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ON MODELING FOR MOVING BOUNDARY PROBLEMS*

A. D. Solomon

Mathematics and Statistics Research Department
Computer Sciences Division
Union Carbide Corporation, Nuclear Division
Oak Ridge, Tennessee 37830

Sponsor: D. M. Eissenberg
Originator: A. D. Solomon

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ABSTRACT

An overview of the area of moving boundary problems emphasizing their appearance in latent heat storage is given.

INTRODUCTION

The classical problems in partial differential equations involve solving an equation within a fixed spatial region. However, when attempting to model such phenomena as melting and freezing, we find that as time varies the region in which, e.g., material in the liquid phase is present, will also vary and must be determined. Such problems--for which the solution of a partial differential equation is sought in a region which is itself varying in an unknown manner--are referred to as moving boundary problems.

The purpose of this note is to describe the current "state of the art" of moving boundary problems as it applies to the storage of heat as latent heat. Assuming that the storage concepts are known to the reader, we will stress the mathematical techniques currently available. We begin (in Section 1) with a quick overview of analytical techniques which are available for such problems in the context of one-dimensional melting of a semi-infinite slab. We then

turn to some simple "rule-of-thumb" approximations for such processes (in Section 2). When all else fails, one is driven to numerical methods; one such method is described in Section 3. Section 4 is devoted to the use of elementary bounds, while in Section 5 we remark on what really happens in a system and how this interacts with the mathematical models. We close with a bibliography of the field.

SECTION 1. SOME ELEMENTARY PROCESSES AND THEIR MODELS

Throughout this section we consider a semi-infinite slab of phase-change-material (PCM), occupying the interval $x > 0$. Initially, at time $t = 0$, the PCM is to be in its solid state at the melting temperature T_{cr}. Due to heat input at the surface $x = 0$ a melting front $x = X(t)$ propagates into the slab. At any time t, to its left ($x < X(t)$) we find liquid PCM, at temperatures above T_{cr}; to its right ($x > X(t)$) the PCM is yet solid at temperature T_{cr}. Assume that the thermal parameters c, ρ, k, α are constants, and that the material undergoes a phase change at temperature T_{cr} with the latent heat H; we find that in the liquid region

$$T_t = \alpha T_{xx} \quad , \qquad x < X(t) \quad ; \tag{1a}$$

in the solid

$$T(x,t) = T_{cr} \quad , \qquad x > X(t) \quad ; \tag{1b}$$

at the initial time,

$$T(x,0) = T_{cr} \quad , \qquad x > 0 \quad ; \tag{1c}$$

at the phase boundary

$$T(X(t),t) = T_{cr} \quad , \qquad t > 0 \tag{1d}$$

and

$$\rho H X'(t) = - K T_x (X(t),t) \quad . \tag{1e}$$

The boundary condition at $x = 0$ may be of a variety of forms. The following cases will be discussed:

$$T(0,t) = T_L > T_{cr} \quad \text{(Dirichlet B.C.)} \tag{2a}$$

$$- K T_x (0,t) = q_o > 0 \quad \text{(flux B.C.)} \tag{2b}$$

$$- K T_x (0,t) = h(T_L - T(0,t) \quad \text{(convection B.C.)} \tag{2c}$$

$$- K T_x (0,t) = \omega(T_L^4 - T(0,t)^4) \quad \text{(radiation B.C.)} \tag{2d}$$

Process 1. Dirichlet B.C. (2a)

In this case functions $X(t)$ and $T(x,t)$ satisfying (1a-e) and (2a) can be found in the form

$$X(t) = 2\lambda \sqrt{\alpha t} \tag{3a}$$

$$T(x,t) = T_L + (T_{cr} - T_L) \frac{\text{erf } (x/2\sqrt{\alpha t})}{\text{erf } (\lambda)} \tag{3b}$$

where λ is the root of the equation

$$\lambda e^{\lambda^2} \text{erf } (\lambda) = \frac{c(T_L - T_{cr})}{H\sqrt{\pi}} \quad . \tag{3c}$$

In latent heat storage the righthand side of this equation is small (since the latent heat should dominate the sensible heat) and so

$$\lambda \approx \sqrt{\frac{c(T_L - T_{cr})}{2H}} \tag{3d}$$

where "$\approx$" denotes approximate equality.

Process 2. Flux B.C. (2b)

In this case the method of Megerlin yields the approximate relation

$$t \approx \frac{h\rho X}{2q_o} + \frac{H^2\rho K}{12cq_o^2} \left\{ \left[1 + \frac{4X\, q_o c}{HK} \right]^{3/2} - 1 \right\} \tag{4a}$$

which for large H and small c implies

$$X(t) \approx q_o t/\rho H \tag{4b}$$

$$T \approx T_{cr} - \frac{HX'}{\alpha c}(x - X) + \frac{H}{2c}\left(\frac{X'}{\alpha}\right)^2 (x - X)^2 \quad . \tag{4c}$$

Comparison with numerical experiments shows the relations to be of high accuracy over the parameter ranges for thermal energy storage PCM's.

Process 3. Convection B.C. (2c)

Using a power-series expansion yields relations for X,T whose first few terms are

$$X(t) \approx \frac{ht(T_L - T_{cr})}{\rho H} - \frac{h^3 t^2 (T_L - T_{cr})^2 \left[1 + \frac{c(T_L - T_{cr})}{H}\right]}{2K(\rho H)^2} \tag{5a}$$

$$T(x,t) \approx T_{cr} - \frac{hx(T_L - T_{cr}}{K} + \frac{h^2(T_L - T_{cr})^2 t}{K\rho H} + \frac{h^2(T_L - T_{cr})^2 x^2}{2\alpha K\rho H} \tag{5b}$$

$$+ \frac{h^3(T_L - T_{cr})^2 xt}{K^2 \rho H} + \frac{\left[1 - 2\frac{c(T_L - T_{cr})}{H}\right] h^4 (T_L - T_{cr})^3 t^2}{2(K\rho H)^2}$$

Process 4. Radiation B.C. (2d)

With the help of a quasi-stationary approach, we find the approximations

$$T(x,t) \approx A(t) + (T_{cr} - A(t))\, x/X(t) \tag{6a}$$

where

$$A = T_{cr} + \frac{\rho H X X'}{K} \tag{6b}$$

and X(t) solves the ordinary differential equation

$$\frac{\rho H X'}{\omega T_L^4} + \left(\frac{T_{cr}}{T_L} + \frac{\rho H X X'}{K T_L}\right)^4 = 1 \tag{6c}$$

All of the approximation techniques are highly accurate so long as the dimensionless Stefan number

$$St = \frac{c\Delta T}{H} \tag{7}$$

is small (e.g., St < 1). Here ΔT is a typical system temperature drop.

SECTION 2. RULES OF THUMB

Under certain circumstances we would like to be able to obtain quick and easily computable (e.g., on a pocket calculator) estimates of the behavior of phase change processes. Thus a contractor might need only a rough estimate of how much PCM is required for a given handware configuration, but he would like to derive it within minutes and if possible, at no cost. Using the methods of the last section, supported by computations, it is possible to derive such "rules of thumb" for simple configurations. Let us now describe one such result.

Consider again the process 3 with a convection B.C. (2c). Then it can be shown that the wall temperature

$$T_{wall} = T(o,t)$$

and the time t are related by

$$t = \frac{Kc\rho}{h^2}\left\{.59\left(\frac{T_{wall} - T_{cr}}{T_L - T_{wall}}\right)^{1.83} + \frac{1}{2St}\left[\left(\frac{T_L - T_{cr}}{T_L - T_{wall}}\right)^2 - 1\right]\right\} \tag{144}$$

with a relative error below 10%, and in most cases less than 3%. Here

$$St = \frac{c\,(T_L - T_{cr})}{H} \quad .$$

Other similar relations can be found for a variety of cases.

SECTION 3. NUMERICAL METHODS

Since the early 1950's a variety of numerical methods for phase change processes have been developed. The need for special methods is clear since the key unknown in these processes is the phase boundary itself.

The numerical method which offers the best hope for dealing with general phase change processes is the "weak-solution" (or "enthalpy") approach. This is based on introducing the specific internal energy e as the key variable of the process. Choosing e = 0 as an arbirary reference value, we associate "solid" with $e \leq 0$ and an "interphase state" with $0 < e < H$. The relation between e and T is

$$T = \begin{cases} T_{cr} + e/c_s, & e \leq 0 \\ T_{cr}, & 0 < e < H \\ T_{cr} + (e - H)/c_L, & e \geq H \end{cases}$$

Here the subscripts s,L refer to solid and liquid phases, respectively. Introduce the diffusivity function $\alpha = \alpha(e)$ as

$$\alpha(e) = \begin{cases} \alpha_s, & e \leq 0 \\ 0, & 0 < e < H \\ \alpha_L, & e \geq H \end{cases}.$$

Then one may replace our original phase change process by the single equation

$$e_t = (\alpha(e)e_x)_x$$

with appropriate boundary and initial conditions. The equation can be discretized and e (and hence T) values computed. The phase boundary is located where $0 \leq e \leq H$ and is "smudged" to a region of very small width.

The method has been applied with success to a variety of problems, although further investigation is still needed.

SECTION 4. BOUNDS ON PROCESSES

One can often derive qualitative information about phase change processes without finding the temperature and the phase boundary. As an example, using a variety of analytical tools, we can show that for the convective B.C. process (2c), the phase boundary X(t) obeys the inequalities

$$X(t) \leq \frac{\text{th}(T_L - T_{cr})}{\rho H}$$

and

$$X(t) \geq \frac{K\,St}{h(1+St)} \left\{ e^{\alpha h^2 t/K^2}\, \text{erfc}\left[\frac{h\sqrt{\alpha t}}{K}\right] + \frac{2h\sqrt{\alpha t}}{K\sqrt{\pi}} - 1 \right\}.$$

Such bounds are of value in sizing systems and as a confirmation of approximations as in Sections 1 and 2.

SECTION 5. REALITY

The models introduced in previous sections ignore some very real effects in phase change processes. These include for various materials in different configurations:

a) natural convection

b) property dependence on temperature

c) additional phase transitions

d) anisotropy of solid properties

e) incongruent melting and degrading of H

f) supercooling

g) multidimensionality

h) inhomogeneity of PCM's.

The precise quantitative understanding of a real storage system requires that one understand how to model these effects-albeit roughly. The limited references to them are given in the Bibliography.

NOMENCLATURE

c	specific heat	(KJ/Kg-°c)
e	specific internal energy	(KJ/Kg)
h	film coefficient	(KJ/m^2-s-°c)
H	latent heat	(KJ/Kg)
K	conductivity	(KJ/m-s-°c)
q	heat flux	(KJ/m^2-s)
t	time variable	(s)
T	temperature	(°c)
T_{cr}	melting temperature	(°c)
T_L	ambient flow temperature	(°c)
x	space variable	(m)
$X(t)$	phase boundary location at time t	(m)
α	thermal diffusivity	(m^2/s)
ρ	density	(Kg/m^3)

$\omega = \dfrac{\sigma}{1 + \dfrac{1}{\varepsilon_1} + \dfrac{1}{\varepsilon_2}}$ for σ the Stefan-Boltzmann constant and ε_1, ε_2 the emissivities of surfaces in raidation processes (KJ/m^2-s-$°c^4$)

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Literally hundreds of papers dealing with phase change modeling have appeared in recent years. In the following lines we present a representative list of these references. Our list is divided roughly in accordance with the material of this report. However, references are also given to material that we have not discussed, including multidimensional phase change processes, and a spectrum of applications. The broad theoretical literature concerned with questions of well-posedness of the mathematical model is greatly under-represented, although the interested reader will find appropriate references in the recent symposium proceedings of Ockendon and of Wilson. Similarly, very recent work of Friedman and others on the use of variational concepts is not referenced here. Only one example of the extensive work of Boley is listed under the heading of "bounds." Similarly, the recent and growing attention to natural convection in melting processes is not well represented by works listed. We have not listed the individual papers of the Ockendon and Wilson proceedings, but we do point out that they include an extensive range of theoretical and applied results. In particular, we can indicate the papers on glass and related work on semi-transparent materials contained in Ockendon's work, and the papers on coupled processes (heat transfer and mass diffusion) given in that of Wilson. The interesting applications of phase-change modeling techniques to statistical decision processes is similarly mentioned among the references of the proceedings and not indicated by us.

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