F(y) - G(y)]/(K\mu - 1)$.

From Eq. (9) it follows that if the initial conditions g_1, g_2 belong to the class of functions W defined in Lemma 3 and have Laplace transforms, the same is true for g. The function $g(y)$ in (9) then solves Eq. (6) and provides solutions, via (5), to Problem A. Uniqueness of such solutions is clear from Eq. (7). Thus we have

THEOREM: For initial conditions $g_i(x)$ in class W with $|g_i(x)| \le M_i \exp(m_i x)$ for large x, Problem A has a unique solution with interface function satisfying the same conditions. The solution is given by (5) for $g(y)$ in (9).

The formulas in (5) and (9) are less than elegant. However, for any particular problem one can usually perform some additional simplifications, transform (5) back to problem M or S using (1) or (2) and study the solutions numerically. Approximations are also easily accessible. For example, one can choose a simple approximation for $g(y)$ in (9), select one of the initial conditions g_1 or g_2 and solve for the remaining function (g_2 or g_1) using (7). Then Eq. (5) gives solutions to problem A except that one of the initial conditions differs from the original. If the difference is small, an approximate solution is obtained.

A study of problem M for specific initial conditions using the above procedure is given in [5].

References

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