

ON THE FORMULATION OF HYPERBOLIC STEFAN PROBLEMS*

By

A. D. SOLOMON (*Oak Ridge National Laboratory*),

V. ALEXIADES (*Oak Ridge National Laboratory and University of Tennessee*),

D. G. WILSON AND J. DRAKE (*Oak Ridge National Laboratory*)

Abstract. The study of phase change processes governed by hyperbolic heat transfer is at an embryonic stage. We raise here some of the relevant questions and make some remarks on the formulation and qualitative behavior of hyperbolic Stefan problems. In particular, we correct an error in the interface condition appearing in two earlier studies, and present an explicit solution to a simple one-phase problem and study its behavior. Finally we describe an enthalpy (weak) formulation for a two-phase problem and report on a few numerical experiments based on it.

1. Introduction. In [1], [2] a model of a phase change process based on hyperbolic heat transfer in the material is given. Upon examination one finds that the Stefan condition at the phase change front used in these studies is incorrect. Developing the correct condition is an exercise in calculus which is carried out in Sec. 2.

If our interest in understanding phase change processes is sufficiently strong, correction of the earlier calculus error cannot satisfy us; indeed, this first step can awaken us to the fact that this "hyperbolic Stefan problem" represents an entirely new facet of the area of phase change models associated with the Stefan problem. Every question relevant to the usual parabolic case is open for the hyperbolic case. Examples of relevant questions one may ask are the following:

- (a) What is the form of a well-posed problem?
- (b) On what basis can we assign a value to the time derivative of the temperature at the initial time as required for solving a hyperbolic equation of second order?
- (c) What is the nature of the "temperature" that obeys the Telegraphers equation?
- (d) What happens if the phase change front moves at a speed greater than the characteristic signal speed? Is this at all possible?
- (e) Is the model of physical relevance?

*Received April 6, 1984. This work was supported by the Applied Mathematical Sciences subprogram of the Office of Energy Research, U. S. Department of Energy under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

The answers to such questions are not clear to us. Formulation of well-posed hyperbolic phase change problems appears to be difficult in view of the fact that there are known non-well-posed parabolic Stefan problems [3]. Having to assign the time derivative of the temperature initially seems to violate one's intuition and (b) is a serious question. Many of the familiar features of parabolic temperature profiles are due to the maximum principle, which is not necessarily obeyed by hyperbolic equations, whence question (c) arises. A "boundary" for a hyperbolic problem must be time-like [5]; does then a phase change front have to move slower than a characteristic? Finally, in spite of a fairly extensive literature in recent years (see references in [1, 2]), and occasional appeals to intuition as in [6], there is still a dearth of reliable evidence that the Telegraphers equation is indeed relevant (cf. [7]).

In this paper we make a first attempt at examining some of these questions. In Sec. 3 we study a simple one-phase problem. We construct an explicit solution to it and make various observations on its qualitative behavior. Sec. 4 is devoted to fragmentary remarks about the nature of a well-posed one-phase problem. Our remarks include the derivation of a necessary condition on imposed surface flux in order that the solution to the Stefan problem be physically meaningful. The last section is devoted to a weak formulation of a two-phase problem in terms of enthalpy, which is appropriate for numerical solution. We report on a numerical experiment based on this approach.

We wish to express our appreciation to A. Geist, G. Giles and R. Wood for a number of discussions, advice and support for the work described.

2. Nomenclature and derivation of the model. We will be modeling the thermal behavior of a one-dimensional material which undergoes a phase change (say melting) at temperature T_{cr} with latent heat H (kJ/kg). The temperature at a point x (meters) at time t (seconds) is denoted by $T(x, t)$ ($^{\circ}\text{C}$). The relevant thermophysical properties of the material are:

density ρ (kg/m^3), specific heat c ($\text{kJ/kg} - ^{\circ}\text{C}$),
 thermal conductivity k ($\text{kJ/m} - \text{s} - ^{\circ}\text{C}$), diffusivity $\alpha = k/\rho c$ (m^2/s).

Whenever two phases are present we distinguish their thermophysical properties via the subscripts "L" (liquid) and "S" (solid). Unless stated otherwise, we will assume throughout that $c_S, c_L, k_S, k_L, \rho_S, \rho_L$ are constants with $\rho_S = \rho_L$. The heat flux will be denoted by q ($\text{kJ/m}^2 - \text{s}$), and the phase change front separating solid and liquid will be represented by a curve $x = X(t)$.

The hyperbolic heat transfer model is an attempt to overcome the physically unreasonable infinite propagation speed inherent in the heat equation which results from Fourier's law

$$q = -kT_x. \quad (2.1)$$

Instead, we can assume that a temperature gradient induces heat to flow after a delay τ , namely

$$q(x, t + \tau) = -kT_x(x, t).$$

The delay τ is called the response or relaxation time of the material. Keeping only the first order correction term in an expansion of $q(x, t + \tau)$, we replace Fourier's law (2.1) by

$$q + \tau q_t = -kT_x. \tag{2.2}$$

Eliminating q from (2.2) and the energy conservation equation

$$\rho c T_t = -q_x, \tag{2.3}$$

yields the "Telegrapher's" equation

$$\tau \rho c T_{tt} + \rho c T_t = k T_{xx}. \tag{2.4}$$

Note that the wave speed of this hyperbolic equation is $(\alpha/\tau)^{1/2}$ and that when $\tau = 0$, (2.4) reduces to the usual heat equation.

Next we derive the appropriate interface condition, first in the one-phase case and then in the two-phase. Without specifying initial and boundary conditions, let us suppose that a slab of material in its solid phase at the melt temperature T_{cr} is melting from the left. Let $x = X(t)$ be the melt front location (Fig. 1). Then conservation of energy requires that

$$\rho H X'(t) = q^- [t]. \tag{2.5}$$

Here all material properties are assumed to be those of the liquid and $T \equiv T_{cr}$ in the solid. In addition for any function $f(x, t)$ we use the notation

$$f^\mp [t] = \text{Lim } f(x, t), \text{ for } x \rightarrow X(t), x \lessgtr X(t).$$

Following [1, 2] we wish to rewrite (2.5) in terms only of the temperature gradient limit $T_x^- [t]$. Differentiating (2.5) yields

$$\rho H X''(t) = q_x^- [t] X'(t) + q_t^- [t].$$

Letting $x \rightarrow X(t)$ for $x < X(t)$ in (2.2) and (2.3) and eliminating q_x^-, q_t^- yields

$$\begin{aligned} \rho H X''(t) &= -c \rho T_t^- [t] X'(t) - (1/\tau) [k T_x^- [t] + q^- [t]] \\ &= -c \rho T_t^- [t] X'(t) - (k/\tau) T_x^- [t] - (\rho H/\tau) X'(t). \end{aligned}$$

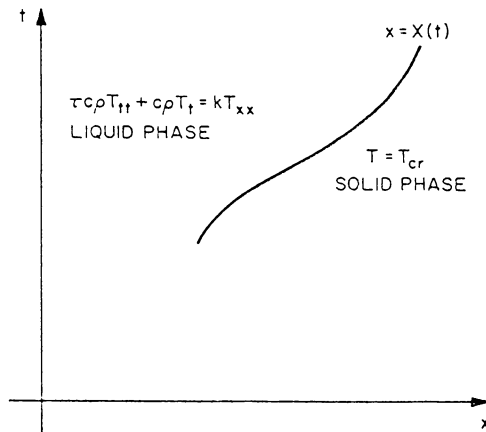


FIG. 1. The Phase Boundary In the One-Phase Case.

Since $x = X(t)$ is an isotherm of T ,

$$T(X(t), t) = T_{cr}, \tag{2.6}$$

we find

$$T_t^-[t] = -X'(t)T_x^-[t],$$

whence we obtain

$$\rho H X''(t) = c_p X'(t)^2 T_x^-[t] - (k/\tau) T_x^-[t] - (\rho H/\tau) X'(t)$$

or

$$X''(t) + (1/\tau) X'(t) = (c/H) T_x^-[t] [X'(t)^2 - (\alpha/\tau)]. \tag{2.7}$$

We note that the quadratic term $X'(t)^2$ was erroneously omitted in [1, 2]. this term though plays an essential role as it is balanced against the signal speed $(\alpha/\tau)^{1/2}$.

Condition (2.7) represents the hyperbolic counterpart to the ordinary 1-phase Stefan condition

$$\rho H X'(t) = -k T_x^-[t]. \tag{2.8}$$

Clearly (2.7) reduces to (2.8) for $\tau = 0$.

For the two-phase case we may not be able to reach a condition in which only current values of T_x^\pm appear. Indeed, for liquid to the left and solid to the right of the front, instead of (2.5) we have

$$\rho H X'(t) = q^-[t] - q^+[t].$$

As before,

$$\rho H X''(t) = q_t^-[t] + q_x^-[t] X'(t) - q_t^+[t] - q_x^+[t] X'(t).$$

If the phases have distinct response times τ_L, τ_S , then we obtain

$$\begin{aligned} \rho H X''(t) = & X'(t)^2 [c_L T_x^-[t] - c_S T_x^+[t]] + [(k_S/\tau_S) T_x^+[t] - (k_L/\tau_L) T_x^-[t]] \\ & + [q^+[t]/\tau_S - q^-[t]/\tau_L]. \end{aligned} \tag{2.9}$$

For $\tau_S = \tau_L = \tau$ this yields, however,

$$\begin{aligned} (2.10) \quad X''(t) + (1/\tau) X'(t) = & (c_L/H) T_x^-[t] [X'(t)^2 - (\alpha_L/\tau)] \\ & - (c_S/H) T_x^+[t] [X'(t)^2 - (\alpha_S/\tau)]. \end{aligned} \tag{2.10}$$

The formulation of the hyperbolic Stefan problem is discussed in Sec. 4.

3. A model with an explicit solution. Consider now the process of melting a semi-infinite slab $x \geq 0$ of material that is initially solid at T_{cr} , due to heat being input at $x = 0$, which we leave unspecified for the moment. We assume the process to be of one phase, with liquid to the left of the front $X(t)$, while to its right we find solid at T_{cr} :

$$T(x, t) = T_{cr}, \quad x \geq X(t), t > 0. \tag{3.1}$$

Recalling (2.4, 7), the functions $T(x, t), X(t)$ are to satisfy the equation

$$\tau T_{tt} + T_t = \alpha T_{xx}, \quad 0 < x < X(t), t > 0, \tag{3.2}$$

and the front conditions

$$T(X(t), t) = T_{cr}, \quad t > 0, \tag{3.3}$$

$$X'(t) + (1/\tau)X(t) = (c/H)T_x^-[t] [X'(t)^2 - (\alpha/\tau)]. \tag{3.4}$$

We assume the relaxation time τ to be a constant.

In order to gain some insight into the nature of the process modeled by these equations, we try to find a function pair $T(x, t)$, $X(t)$, with a straight line as a front, other than a characteristic. Thus we take

$$X(t) = Mt, \quad t > 0, \text{ with } 0 < M, M \neq (\alpha/\tau)^{1/2}, \tag{3.5}$$

and look for the temperature T . It is easy to check that the function

$$T(x, t) = T_{cr} + (H/c) [\exp [M(x - Mt)/(\tau M^2 - \alpha)] - 1] \tag{3.6}$$

satisfies (3.2)–(3.4). The boundary value of T is

$$T(0, t) = T_{cr} + (H/c) [\exp [M^2 t/(\alpha - \tau M^2)] - 1] =: T_L(t). \tag{3.7}$$

Looking at this backwards, we can view (3.5), (3.6) as an explicit solution of (3.2)–(3.4) with boundary condition (3.7) driven by the imposed temperature $T_L(t)$ at $x = 0$, with $M \neq (\alpha/\tau)^{1/2}$ an input parameter. We discuss this further in Sec. 4.

Let us examine this explicit solution in a little more detail. We distinguish two cases, according to the value of the input parameter $M \neq (\alpha/\tau)^{1/2}$.

Case 1. $M < (\alpha/\tau)^{1/2}$. In this case the phase change front propagates slower than the characteristics of the equation. To the left of the front, i.e. for $x < X(t) = Mt$, we see from (3.6) that $T(x, t) > T_{cr}$, so we have liquid there. This is in great contrast with

Case 2. $M > (\alpha/\tau)^{1/2}$. Now the front speed exceeds the characteristic signal speed of the hyperbolic equation (3.2). To the left of the front ($x < Mt$), we find from (3.6), $T(x, t) < T_{cr}$, so that we have “supercooled” liquid there. This “temperature” decreases exponentially fast, with $T_x(x, t) > 0$. Substituting T_x from (3.6) into (2.2), multiplying by the integrating factor $e^{t/\tau}$, integrating in t , and using (2.5) to evaluate the integration constant, we arrive at

$$q(x, t) = \rho HM \exp [M(x - Mt)/(\tau M^2 - \alpha)], \quad 0 \leq x \leq Mt. \tag{3.8}$$

Thus, even though $T_x > 0$, the heat flux q is still positive and heat is flowing to the front from within the “supercooled” liquid phase. This unphysical situation is apparently an acceptable solution of the mathematical problem. We discuss this further in the next section.

What of the case where $M = (\alpha/\tau)^{1/2}$? In this case we can show that the phase change front $x = X(t) = Mt$ cannot be found to meet all of the conditions required of it. Indeed, suppose

$$X(t) = (\alpha/\tau)^{1/2} t, \quad t \geq 0.$$

Then (3.3) implies

$$T_x^-[t] (\alpha/\tau)^{1/2} + T_t^-[t] = 0.$$

Substituting T_x and T_t along $x = X(t)$ from (2.2) and (2.3) we find

$$q_t^-[t] + (\alpha/\tau)^{1/2} q_x^-[t] = -q^-[t]/\tau,$$

or

$$\frac{d}{dt} q^-[t] + (1/\tau) q^-[t] = 0,$$

whence

$$q^-[t] = Ae^{-t/\tau}, \quad A = \text{arbitrary constant.}$$

This however is in violation of the interface condition (2.5), showing that, as one would expect, our basic conditions constitute an overdetermined set of constraints if the front is a characteristic of the equation [5].

REMARK. Letting $\tau \rightarrow 0$ in (3.6), we obtain a function pair

$$X(t) = Mt, \\ T(x, t) = T_{cr} + (H/c) [\exp[M(Mt - x)/\alpha] - 1],$$

which satisfies both the ordinary heat equation and the interface condition (2.8) of the parabolic Stefan problem, as it should.

4. Formulation of hyperbolic Stefan problems. Led by the results of Sec. 2 and the example of Sec. 3, we may pose the following one-phase melting problems involving hyperbolic heat transfer.

Find $X(t)$ and $T(x, t)$ satisfying (3.1)–(3.4) and

Problem I. The imposed temperature boundary condition

$$T(0, t) = T_L(t), \quad t > 0, \quad (4.1)$$

with prescribed $T_L(t) > T_{cr}$;

Problem II. The imposed flux boundary condition

$$q(0, t) = q_0(t), \quad t > 0, \quad (4.2)$$

with prescribed $q_0(t) > 0$;

Problem III. The convective boundary condition

$$q(0, t) = h [T_L(t) - T(0, t)], \quad t > 0 \quad (4.3)$$

with prescribed $T_L(t) > T_{cr}$ and $h > 0$ (heat transfer coefficient).

Recall that here the flux q is not simply $-kT_x$ as in the parabolic case; instead, q and T are related via (2.2), the generalization of Fourier's law.

Two-phase problems may be formulated similarly. They would consist of Eq. (2.4) in the liquid and in the solid (the parameters having their liquid and solid values respectively), interface conditions (2.6) and (2.9), together with boundary conditions like (4.1, 2 or 3) at both ends of the slab; moreover, the equation (2.4) being of second order in time, requires as initial data both $T(x, 0)$ and $T_t(x, 0)$ to be prescribed, which seems physically unreasonable to us, as we have already mentioned in the Introduction (cf. question (b)).

It is reasonable to conjecture that if the data $T_L(t)$ or $q_0(t)$ are sufficiently smooth then Problems I, II or III are well-posed in the classical sense, but we are not aware of any

existing works along these lines. Our example in Sec. 3 indicates that “strange” things may happen in some cases and may help to explain the lack of existing work. In particular, taking as $T_L(t)$ the right hand side of (3.7) [or as $q_0(t)$ the right-hand side of (3.8)] at $x = 0$, with $M > (\alpha/\tau)^{1/2}$, the pair (3.5), (3.6) constitutes a solution of Problem I [or II respectively]. Such a solution is of course physically unacceptable since heat flows backwards in it, violating the second axiom of thermodynamics.

Following [7], the condition of positive entropy production implies that

$$-T_x(x, t)q(x, t) \geq 0 \tag{4.4}$$

must hold at each point of the liquid $0 \leq x \leq X(t)$. Thus, solutions violating (4.4) will be physically unacceptable. Note that this condition is obeyed in our example if $M < (\alpha/\tau)^{1/2}$ but it is violated if $M > (\alpha/\tau)^{1/2}$ (cf. Sec 3).

In parabolic problems, (4.4) is of course automatic by Fourier’s law. Apparently, in hyperbolic problems such a condition may not hold always, and therefore it may be necessary to impose it as an additional condition in order to ensure a physically acceptable solution. This, in turn may impose restrictions on the data of the problem, as we now show for the case of Problem II.

In fact, consider Problem II with the additional requirement that (4.4) hold for $0 \leq x \leq X(t)$. Evaluating (4.4) at $x = 0$ and replacing $T_x(0, t)$ from (2.2) we obtain

$$0 \leq -(1/k)[q_0(t) + \tau q'_0(t)]q_0(t)$$

whence

$$\frac{d}{dt} [q_0(t)e^{t/\tau}] \geq 0, \quad t \geq 0. \tag{4.5}$$

Therefore, the imposed boundary flux must not decrease faster than $e^{-t/\tau}$. Is this a reasonable requirement on the data of the problem? Note that the unphysical solution in our example of Sec. 3 is generated by the flux

$$q_0(t) = \rho HM \exp[M^2 t / (\alpha - \tau M^2)], \quad t \geq 0, \text{ with } M > (\alpha/\tau)^{1/2},$$

which violates (4.5). On the other hand, if $M < (\alpha/\tau)^{1/2}$ then (4.5) is satisfied.

One would think that the front speed, $X'(t)$, cannot be greater than the signal speed $(\alpha, \tau)^{1/2}$, because then the front becomes a space-like wave [5] and conditions (3.3), (3.4) are too few for the problem to be well-posed. It is therefore disturbing that in our example we can find solutions with $X'(t) > (\alpha/\tau)^{1/2}$, unless we impose additional restrictions like (4.5) on the data.

We close this section with an observation concerning the reasonable case $X'(t) < (\alpha/\tau)^{1/2}$. If this holds and also $T(x, t) \geq T_{cr}$ in the liquid, then $T_x^-[t] \leq 0$ and (3.4) implies

$$X''(t) + (1/\tau)X'(t) \geq 0$$

whence

$$d [X'(t)e^{t/\tau}/dt] \geq 0.$$

Thus $X'(t)e^{t/\tau}$ as well as $q [t]e^{t/\tau}$ will be nondecreasing functions of t .

5. Enthalpy formulation of two-phase problems. Similarly to the parabolic case, hyperbolic phase-change problems may be formulated in a weak form by means of the enthalpy. Such formulations are physically more reasonable and more general, as experience has shown (see for example, [8]).

We formulate here a two-phase problem for a one dimensional slab of pure material initially solid, occupying $0 \leq x \leq 1$, insulated at $x = 0$, being heated at $x = 1$ by imposing a flux $q_0(t)$.

Conservation of energy is described by

$$\rho E_t + q_x = 0 \quad (5.1)$$

where $q(x, t)$ is the thermal flux given by the generalized Fourier law (2.2),

$$q + \tau q_t = -kT_x, \quad (5.2)$$

and $E(x, t)$ is the enthalpy, given by [9]

$$E = \begin{cases} 0, & \text{for } T = T_{cr} \text{ (solid),} \\ c_S(T - T_{cr}), & \text{for } T < T_{cr} \text{ (solid)} \\ H + c_L(T - T_{cr}), & \text{for } T > T_{cr} \text{ (liquid),} \\ H, & \text{for } T = T_{cr} \text{ (liquid),} \end{cases} \quad (5.3)$$

with a jump of magnitude H , the latent heat, at $T = T_{cr}$. In terms of E the phases are characterized by $E \leq 0$: solid, $0 < E < H$: interphase, $E \geq H$: liquid. Note that, E and q being discontinuous across the phase change front, the derivatives in (5.1) and (5.2) must be interpreted in distributional sense over the whole region occupied by the material. Formally eliminating q between them we obtain

$$\rho \tau E_{tt} + \rho E_t = (kT_x)_x, \quad (5.4)$$

again in distribution sense. This relation can be implemented numerically in various ways. Knowing the temperature distribution T at time t , it allows us to update E at $t + \Delta t$ and then T is found from (5.3). The great advantage is that no tracking of the front is required. The enthalpy formulation of the two-phase problem mentioned above is formally given by:

$$\begin{aligned} \rho \tau E_{tt} + \rho E_t &= (kT_x)_x, & t > 0, 0 \leq x \leq L, \\ T(x, 0) &= T_0(x), & 0 < x < L, q(0, t) = q_0(t), & q(L, t) = 0, \\ \rho E_t &= (kT_0'(x))', & 0 < x < L, t = 0. \end{aligned} \quad (5.5)$$

Note that the lower order term E_t in (5.4) may be replaced by a term involving no derivative via a change of variables.

Alternatively (5.4) may be written as a first order system. In fact, the original system (5.1, 2) itself may be implemented numerically in the form

$$Q_t = -(k/\tau)U_x, \quad V_t = (1/\tau)V - Q_x/\rho,$$

where $Q = qe^{t/\tau}$, $U = Te^{t/\tau}$, $V = Ee^{t/\tau}$. Indeed, knowing U, V and Q at time t , we can update Q from the first equation, then update V from the second and then U from (5.3).

The relations (5.5) can be implemented numerically in a number of ways. In studies made thusfar, we have observed that as expected, as $\tau \rightarrow 0$ the computed solution tends to

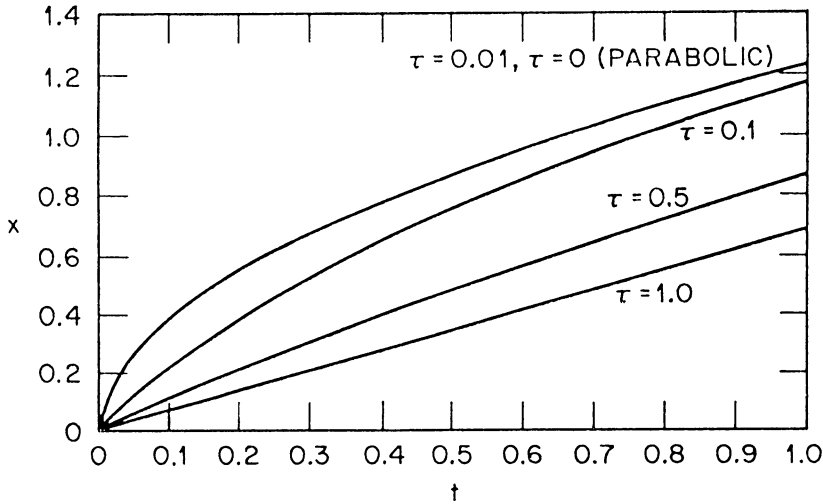


FIG. 2. Computed front histories for hyperbolic one-phase problem in dimensionless case: $k = c\rho = \alpha = 1, J = 1, T_{cr} = 0$ for imposed temperature $T(0, t) = 1$, As $\tau \rightarrow 0$.

that of the parabolic Stefan problem. A typical result for an imposed constant surface temperature (condition (3.8a)) is seen in Fig. 2.

While superficially, Fig. 2 tends to buttress the conjecture of the “correct” parabolic behavior as the limiting case of hyperbolic heat transfer, the numerical implementation is not straightforward. Let us discuss this point.

The enthalpy equation can be differenced using second order central differences for both time and space derivatives. The resulting difference approximation is conditionally stable with the same restrictions on time step and mesh spacing as the corresponding wave equation without the first order time derivatives, i.e. $(\alpha/\tau)^{1/2}(\Delta t/\Delta x)$.

Unfortunately, since the Telegraphers equation admits discontinuous solutions, other numerical difficulties enter. A constant imposed surface temperature different from the initial temperature creates a discontinuous enthalpy wave traveling at the signal speed $(\alpha/\tau)^{1/2}$. The difference approximations at this wave front introduce parasitic waves or wave packets. These parasitic waves are non-physical. In [10], various situations are mentioned which give rise to these parasitic waves. For the hyperbolic enthalpy formulation, special care must be taken with the phase change front, where the enthalpy varies rapidly, with material interfaces and with discontinuities in the temperature profiles. Future numerical work will address these problems.

REFERENCES

- [1] M. Sadd and J. Didlake, *Non-fourier melting of a semi-infinite solid*, Journal of Heat Transfer, 25–28 (1977)
- [2] L. DeSocio and G. Gualtieri, A Hyperbolic Stefan Problem Quarterly of Applied Mathematics **41**, 253–259 (1983)
- [3] A. Solomon, V. Alexiades and D. Wilson, *Explicit solutions to phase change problems*, Quarterly of Applied Mathematics **41**, 237–243 (1983)
- [4] M. Protter and H. Weinberger, *Maximum principles in differential equations*, Prentice Hall, Englewood Cliffs, 1967

- [5] R. Courant and D. Hilbert, *Methods of mathematical physics*, Vol. II, Interscience, New York, 1962
- [6] P. Morse and H. Feshbach, *Methods of theoretical physics*, Pt. I, McGraw Hill, New York, 1953, p. 865
- [7] D. Bogy and P. Naghdi, *On heat conduction and wave propagation in rigid solids*, *Journal of Mathematical Physics* **11**, 917–923 (1970)
- [8] A. Solomon, *Numerical methods for solving Stefan-type problems*, *Res Mechanica*, to appear
- [9] A. Solomon, *Some remarks on the Stefan problem*, *Mathematics of Computation* **20**, 347–360 (1966)
- [10] L. Trefethen, *Group velocity in finite difference schemes*, *SIAM Review* **24**, 113–136 (1982)