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# DETERMINATION OF ONE OR TWO UNKNOWN THERMAL COEFFICIENTS OF A SEMI-INFINITE MATERIAL THROUGH A TWO-PHASE STEFAN PROBLEM

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**Abstract**—This paper consists of two parts:

(1) We consider the two-phase (fusion) Stefan problem for a semi-infinite material with one unknown thermal coefficient. We have an overspecified condition of type

$$k_2 \frac{\partial T_2}{\partial x}(0, t) = -ho/\sqrt{t}$$

with $ho > 0$ on the fixed face $x = 0$ of the phase-change material. We obtain: (i) if $\rho$ is unknown, then the corresponding free boundary problem always has a unique solution of the Neumann type; (ii) if one of the remaining five coefficients is unknown, then the corresponding free boundary problem has a unique solution of the Neumann type iff a complementary condition is verified.

(2) We consider the inverse two-phase (fusion) Stefan problem for a semi-infinite material with an overspecified condition

$$k_2 \frac{\partial T_2}{\partial x}(0, t) = -ho/\sqrt{t}$$

with $ho > 0$ on the fixed face and with two unknown thermal coefficients.

We obtain: (i) if $(\rho, k_2)$ are unknown, the corresponding moving boundary problem always has a unique solution of the Neumann type; (ii) if $(l, k_1)$, $(l, c_1)$ or $(k_1, c_1)$ are unknown, the corresponding moving boundary problem has infinite solutions whenever the complementary conditions are verified; (iii) in the remaining eleven cases, the corresponding moving boundary problem has a unique solution of the Neumann type iff complementary conditions are verified.

Moreover, in both parts, we obtain formulas for the unknown thermal coefficients.

## I. INTRODUCTION

Heat transfer problems with phase-change such as melting and freezing have been studied in the last century because of their wide scientific and technological applications. For example, a review of a long bibliography on moving and free boundary problems for the heat equation, particularly concerning the Stefan problem, is presented in [34]. That bibliography is analysed and classified into the theoretical, numerical and experimental papers and also into those concerning possible applications. A bibliography on moving free boundary problems with key-word index is given in [37]. It is important to point out, that the subject has been reviewed in many other papers, for example [1, 4, 7, 10–14, 20–24, 26, 27, 36].

We consider the melting of a solid in a semi-infinite region $0 < x < +\infty$. Initially, the solid is at uniform temperature $-d < 0$ below the melting temperature $T_m = 0°C$ (we shall assume from now on, without loss of generality, that the phase-change temperature of the material is 0°C). For time $t > 0$, a constant temperature $b > 0$, higher than the melting temperature of the substance, is maintained at the fixed face $x = 0$. As a result, the liquid phase is formed in the region $0 < x < s(t)$ (we shall assume that the solid and liquid phases are separated by a sharp interphase $x = s(t)$ at time $t > 0$ with the initial condition $s(0) = 0$) and the solid phase remains in the region $s(t) < x$, as shown in Fig. 1.

We shall also assume that the thermal properties are constant in each phase, but that they may take different values in the liquid and solid phases. In general, the solid and liquid densities are not the same, therefore, some motion of solid resulting from the density change is expected in actual situations. In the following analysis, we assume the density $\rho$ to be the same

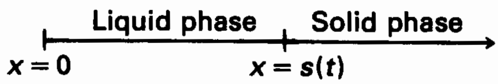


Fig. 1. Physical model of the problem.

for both phases so that the convective velocity resulting from the volumetric effects can be neglected, i.e., there is no expansion nor contraction in the melting process.

We suppose that the temperature $T = T(x, t)$ of the material is defined by

$$T(x,t)=\begin{cases} T_2(x,t)>0 & \text{if } 0<x<s(t), \quad t>0 \\ 0 & \text{if } x=s(t), \quad t>0 \\ T_1(x,t)<0 & \text{if } s(t)<x, \quad t>0 \end{cases} \tag{1}$$

The governing differential equations take the following forms for the liquid and solid phases:

$$T_{2_t} - \alpha_2 T_{2_{xx}} = 0, \qquad 0<x<s(t), \qquad t>0 \tag{2i}$$

$$T_{1_t} - \alpha_1 T_{1_{xx}} = 0, \qquad s(t)<x, \qquad t>0. \tag{2ii}$$

The conditions at the liquid–solid interface $x = s(t)$ are given by the requirement of the continuity of temperature and the energy equation (Stefan's condition), i.e.

$$T_1(s(t),t) = T_2(s(t),t) = 0, \qquad t>0 \tag{2iii}$$

$$k_1 T_{1_x}(s(t),t) - k_2 T_{2_x}(s(t),t) = \rho l \dot{s}(t), \qquad t>0 \tag{2iv}$$

The initial and boundary conditions are given by

$$T_1(x,0) = T_1(+\infty,t) = -d<0, \qquad x>0, \qquad t>0 \tag{2v}$$

$$T_2(0,t) = b>0, \qquad t>0 \tag{2vi}$$

$$s(0) = 0. \tag{2vii}$$

In this paper we consider the two-phase Stefan problem (2i–vii) [7, 11, 27, 29, 32, 38] for a semi-infinite material $0<x<\infty$ with one or two unknown coefficients with an overspecified heat flux condition on the fixed face $x = 0$, given by

$$k_2 T_{2_x}(0,t) = -\frac{ho}{\sqrt{t}}, \qquad t>0 \tag{2viii}$$

for $ho>0$ given. We point out that when the boundary condition on the fixed face $x = 0$ is the heat flux (2viii) then the temperature of the corresponding two-phase Stefan problem is constant at the fixed face and $s(t)$ is proportional to $t^{\frac{1}{2}}$ under an appropriate condition for the data $ho$ [32]. For this reason, we have introduced the overspecified (2viii) on the fixed face $x = 0$. The idea of using an overspecified condition on the boundary was introduced in [8, 9, 15, 16] (see more details in [10]).

If by means of a phase-change experiment (e.g., fusion), we are able to measure the quantities $b>0$ and $ho>0$ given by the conditions (2vi) and (2viii) respectively, then we shall be able to find formulas for the determination of only one unknown thermal coefficient among $l$, $\rho$, $c_1$, $c_2$, $k_1$, $k_2$ (see Section II). If, moreover, we are able to measure the quantity $\sigma>0$ (i.e., $s(t)$), given by the condition (4), then we can find formulas for the simultaneous determination of two unknown thermal coefficients among $k_1$, $k_2$, $c_1$, $c_2$, $\rho$, $l$ (see Section III). Summing up, if $\sigma$ is known, then we have two overspecified conditions and, therefore, two unknown thermal coefficients may be found under appropriate conditions. If $\sigma$ is not known, at most one thermal coefficient can be found.

In Section II, we study problem (P1) where we want to find the function $s = s(t)>0$ (free boundary), defined for $t>0$; the temperature $T = T(x, t)$, defined as (1), and one of the six thermal coefficients $l$, $\rho$, $c_1$, $c_2$, $k_1$, $k_2$ so that the conditions (2i–viii) are satisfied. The results obtained for the six cases already mentioned are summarized in Table 1. The solution of

Table 1

| Case No. | Unknown coefficient | Necessary and sufficient conditions for the existence and unicity of the solution | Solution |
|---|---|---|---|
| 1 | $l$ | (R2) | $l=\frac{1}{\rho a_2\xi_2}T(\xi_2),\quad \sigma=a_2\xi_2.$ with $\xi_2=f^{-1}(k_2b/hoa_2\sqrt{\pi})$ |
| 2 | $\rho$ | — | $\rho=\frac{\pi}{k_2c_2}\left[\frac{ho}{b}f(\xi_2)\right]^2,\quad \sigma=\frac{k_2b}{ho\sqrt{\pi}}\frac{\xi_2}{f(\xi_2)}$ where $\xi_2$ is the solution of the equation $\begin{cases} x=(1/l\sqrt{\pi})P(x,\alpha,1,\gamma,1/\beta), & x>0 \\ \text{with } \alpha=bc_2,\ \beta=\sqrt{c_2k_1/c_1k_2}, & \gamma=d\sqrt{c_1c_2k_1/k_2}\end{cases}$ |
| 3 | $c_1$ | (R3) | $c=(k_1/\rho a_2^2)(\xi_1/\xi_2)^2,\quad \sigma=a_2\xi_2$ where $\xi_2$ is given as in case 1, and $\xi_1$ is the solution of the equation $\begin{cases} V(x)=A_1, & x>0 \\ \text{with } A_1=\frac{\rho la_2\xi_2\sqrt{\pi}}{dk_1}k(\xi_2,0)\end{cases}$ |
| 4 | $c_2$ | (R5) | $c_2=\frac{k_2}{\rho a_1^2}\left(\frac{G^{-1}(\xi_1)}{\xi_1}\right)^2,\quad \sigma=a_1\xi_1$ where $\xi_1$ is the solution of the equation $h(G^{-1}(x),ho/\rho la_1)=U(x),\ x>\frac{k_2b}{2hoa_1}$ |
| 5 | $k_1$ | (R4) | $k_1=\rho c_1a_2^2(\xi_2/\xi_1)^2,\quad \sigma=a_2\xi_2$ where $\xi_2$ is given as in case 1, and $\xi_1$ is the solution of the equation $\begin{cases} Q(x)=B, & x>0 \\ \text{with } B^{-1}=\frac{l}{dc_1a_2\xi_2}k(\xi_2,0)\end{cases}$ |
| 6 | $k_2$ | (R1) | $k_2=\rho c_2\left(\frac{a_1\xi_1}{H^{-1}(\xi_1)}\right)^2,\quad \sigma=a_1\xi_1$ where $\xi_1$ is the solution of the equation $h\left(H^{-1}(x),\frac{ho}{\rho la_1}\right)=U(x),\quad x>0$ |

problem (P1) is given by

$$\left.\begin{aligned} T_2(x,t)&=b-\frac{b}{f(\sigma/a_2)}f(x/2a_2\sqrt{t}),\qquad a_i=\sqrt{\alpha_i}\,(i=1,2)\\ T_1(x,t)&=\frac{df(\sigma/a_1)}{1-f(\sigma/a_1)}-\frac{d}{1-f(\sigma/a_1)}f(x/2a_1\sqrt{t})\end{aligned}\right\}\tag{3}$$

$$s(t)=2\sigma\sqrt{t},\qquad \sigma>0\tag{4}$$

where $\sigma$ and the unknown thermal coefficient are obtained for the following system of equations

$$\frac{ho}{\rho l}\exp(-\sigma^2/a_2^2)-\frac{dk_1}{\rho la_1\sqrt{\pi}}\frac{\exp(-\sigma^2/a_1^2)}{1-f(\sigma/a_1)}=\sigma\tag{5i}$$

$$f(\sigma/a_2)=\frac{k_2b}{hoa_2\sqrt{\pi}}\tag{5ii}$$

We shall prove that problem (P1) does not always have a solution of the Neumann type (3, 4). Moreover, the explicit solution exists for cases 1, 3, 4, 5 and 6 iff a complementary condition is satisfied. Otherwise, it always exists for case 2($\rho$ unknown). Complementary conditions for the calculation of the explicit solution have been obtained for Stefan type problems in papers [32, 33, 35].

Table 2(a)

| Case No. | Unknown coefficients | Necessary and sufficient conditions for the existence and unicity of the solution | Solution |
|---|---|---|---|
| 1 | $\rho, l$ | (R6) | $\rho = \frac{k_2}{c_2 \sigma^2} \xi_2^2$, $l = \frac{\lambda_2 \sigma}{k_2 \xi_2^2} \xi_2^2 W(\xi_2)$ where $\xi_2$ is the unique solution of the equation $F(x) = \frac{k_2 b}{h o \sigma \sqrt{\pi}}$, $x > 0$ |
| 2 | $\rho, c_2$ | (R7) | $\rho = \frac{k_1}{c_1 \sigma^2} \xi_1^2$, $c_2 = \frac{k_2 c_1}{k_1} (\xi_2/\xi_1)^2$ where $\xi_2$ is given as in case 1, and $\xi_1$ is the unique solution of the equation $W_1(x) = h\left(\xi_2, \frac{\sigma c_1 h o}{l k_1}\right)$, $x > 0$ |
| 3 | $\rho, k_2$ | — | $\rho = \frac{h o \sqrt{\pi}}{b \sigma c_2} \xi_2 f(\xi_2)$, $k_2 = \frac{\sigma h o \sqrt{\pi}}{b} \frac{f(\xi_2)}{\xi_2}$ where $\xi_2$ is the unique solution of the equation $W_1(I(x)) = h\left(x, \frac{\sigma c_1 h o}{l k_1}\right)$, $x > 0$ |
| 4 | $k_2, c_2$ | (R8) | $k_2 = \frac{\sigma h o \sqrt{\pi}}{b} \frac{f(\xi_2)}{\xi_2}$, $c_2 = \frac{h o \sqrt{\pi}}{\rho \sigma b} \xi_2 f(\xi_2)$ where $\xi_2 = t\left(\frac{h o}{\rho l}\left[\sigma + \frac{d k_1}{\rho l a_1 \sqrt{\pi}} K\left(\frac{\sigma}{a_1}\right)\right]^{-1}\right)$. |
| 5 | $k_2, l$ | (R10) | $k_2 = \frac{\rho \sigma^2 c_2}{\xi_2^2}$, $l = \frac{1}{\rho \sigma} Z(\xi_2)$ where $\xi_2$ is the unique solution of the equation $J(x) = \frac{\rho b \sigma c_2}{h o \sqrt{\pi}}$, $x > 0$ |
| 6 | $l, c_2$ | (R11) | $l = \frac{1}{\rho \sigma} Z(\xi_2)$, $c_2 = \frac{k_2}{\rho \sigma^2} \xi_2^2$ where $\xi_2$ is given as in case 1 |
| 7 | $c_1, c_2$ | (R13) | $c_1 = \frac{k_1}{\rho \sigma^2} \xi_1^2$, $c_2 = \frac{k_2}{\rho \sigma^2} \xi_2^2$ where $\xi_2$ is given as in case 1, and $\xi_1$ is the unique solution of the equation $V(x) = \frac{\rho l \sigma^2 \sqrt{\pi}}{d k_1} L(\xi_2)$, $x > 0$ |
| 8 | $k_1, k_2$ | (R15) | $k_1 = \frac{\rho c_1 \sigma^2}{\xi_1^2}$, $k_2 = \frac{\rho c_2 \sigma^2}{\xi_2^2}$ where $\xi_2$ is given as in case 5, and $\xi_1$ is the unique solution of the equation $Q(x) = (d c_1/l)(L(\xi_2))^{-1}$, $x > 0$ |
| 9 | $\rho, c_1$ | (R16) | $\rho = \frac{k_2}{c_2 \sigma^2} \xi_2^2$, $c_1 = \frac{k_1 c_2}{k_2} (\xi_1/\xi_2)^2$ where $\xi_2$ is given as in case 1, and $\xi_1$ is the unique solution of equation $V(x) = \frac{\sigma h o \sqrt{\pi}}{d k_1}\left[\exp(-\xi_2^2) - \frac{l k_2 \xi_2^2}{h o c_2 \sigma}\right]$, $x > 0$ |
| 10 | $\rho, k_1$ | (R17) | $\rho = \frac{k_2}{c_2 \sigma^2} \xi_2^2$, $k_1 = \frac{c_1 k_2}{c_2} (\xi_2/\xi_1)^2$ where $\xi_2$ is given as in case 1 and $\xi_1$, as in case 8 |

Table 2(a) (*continued*)

| Case No. | Unknown coefficients | Necessary and sufficient conditions for the existence and unicity of the solution | Solution |
|---|---|---|---|
| 11 | $k_2, c_1$ | (R18) | $k_2 = \frac{\rho c_2 \sigma^2}{\xi_2^2}$, $c_1 = \frac{k_1}{\rho\sigma^2}\xi_1^2$ where $\xi_2$ is given as in case 5 and $\xi_1$, as in case 7 |
| 12 | $c_2, k_1$ | (R19) | $c_2 = \frac{k_2}{\rho\sigma^2}\xi_2^2$, $k_1 = \frac{\rho c_1 \sigma^2}{\xi_1^2}$ where $\xi_2$ is given as in case 1 and $\xi_1$, as in case 8 |

Table 2(b)

| Case No. | Unknown coefficients | Necessary and sufficient conditions for the existence of at least one solution | Solution |
|---|---|---|---|
| 13 | $c_1, k_1$ | (R20), (R21) | $k_1 > 0$, $c_1 = c_1(k_1) = \frac{k_1}{\rho\sigma^2}\xi_1^2(k_1)$ where, for each $k_1 > 0$, $\xi_1(k_1)$ is the unique solution of the equation $V(x) = \frac{\rho l \sigma^2\sqrt{\pi}}{dk_1} L\left(\frac{\sigma}{a_2}\right)$, $x > 0$ |
| 14 | $l, k_1$ | (R20), (R22) | $l = l(\xi_1) = \frac{ho}{\rho\sigma}\exp\left(-\left(\frac{\sigma}{a_2}\right)^2\right) - \frac{dc_1}{Q(\xi_1)}$, $k_1 = k_1(\xi_1) = \frac{\rho c_1\sigma^2}{\xi_1^2}$ with $\xi_1 > \xi_1^0$, where $\xi_1^0$ is the unique solution of the equation $Q(x) = \frac{\rho\sigma d c_1}{ho}\exp(\sigma/a_2)^2$, $x > 0$ |
| 15 | $l, c_1$ | (R20) | $l = l(\xi_1) = \frac{ho}{\rho\sigma}\exp\left(-\left(\frac{\sigma}{a_2}\right)^2\right) - \frac{dk_1}{\rho\sigma^2\sqrt{\pi}}V(\xi_1)$, $c_1 = c_1(\xi_1) = \frac{k_1}{\rho\sigma^2}\xi_1^2$ with $0 < \xi_1 < \xi_1^0$, where $\xi_1^0 = V^{-1}\left(\frac{ho\sigma\sqrt{\pi}}{dk_1}\exp\left(-\left(\frac{\sigma}{a_2}\right)^2\right)\right)$ |

Because of physical considerations, in Section III, we take the moving boundary $s(t)$ defined by (4), with $\sigma > 0$ given, and we face the problem (P2): to find the temperature $T = T(x, t)$ as in (1) and two of the six thermal coefficients of the material, so that condition (2) is satisfied.

Results obtained for all fifteen cases are summarized in Tables 2(a) and 2(b). The solution for problem (P2) is given by (3), where the two thermal coefficients to be determined are obtained as a solution for system of equations (5). We shall prove that:

(i) if $(\rho, k_2)$ are unknown, the corresponding moving boundary problem always has a unique solution of the Neumann type;

(ii) if $(l, k_1)$, $(l, c_1)$ or $(k_1, c_1)$ are unknown, the corresponding moving boundary problem has infinite solutions whenever the complementary conditions are verified;

(iii) in the remaining eleven cases, the corresponding moving boundary problem has a unique solution of the Neumann type iff complementary conditions are verified.

In Section IV, we obtain estimations for the coefficient $\sigma$ which characterizes the free boundary of the Neumann solution for a semi-infinite material undergoing a phase-change process as the one described in this paper.

The experimental determination of the coefficients $ho > 0$ and $\sigma > 0$ (when necessary) can be obtained respectively through the least squares in the following expressions

$$ho = -t^{\frac{1}{2}}k_2 T_{2_x}(0, t) = -t^{\frac{1}{2}} \cdot (\text{heat flux in } x = 0 \text{ at time } t) \qquad \text{(2viii } bis\text{)}$$

for all $t>0$

$$\sigma=\frac{s(t)}{2t^{\frac{1}{2}}}, \quad \text{for all } t>0, \tag{4 bis}$$

through a discrete number of measurement at time $t_1, t_2, \dots, t_n$ of the corresponding quantities. An experimental work [2] is in preparation to evaluate the theoretical results of this paper. Other methods for the calculation of thermal coefficients have been given, for example, in [3, 5, 6] (in [35] we can obtain numerous references on physical and mathematical methods for the determination of thermal coefficients).

The results of this paper have been presented in [28] and generalize those obtained for the Lamé–Clapeyron problem [7, 11, 17, 27, 29–31] in [33, 35].

From now on, we shall consider the new variables:

$$\text{(i) } \xi_1=\frac{\sigma}{a_1} \qquad \text{(ii) } \xi_2=\frac{\sigma}{a_2} \tag{6}$$

## II. DETERMINATION OF A THERMAL COEFFICIENT. SOLUTION OF PROBLEM (P1)

To simplify the building of Table 1, let us consider the following restrictions:

$$\frac{dk_1}{hoa_1\sqrt{\pi}}<1 \tag{R1}$$

$$\left.\begin{array}{l}\text{(R1) with}\\ \dfrac{bk_2}{hoa_2\sqrt{\pi}}<f(So), \quad \text{where } S_0 \text{ is the unique positive zero of } T.\end{array}\right\} \tag{R2}$$

$$\frac{bk_2}{hoa_2\sqrt{\pi}}<f(x_0), \quad \text{where } x_0 \text{ is the unique positive zero of } k(x,0). \tag{R3}$$

$$\frac{bk_2}{hoa_2\sqrt{\pi}}<f(x_1), \quad \text{where } x_1 \text{ is the unique positive zero of } k(x, dc_1). \tag{R4}$$

$$\frac{bk_2}{2ho}+\frac{dk_1}{\rho la_1\sqrt{\pi}}K\left(\frac{k_2b}{2hoa_1}\right)<\frac{ho}{\rho l} \tag{R5}$$

The six possible cases for determining the thermal coefficients are considered in Table 1 (in all cases $\sigma$ is also unknown). The necessary and sufficient condition to be verified by the data for the existence and uniqueness of problem (P1) are given together with the expression of $\sigma$ and the corresponding unknown coefficient.

Now we shall only prove the following property for case 3 (determination of $c_1$):

*Property 1*

The necessary and sufficient condition for problem (P1) with $c_1$ unknown to have a unique solution is that data $ho>0$, $b>0$, $d>0$ and coefficients $l$, $\rho$, $c_2$, $k_1$, $k_2$ of the phase-change material do verify condition (R3). In such a case, the solution is given by (3), (4), where

$$\sigma=a_2\xi_2, \qquad c_1=\frac{k_1}{\rho a_2^2}\left(\frac{\xi_1}{\xi_2}\right)^2 \tag{7}$$

with

$$\xi_2=f^{-1}(k_2b/a_2ho\sqrt{\pi}) \tag{8}$$

$$\left.\begin{array}{l}V(\xi_1)=A_1, \qquad \xi_1>0\\ \text{where } A_1=\dfrac{\rho la_2\xi_2\sqrt{\pi}}{dk_1}k(\xi_2, 0).\end{array}\right\} \tag{9}$$

PROOF. If

$$\frac{k_2b}{hoa_2\sqrt{\pi}}<1$$

is verified, from (5ii) and (6ii), we obtain (8). Therefore, from (5i) it follows that $\xi_1$ should verify equation (9). The latter has a unique solution iff $A_1>0$ (because $V(0)=0$, $V(+\infty)=+\infty$, $V'>0$), that is, iff

$$\xi_2<x_0 \tag{10}$$

where $x_0$ is the only positive root of $k(x, 0)$. Now, considering (8), condition (10) is equivalent to (R3), and so the property is proved.

## III. DETERMINATION OF TWO UNKNOWN COEFFICIENTS. SOLUTION OF PROBLEM (P2)

Let us consider the following restrictions, to be used in Table 2 [we denote by $f_0 g$ the composition of functions $f$ and $g$, i.e. $(f_0 g)(x)=f(g(x))$]:

$$F(s_0)<\frac{k_2 b}{ho\sigma\sqrt{\pi}}<\frac{2}{\sqrt{\pi}}, \text{ where } s_0 \text{ is the unique positive zero of } W. \tag{R6}$$

$$\frac{k_2 b}{2ho\sigma}<1 \tag{R7}$$

$$\frac{\rho l\sigma}{ho}+\frac{dk_1}{hoa_1\sqrt{\pi}}K(\sigma/a_1)<1. \tag{R8}$$

$$\frac{a_1 ho\sqrt{\pi}}{dk_1}>K(\sigma/a_1). \tag{R9}$$

$$\left.\begin{array}{l}\text{(R9) with}\\ \dfrac{\rho b\sigma c_2}{ho\sqrt{\pi}r_0 f(r_0)}<1, \quad \text{with } r_0=t(a_1 h_0\sqrt{\pi}/dk_1 K(\sigma/a_1))\end{array}\right\} \tag{R10}$$

$$\begin{array}{l}\text{(R9) with}\\ F(r_0)<\dfrac{k_2 b}{\sigma h_0\sqrt{\pi}}<\dfrac{2}{\sqrt{\pi}}, \text{ where } r_0 \text{ was defined in (R10).}\end{array} \tag{R11}$$

$$\frac{\rho l\sigma}{ho}<1. \tag{R12}$$

$$\left.\begin{array}{l}\text{(R12) with}\\ (F_0 t)(ho/\rho l\sigma)<\dfrac{k_2 b}{\sigma h_0\sqrt{\pi}}<\dfrac{2}{\sqrt{\pi}}.\end{array}\right\} \tag{R13}$$

$$\frac{\rho\sigma(dc_1+l)}{ho}<1. \tag{R14}$$

$$\left.\begin{array}{l}\text{(R14) with}\\ (J_0 t)(ho/\rho\sigma(dc_1+l))>\dfrac{\rho c_2 b\sigma}{ho\sqrt{\pi}}\end{array}\right\} \tag{R15}$$

$$(F_0 g^{-1})(ho\sigma c_2/lk_2)<\frac{k_2 b}{\sigma ho\sqrt{\pi}}<\frac{2}{\sqrt{\pi}} \tag{R16}$$

$$(F_0 g^{-1})(ho\sigma c_2/k_2(dc_1+l))<\frac{k_2 b}{\sigma ho\sqrt{\pi}}<\frac{2}{\sqrt{\pi}} \tag{R17}$$

$$\left.\begin{array}{l}\text{(R12) with}\\ (J_0 t)(ho/\rho l\sigma)>\dfrac{\rho c_2 b\sigma}{ho\sqrt{\pi}}.\end{array}\right\} \tag{R18}$$

$$\left.\begin{array}{l}\text{(R14) with}\\ (F_0 t)(ho/\rho\sigma(dc_1+l))<\dfrac{k_2 b}{\sigma ho\sqrt{\pi}}<\dfrac{2}{\sqrt{\pi}}.\end{array}\right\} \tag{R19}$$

$$ho = \frac{k_2 b}{a_2 f(\sigma/a_2)\sqrt{\pi}}. \tag{R20}$$

$$\frac{ho}{\rho l \sigma} > \exp(\sigma^2/a_2^2). \tag{R21}$$

$$\frac{ho}{\rho \sigma d c_1} > \exp(\sigma^2/a_2^2) \tag{R22}$$

In Table 2, we consider the fifteen possible cases for the determination of two thermal coefficients. The first part [Table II(a)] corresponds to the twelve cases where, with or without restrictions, the existence and uniqueness of the solution for problem (P2) is assured. In the second part [Table II(b)], the sufficient and necessary conditions that assure the existence of the solution in the three remaining cases are given, together with the expression of the infinite pairs of the corresponding unknown coefficients.

Next, only five of the fifteen results (corresponding to cases 3, 5, 13, 8 and 7) are proved, through the following Properties:

*Property 2 (determination of $\rho$ and $k_2$)*

Whatever the data $ho$, $\sigma$, $b$, $d>0$ and whatever the coefficients of the phase-change material $l$, $k_1$, $c_1$, $c_2>0$, problem (P2) with $\rho$ and $k_2$ unknown, has solution (3), where $\rho$ and $k_2$ are given by

$$\text{(i)}\ \rho = \frac{ho\sqrt{\pi}}{b\sigma c_2}\xi_2 f(\xi_2), \qquad \text{(ii)}\ k_2 = \frac{\sigma ho\sqrt{\pi}}{b}\frac{f(\xi_2)}{\xi_2} \tag{11}$$

being $\xi_2$ the unique solution for the equation

$$\left.\begin{array}{ll} (W_{1_0} I)(x) = h(x, A), & x>0 \\ \text{with}\quad A = \dfrac{\sigma c_1 ho}{l k_1} & \end{array}\right\} \tag{12}$$

PROOF: From (6) we obtain:

$$\rho = \frac{k_1 \xi_1^2}{\sigma^2 \lambda_1}, \qquad k_2 = \frac{k_1 c_2}{c_1}\left(\frac{\xi_1}{\xi_2}\right)^2.$$

On the other hand, from (5ii) we obtain (11i) and system (5) is equivalent to finding $\xi_1$, $\xi_2$ so that they verify

$$\frac{ho}{l}\exp(-\xi_2^2) - \frac{dk_1}{\sigma l\sqrt{\pi}}\xi_1\frac{\exp(-\xi_1^2)}{1-f(\xi_1)} = \frac{k_1}{\sigma c_1}\xi_1^2 \tag{13i}$$

$$\xi_1^2 = \frac{\sigma c_1 ho\sqrt{\pi}}{b k_1 c_2}\xi_2 f(\xi_2). \tag{13ii}$$

From (13ii) it follows that $\xi_1 = I(\xi_2)$, where $I$ is a strictly increasing positive function that verifies $I(0)=0$ and $I(+\infty)=+\infty$. Then, by replacing $\xi_2 = I^{-1}(\xi_1)$ in (13i), we obtain for $\xi_1$, equation (12). It is easy to verify that $W_1$ is a strictly increasing function that verifies $W_1(0)=0$ and $W_1(+\infty)=+\infty$, thus there exists a unique solution of equation (12), and so the property has been proved.

*Property 3 (determination of $k_2$ and $l$)*

The necessary and sufficient condition for problem (P2), with $k_2$ and $l$ unknown, to have a unique solution is that data $ho>0$, $b>0$, $d>0$, $\sigma>0$ and coefficients $\rho$, $c_1$, $c_2$, $k_1$ of the phase-change material do verify condition (R10). In such case, the solution is given by (3), where

$$\text{(i)}\quad l = \frac{Z(\xi_2)}{\rho\sigma}, \qquad \text{(ii)}\quad k = \frac{\rho\sigma^2 c_2}{\xi_2^2} \tag{14}$$

being $\xi_2$ the unique solution of equation

$$J(x) = \frac{\rho b \sigma c_2}{ho\sqrt{\pi}}, \qquad x > 0 \tag{15}$$

PROOF: Condition (5ii) is equivalent to (15), which obviously possesses a unique solution $\xi_2$. (14ii) is obtained trivially and (14i) by solving for $l$ from (5i). Since we expect to find $l > 0$, it should be $Z(\xi_2) > 0$.

As $Z$ is a strictly decreasing function,

$$Z(0) = ho - \frac{dk_1}{a_1\sqrt{\pi}} \frac{\exp(-\xi_1^2)}{1 - f(\xi_1)}, \qquad Z(+\infty) = -\frac{dk_1}{a_1\sqrt{\pi}} \frac{\exp(-\xi_1^2)}{1 - f(\xi_1)} < 0,$$

then $l > 0$ exists (and it is unique) iff

$$\begin{cases} Z(0) > 0 & \text{(i.e., (R9))} \\ \xi_2 < r_0, & \text{where } r_0 \text{ is the unique zero of } Z. \end{cases}$$

Condition $\xi_2 < r_0$ is equivalent to $\xi_2 f(\xi_2) < r_0 f(r_0)$, and, from (15), the latter is equivalent to (R10).

*Property 4 (determination of $c_1$ and $k_1$)*

The necessary and sufficient condition for problem (P2), with $c_1$ and $k_1$ unknown, to have at least one solution is that conditions (R20) and (R21) are verified. In such case, there exist infinite solutions that, for each $k_1 > 0$ have the form (3) with

$$c_1 = c_1(k_1) = \frac{k_1}{\rho\sigma^2} \xi_1^2(k_1) \tag{16}$$

where $\xi_1(k_1)$ is the unique solution of equation

$$V(x) = \frac{\rho l \sigma^2 \sqrt{\pi}}{dk_1} L(\sigma/a_2), \qquad x > 0. \tag{17}$$

PROOF: In this case, none of the two unknowns appears in (5ii). Therefore, (R20) is a necessary condition for the existence of at least one solution.

On the other hand, (5i) is equivalent to (17), which, for each $k_1 > 0$, is an equation on $\xi_1$. The necessary and sufficient condition for that equation to have a solution is

$$L\left(\frac{\sigma}{a_2}\right) > 0,$$

that is, (R21).

*Property 5 (determination of $k_1$ and $k_2$)*

The necessary and sufficient condition for problem (P2), with $k_1$ and $k_2$ unknown, to have a unique solution is that data $ho > 0$, $b > 0$, $d > 0$, $\sigma > 0$ and coefficients $\rho$, $l$, $c_1$, $c_2$ of the phase-change material do verify condition (R15). In such case, the solution is given by (3), with

$$\text{(i) } k_1 = \rho c_1 \left(\frac{\sigma}{\xi_1}\right)^2, \qquad \text{(ii) } k_2 = \rho c_2 \left(\frac{\sigma}{\xi_2}\right)^2 \tag{18}$$

where

$$\xi_2 = J^{-1}\left(\frac{\rho c_2 b \sigma}{ho\sqrt{\pi}}\right) \tag{19}$$

and $\xi_1$ is the unique solution of equation

$$Q(x) = \frac{dc_1}{l}\left[\frac{ho}{\rho l \sigma}\exp(-\xi_2^2) - 1\right]^{-1}, \quad x > 0 \tag{20}$$

PROOF: Using (6) we obtain (18) and system (5) is equivalent to finding $\xi_1 > 0$, $\xi_2 > 0$ so that they verify

$$\frac{ho}{\rho l}\exp(-\xi_2^2) - \frac{dc_1\sigma}{\rho l\sqrt{\pi}}\frac{1}{\xi_1}\frac{\exp(-\xi_1^2)}{1-f(\xi_1)} = \sigma \tag{21i}$$

$$f(\xi_2) = \frac{bc_2\sigma}{ho\sqrt{\pi}}\frac{1}{\xi_2} \tag{21ii}$$

From (21ii) it follows (19). Let us point out that $J$ is a strictly increasing function that verifies $J(0)=0$, $J(+\infty)=+\infty$. By replacing $\xi_2$ in (21i) we obtain an equation which is equivalent to (20).

Since $Q$ is a strictly increasing function with $Q(0)=0$, $Q(+\infty)=1$, equation (20) has a solution (and in this case, it is unique) iff $0<A<1$, where $A$ is the constant which appears in the second member of (20). This condition is nothing but (R15). In fact,

$$0<A<1 \Leftrightarrow \frac{1}{A}>1 \Leftrightarrow \exp(-\xi_2^2) > \frac{\rho l\sigma}{ho}\left(\frac{dc_1}{l}+1\right) \Leftrightarrow$$

$$\frac{ho}{\rho\sigma(dc_1+l)}>1, \qquad \xi_2<t\left(\frac{ho}{\rho\sigma(dc_1+l)}\right) \Leftrightarrow \text{(R15)}$$

*Property 6 (determination of $c_1$ and $c_2$)*

The necessary and sufficient condition for problem (P2), with $c_1$ and $c_2$ unknown, to have a unique solution is that data $ho>0$, $b>0$, $d>0$, $\sigma>0$ and coefficients $\rho$, $l$, $k_1$, $k_2$ of the phase-change material do verify condition (R13). In such case, the solution is given by (3), with

$$\text{(i) } c_1 = \frac{k_1}{\rho}\left(\frac{\xi_1}{\sigma}\right)^2, \qquad \text{(ii) } c_2 = \frac{k_2}{\rho}\left(\frac{\xi_2}{\sigma}\right)^2 \tag{22}$$

where

$$\xi_2 = F^{-1}\left(\frac{k_2 b}{ho\sigma\sqrt{\pi}}\right) \tag{23}$$

and $\xi_1$ is the unique solution of equation

$$V(x) = \frac{\rho l\sigma^2\sqrt{\pi}}{ck_1}\left[\frac{ho}{\rho l\sigma}\exp(-\xi_2^2)-1\right], \quad x>0. \tag{24}$$

PROOF: Using (6) we obtain (22) and system (5) becomes one of finding $\xi_1>0$, $\xi_2>0$ so that they verify

$$\frac{ho}{\rho l}\exp(-\xi_2^2) - \frac{dk_1}{\rho l\sigma\sqrt{\pi}}\xi_1\frac{\exp(-\xi_1^2)}{1-f(\xi_1)} = \sigma \tag{25i}$$

$$f(\xi_2) = \frac{k_2 b}{ho\sigma\sqrt{\pi}}\xi_2 \tag{25ii}$$

Since $F$ is a strictly decreasing function, with $F(0)=\frac{2}{\sqrt{\pi}}$, $F(+\infty)=0$, if (R7) is verified, then we can solve $\xi_2$ from equation (25ii) and we obtain (23).

Now, assuming that (R7) is verified and replacing $\xi_2$ in (25i), we obtain for $\xi_1$ an equation which is equivalent to (24). Since $V$ is a strictly increasing function with $V(0)=0$, $V(+\infty)=+\infty$, the necessary and sufficient condition for (24) to have a unique solution is that

$$\frac{ho}{\rho l\sigma}\exp(-\xi_2^2)-1>0$$

that is,

$$\xi_2<t\left(\frac{ho}{\rho l\sigma}\right), \qquad \frac{ho}{\rho l\sigma}>1$$

and this is equivalent to

$$F(\xi_2) > (F_0 t)\left(\frac{ho}{\rho l \sigma}\right), \qquad \frac{ho}{\rho l \sigma} > 1$$

that is,

$$\frac{k_2 b}{ho\sigma\sqrt{\pi}} > (F_0 t)\left(\frac{ho}{\rho l \sigma}\right), \qquad \frac{ho}{\rho l \sigma} > 1. \tag{26}$$

In short, we have proved that the necessary and sufficient condition for system (25) to have a unique solution is that (R7) and (26) are verified, that is, that (R13) is verified.

## IV. ESTIMATIONS FOR THE THERMAL COEFFICIENTS

Restrictions (R1)–(R19) are necessary and sufficient conditions for the existence and uniqueness of the various problems presented. Now, let us assume that we have a unidimensional, homogeneous, semi-infinite material, all its thermal coefficients being constant, which undergoes a phase-change process as the one described in the present paper. We can assume that any of its coefficients is unknown, for example, $c_1$. We now wonder whether restriction (R3) is satisfied or not. If we assume that the mathematical model corresponds exactly to the physical reality, then we would have an affirmative answer to our previous question, since the fact that (R3) does not occur would indicate the non-existence of $c_1$; however, coefficient $c_1$ exists and it constitutes nothing but the specific heat of the solid phase of the material we are considering. More precisely, there are two possibilities: either restriction (R3) is satisfied or the mathematical problem corresponding to the determination of $c_1$, as is presented in this paper, fits in the category of the so-called improperly-posed problems [18, 19, 25]. The same can be said in relation to any of the restrictions (R1)–(R19).

Conversely, the problems used for determining $(c_1, k_1)$, $(l, k_1)$, $(l, c_1)$ are improperly-posed problems, whether the corresponding restrictions (R20, R21, R22) are satisfied or not, since, in the cases where the corresponding restriction occurs, the problem has infinite solutions and in the cases where it does not occur, the problem has no solution. On the other hand, restrictions (R1)–(R22) can be interpreted in the following way: by using (5ii) to elminate $ho$, we obtain estimations in which the thermal coefficients $(k_1, k_2, c_1, c_2, l, \rho)$, the coefficient $\sigma$ which characterizes the free boundary, the initial temperature $-d$ and the fixed face temperature $b$ are present. We obtain estimations that can be interpreted as a priori bounds for the thermal coefficients and, in particular, for the coefficient which characterizes the free boundary. For example:

$$(\mathrm{R1}) \Leftrightarrow f(\sigma/a_2) < \frac{b}{d}\sqrt{\frac{k_2 c_2}{k_1 c_1}} \quad \text{(see (30) in [14])},$$

$$(\mathrm{R4}) \Rightarrow \frac{\sigma}{a_2} < J^{-1}(bc_2/(l + dc_1)\sqrt{\pi}),$$

$$(\mathrm{R8}) \Leftrightarrow \frac{\sigma}{a_2} < Y^{-1}(bc_2/l\sqrt{\pi}),$$

$$(\mathrm{R21}) \Leftrightarrow \frac{\sigma}{a_2} < R^{-1}(bc_2/l\sqrt{\pi}),$$

$$(\mathrm{R22}) \Leftrightarrow \frac{\sigma}{a_2} < R^{-1}(bc_2/dc_1\sqrt{\pi}).$$

We point out that the restrictions (R1)–(R22) are not all independent of each other, for example:

(i) $x_1 < x_0$, so (R4) $\Rightarrow$ (R3);
(ii) $x_1 < S_0$, so (R1) and ($R_4$) $\Rightarrow$ (R2), etc.

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## NOMENCLATURE

| | |
|---|---|
| $k$ | thermal conductivity |
| $c$ | specific heat |
| $l$ | latent heat of fusion |
| $s$ | position of phase-change location |
| $t$ | time variable |
| $x$ | space variable |
| $-d<0$ | initial temperature |
| $b>0$ | temperature of the fixed face $x=0$ |
| $\alpha=a^2=\dfrac{k}{\rho c}$ | thermal diffusivity |
| $h_0>0$ | coefficient which characterizes the heat flux of the fixed face $x=0$ |
| $T$ | temperature |
| *Greek symbols* | |
| $\rho$ | mass density |
| $\sigma$ | coefficient which characterizes $s(t)$ |
| $\xi=\sigma/a$ | dimensionless parameter |
| *Subscripts* | |
| $i=1$ | solid phase |
| $i=2$ | liquid phase |

*Functions*

$$f(x)=\operatorname{erf}(x)=\frac{2}{\sqrt{\pi}}\int_0^x \exp(-u^2)\,du, \qquad g(x)=x^2\exp(x^2),$$

$$h(x,A)=A\exp(-x^2), \qquad k(x,A)=h\left(x,\frac{h_0}{\rho(l+A)}\right)-a_2x,$$

$$L(x)=h\left(x,\frac{h_0}{\rho l\sigma}\right)-1, \qquad t(x)=(\log x)^{\frac{1}{2}},$$

$$F(x)=\frac{f(x)}{x}, \qquad G(x)=\frac{k_2b}{h_0a_1\sqrt{\pi}}\frac{x}{f(x)},$$

$$J(x)=xf(x), \qquad H(x)=\frac{h_0\sqrt{\pi}}{\rho bc_2a_1}J(x),$$

$$I(x)=\left[\frac{\sigma c_1h_0\sqrt{\pi}}{bk_1c_2}J(x)\right]^{\frac{1}{2}}, \qquad K(x)=\frac{\exp(-x^2)}{1-f(x)},$$

$$P(x,\alpha,\beta,\gamma,\delta)=\frac{h(\beta x,\alpha)}{f(\beta x)}-\gamma K(\delta x), \qquad V(x)=xK(x),$$

$$Q(x)=\sqrt{\pi}\,x\exp(x^2)(1-f(x)), \qquad U(x)=x+\frac{dk_1}{\rho la_1^2\sqrt{\pi}}K(x),$$

$$T(x)=h(x,h_0)-\frac{dk_1}{a_1\sqrt{\pi}}K\left(\frac{a_2x}{a_1}\right), \qquad W(x)=h(x,h_0)-\frac{dk_1}{\sigma\sqrt{\pi}}V\left(\left(\frac{k_2c_1}{k_1c_2}\right)^{\frac{1}{2}}x\right),$$

$$W_1(x)=x^2+\frac{dc_1}{l\sqrt{\pi}}V(x), \qquad Z(x)=h(x,h_0)-\frac{dk_1}{a_1\sqrt{\pi}}K\left(\frac{\sigma}{a_1}\right).$$