

DETERMINATION OF UNKNOWN THERMAL COEFFICIENTS
OF A SEMI-INFINITE MATERIAL FOR THE ONE-PHASE
LAME-CLAPEYRON (STEFAN) PROBLEM THROUGH THE
SOLOMON-WILSON-ALEXIADES' MUSHY ZONE MODEL

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ABSTRACT

We use the Solomon-Wilson-Alexiades' mushy zone model (Letters Heat Mass Transfer, 9(1982), 319-324) for the simultaneous determination of unknown coefficients of a semi-infinite material through a phase-change problem with an overspecified condition on the fixed face. We also find formulas for the unknown coefficients and the necessary and sufficient conditions for the existence of a solution.

1. Introduction

We consider a semi-infinite material that is initially assumed to be solid at its melting temperature 0°C without loss of generality. At time $t=0$, a constant temperature $B>0$ is imposed at $x=0$ and then fusion ensues, where three distinct regions can be distinguished (for a complete description of this model see [4]):

H1) Solid, at temperature 0°C , occupying the region $x>r(t)$.

H2) Liquid, at temperature $\theta(x,t)>0$, occupying the region $0<x<s(t)$, where $s(t)\leq r(t)$.

H3) Mushy zone, at temperature $\theta(x,t)\equiv 0$, occupying the region $s(t)\leq x\leq r(t)$. Thus, the mushy region is taken to be isothermal, we make the following two assumptions on this structure:

H3i) the material contains a fixed fraction εl ($0<\varepsilon<1$) of the total latent heat l , i.e.,

$$(1) \quad -k\theta_x(s(t),t) = \rho l [(1-\varepsilon)\dot{s}(t) + \varepsilon\dot{r}(t)], \quad t>0$$

H3ii) its width is inversely proportional to the temperature gradient, i.e.,

$$(2) \quad -\theta_x(s(t), t) (r(t) - s(t)) = \gamma > 0, \quad t > 0.$$

From now on we denote one of the four coefficients k , ρ , ℓ , c of a given material with the words 'thermal coefficient'.

Let us suppose that one or two thermal coefficients of the liquid phase of some given semi-infinite material are unknown (For the solid phase we can consider a solidification process instead of a fusion process which has an analogous formulation). If by means of a phase-change experiment (fusion of the material at its melting temperature) we are able to measure certain quantities (see further), then we shall find formulas for the simultaneous determination of the unknown coefficients. We shall consider a (direct or inverse) one-phase Lamé-Clapeyron problem (or one-phase Stefan problem with constant thermal coefficients) [1,2,3] with an overspecified condition on the fixed face $x=0$ (See more details and references on this subject in [5]). This overspecified condition can be either the specification of the heat flux [5]

$$(3) \quad k\theta_x(0, t) = - \frac{h_0}{\sqrt{t}}, \quad t > 0 \quad (h_0 > 0)$$

or the temperature gradient [6]

$$(3 \text{ bis}) \quad \theta_x(0, t) = - \frac{H_0}{\sqrt{t}}, \quad t > 0 \quad (H_0 > 0)$$

through the fixed face $x=0$ of the material undergoing the phase-change process.

We shall prove that the different problems posed in the next sections for the determination of several unknown coefficients do not always have an explicit solution. Moreover, it does exist iff some complementary conditions for the corresponding data are verified.

2. Determination of One Thermal Coefficient

We shall consider two cases for the determination of one of the four coefficients k , ρ , ℓ , c .

The first one will deal with the simultaneous determination of the two free boundaries $s(t)$ and $r(t)$, and the second will deal with the simultaneous determination of the coefficients ϵ and γ .

2.1. First Case

Problem P1. We shall find the functions $s=s(t)>0$ and $r=r(t)>s(t)$, defined for $t>0$ with $r(0)=s(0)=0$; the temperature $\theta=\theta(x,t)$ of the liquid phase, defined for $0<x<s(t)$, $t>0$ and one of the four thermal coefficients k, ρ, l, c of the phase-change material so that they satisfy the conditions (1)-(7) where

$$\begin{aligned} (4) \quad a^2 \theta_{xx} &= \theta_t, \quad 0 < x < s(t), \quad t > 0 \quad (a^2 = \frac{k}{\rho c}) \\ (5) \quad \theta(0,t) &= B > 0, \quad t > 0; \quad (6) \quad \theta(s(t),t) = 0, \quad t > 0 \\ (7) \quad s(0) &= r(0) = 0, \end{aligned}$$

Where $h_0 > 0$, $B > 0$, $\gamma > 0$ and $0 < \epsilon < 1$ are data and must be known or determined by an experience of change of phase.

The solution of problem (1)-(7) is given by

$$\begin{aligned} (8) \quad \theta(x,t) &= B - \frac{B}{F(\xi)} f\left(\frac{x}{2a\sqrt{t}}\right) \\ (9) \quad s(t) &= 2a\xi\sqrt{t}, \quad (10) \quad r(t) = 2a\mu\sqrt{t} \end{aligned}$$

where the three unknown coefficients ξ, μ and one of the four thermal coefficients k, ρ, l, c satisfy the following system of equations

$$\begin{aligned} (11) \quad \mu &= \xi + \frac{\gamma\sqrt{\pi}}{2B} f(\xi) \exp(\xi^2) \\ (12) \quad F(\xi) &= \frac{cB}{l\sqrt{\pi}}, \quad (13) \quad f(\xi) = \frac{B}{h_0} \frac{\sqrt{k\rho c}}{\sqrt{\pi}} \end{aligned}$$

with

$$\begin{aligned} (14) \quad f(x) &= \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt \\ (15) \quad F(x) &= xf(x)\exp(x^2) + \frac{\epsilon\gamma\sqrt{\pi}}{2B} [f(x)\exp(x^2)]^2. \end{aligned}$$

Since condition (11) expresses μ in function of the element ξ , the two remaining unknown ξ and one of the four thermal coefficients k, ρ, l, c must satisfy the conditions (12) and (13). Then, we obtain the following Property

Property 1. Whatever the data $h_0 > 0$, $B > 0$, $\gamma > 0$, $0 < \epsilon < 1$ we have the following result:

The necessary and sufficient condition for problem P1 with c unknown to have a unique solution is that the coefficients $k, \rho, \ell > 0$ of the phase-change material do verify the condition

$$(16) \quad 1 + \frac{\epsilon \gamma}{B} < \frac{2 h_0^2}{\rho \ell k B}.$$

In such case, the solution is given by (8)-(10), where μ is given by (11), c is given by

$$(17) \quad c = \frac{\pi h_0^2}{k \rho B^2} f^2(\xi)$$

and ξ is the unique solution of the equation

$$(18) \quad G(x) = \frac{h_0^2 \sqrt{\pi}}{\rho \ell k B}, \quad x > 0$$

where function G is defined, for $x > 0$, by the expression

$$(19) \quad G(x) = \frac{F(x)}{f^2(x)}.$$

Moreover, for the problem P1 with k or ρ or ℓ unknown we have analogous results.

2.2. Second Case

Problem P2. We suppose that the two moving boundaries are given by

$$(20) \quad s(t) = 2\sigma\sqrt{t}, \quad r(t) = 2\omega\sqrt{t}, \quad \text{with } 0 < \sigma < \omega.$$

The problem lies in finding the temperature $\theta = \theta(x, t)$ of the liquid phase (defined for $0 < x < s(t)$, $t > 0$), the two coefficients ϵ and γ which characterize the mushy region, and one of the four thermal coefficients k, ρ, ℓ, c of the phase-change material so that they satisfy the conditions (1)-(6), where $h_0 > 0$, $B > 0$, $0 < \sigma < \omega$ are data.

We define

$$(21) \quad \xi = \frac{\sigma}{a}, \quad a = \frac{\sqrt{k}}{\sqrt{\rho c}}$$

which is known or unknown iff ℓ is unknown or known, respectively. Then the temperature θ of the problem P2 is given by (8) and the three unknown coefficients must satisfy the following conditions:

$$(22) \quad \gamma = \frac{2B}{\sigma\sqrt{\pi}} (\omega - \sigma) \frac{\exp(-\xi^2)}{f_2(\xi)}$$

$$(23) \quad \sigma + \varepsilon(\omega - \sigma) = \frac{cB\sigma}{\ell\sqrt{\pi}} \frac{\exp(-\xi^2)}{f_1(\xi)}, \quad (24) \quad f_2(\xi) = \frac{kB}{\sigma h_0 \sqrt{\pi}}$$

where functions f_1 and f_2 are defined for $x > 0$, by the expressions

$$(25) \quad f_1(x) = xf(x), \quad f_2(x) = \frac{f(x)}{x}.$$

Since condition (22) expresses γ in function of the element ξ , the two remaining unknown ε and ξ (or ℓ) must satisfy conditions (23) and (24). Then, we obtain the following Property

Property 2. Whatever the data $h_0 > 0$, $B > 0$, $0 < \sigma < \omega$, we have the following result:

The necessary and sufficient condition for problem P2, with c unknown, to have a unique solution is that the coefficients $k, \ell, \rho > 0$ of the phase-change material do verify the conditions

$$(26) \quad f_2(\sqrt{\log Z_0}) < \frac{kB}{\sigma h_0 \sqrt{\pi}} < f_2(\sqrt{\log Y_0}) \quad \text{if } Y_0 > 1$$

or

$$(27) \quad \begin{cases} f_2(\sqrt{\log Z_0}) < \frac{kB}{\sigma h_0 \sqrt{\pi}} < \frac{2}{\sqrt{\pi}} \\ Z_0 > 1 \end{cases} \quad \text{if } Y_0 < 1$$

where Z_0 and Y_0 are given by

$$(28) \quad Z_0 = \frac{h_0}{\rho \ell \sigma}, \quad Y_0 = \frac{h_0}{\rho \ell \omega}.$$

In such case, the temperature is given by (8), γ is given by (22), ε and c are given by

$$(29) \quad \varepsilon = \frac{\frac{h_0}{\rho l \sigma} \exp(-\xi^2) - 1}{(\omega/\sigma) - 1}, \quad c = \frac{k}{\rho \sigma^2} \xi^2$$

where ξ is the unique solution of the equation

$$(30) \quad f_2(x) = \frac{kB}{\sigma h_0 \sqrt{\pi}}, \quad x > 0.$$

Moreover, for the problem P2 with k or l or ρ unknown we have analogous results.

Proof. The coefficient c is obtained from (21) and the element ξ is given as the solution of equation (30) iff the data verify the condition

$$(31) \quad \frac{kB}{\sigma h_0 \sqrt{\pi}} < \frac{2}{\sqrt{\pi}}.$$

From the expression for $c=c(\xi)$ and condition (23) we obtain, for ε , the expression (29). Then we have:

$$(32) \quad \begin{aligned} \varepsilon > 0 &\Leftrightarrow \xi < \sqrt{\log Z_0}, \quad Z_0 > 1 \quad \Leftrightarrow \\ f_2(\sqrt{\log Z_0}) &< f_2(\xi) = \frac{kB}{\sigma h_0 \sqrt{\pi}}, \quad Z_0 > 1 \end{aligned}$$

because the function f_2 is a decreasing one for $x > 0$, and

$$(33) \quad \varepsilon < 1 \Leftrightarrow Y_0 = \frac{h_0}{\rho l \omega} < \exp(\xi^2).$$

In case $Y_0 < 1$, the condition (33) is always verified and in case $Y_0 > 1$, we have

$$(34) \quad \varepsilon < 1 \Leftrightarrow \frac{kB}{\sigma h_0 \sqrt{\pi}} < f_2(\sqrt{\log Y_0}), \quad Y_0 > 1.$$

Since

$$(35) \quad f_2(x) < \frac{2}{\sqrt{\pi}}, \quad \forall x > 0$$

we deduce the thesis.

3. Determination of Two Thermal Coefficients

Similarly to what we have previously done, we suggest the following problem.

Problem P3. We suppose that the moving boundary $s(t)$ is given

$$(36) \quad s(t) = 2\sigma\sqrt{t}, \quad \sigma > 0.$$

The problem lies in finding the temperature $\theta = \theta(x, t)$ of the liquid phase, defined for $0 < x < s(t)$, $t > 0$; the free boundary $r(t)$ which characterizes the mushy zone defined for $t > 0$ with $r(0) = 0$ and $r(t) > s(t)$ for $t > 0$; and two of the four thermal coefficients k , ρ , ℓ , c of the phase-change material so that they satisfy the conditions (1)-(6), where $h_0 > 0$, $B > 0$, $\sigma > 0$, $\gamma > 0$ and $0 < \epsilon < 1$ are data.

We define ξ by (21) which is unknown iff one of the three thermal coefficients k , ρ , ℓ , c is unknown. Then the temperature θ of the problem P3 is given by (8), the free boundary r is given by

$$(37) \quad r(t) = 2\omega\sqrt{t}, \quad \omega > 0,$$

and the three unknown coefficients (ω and two of the four thermal coefficients k , ρ , ℓ , c) must satisfy conditions (24), (38) and (39) where

$$(38) \quad \omega = \sigma \left(1 + \frac{\gamma}{B} T(\xi) \right) \quad (39) \quad \frac{h_0}{\rho \ell \sigma} \exp(-\xi^2) = 1 + \frac{\epsilon \gamma}{B} T(\xi)$$

with the function $T = T(x)$ is defined for $x > 0$ by

$$(40) \quad T(x) = \frac{\sqrt{\pi}}{2} f_2(x) \exp(x^2).$$

Since condition (38) expresses ω in function of the element ξ and other data, the two remaining unknown coefficients must satisfy conditions (24) and (39). Then we obtain the following Property

Property 3. Whatever the data $h_0 > 0$, $B > 0$, $\sigma > 0$, $\gamma > 0$, $0 < \epsilon < 1$, we have the following result:

The necessary and sufficient condition for problem P3, with k and c unknown, to have a unique solution is that the coef-

ficients $\rho, l > 0$ of the phase-change material do verify the conditions

$$(41) \quad \frac{h_0}{\rho l \sigma} > 1 + \frac{\epsilon \gamma}{B} .$$

In such case, the temperature is given by (8), ω is given by (38), k and c are given by

$$(42) \quad k = \frac{\sigma h_0 \sqrt{\pi}}{B} f_2(\xi) , \quad c = \frac{\sqrt{\pi} h_0}{\rho B \sigma} f(\xi) \xi$$

where ξ is the unique solution of equation

$$(43) \quad 1 + \frac{\epsilon \gamma}{B} T(x) = \frac{h_0}{\rho l \sigma} \exp(-x^2) , \quad x > 0 .$$

Moreover, for the problem P3 with $\{k, l\}$ or $\{k, \rho\}$ or $\{l, c\}$ or $\{l, \rho\}$ or $\{\rho, c\}$ unknown we have analogous results.

Remark 1. We may pose a new problem P'3, analogous to that of problem P3, where $r(t)$ now turns out to be a datum and $s(t)$ an unknown.

The results of both problem P3 or P'3 may be of practical interest if we can determine accurately one of the two boundaries through a phase-change experiment and we want to calculate where the other boundary is located.

Remark 2. When the thermal conductivity is unknown a new variant can be proposed for the determination of coefficients of a semi-infinite material [6]. If we replace condition (3) by (3bis), we can consider problem (P1bis), (P2bis), (P3bis), k always being an unknown coefficient. We can use a similar method to the one developed before so we would not include it here.

For the calculation H_0 , it is necessary to obtain the experimental determination of the temperature gradient on the fixed face $x=0$ with condition (5) of constant temperature. On the other hand, according to condition (3), the experimental determination of the heat flow in $x=0$ is necessary for the calculation of the coefficient h_0 . It is held that this new variant may, to some extent, simplify the experimental results for the application of the present method.

4. Determination of Other Coefficients

There exist two constants $0 < \varepsilon < 1$ and $\gamma > 0$ defined in the Solomon-Wilson-Alexiades' model. It is our interest to compute γ or ε through an experience of phase-change with an overspecified condition (3) on the fixed face, i.e., to find formulas for $\{\theta, r, s, \gamma\}$ or $\{\theta, s, r, \varepsilon\}$. We obtain the following results

Property 4

The necessary and sufficient condition for determining that $\{\theta(x, t), s(t), r(t), \gamma\}$ has a unique solution is that the data $h_0 > 0$, $B > 0$, $0 < \varepsilon < 1$ and the coefficients k, ρ, ℓ, c of the phase-change material do verify the condition

$$(44) \quad \frac{kB}{ah_0\sqrt{\pi}} < f(U^{-1}(\frac{cah_0}{k\ell})) ,$$

where

$$(45) \quad U(x) = x \exp(x^2) , \quad U^{-1} \text{ inverse function of } U \text{ for } x > 0.$$

In such case, the temperature θ is given by (8), $s(t)$ is given by (9), $r(t)$ is given by (10), γ and μ are respectively given by

$$(46) \quad \gamma = \frac{2ah_0}{k\varepsilon} \left[\frac{cah_0}{k\ell} \exp(-\xi^2) - \xi \right] \exp(-\xi^2)$$

$$(47) \quad \mu = \xi + \frac{1}{\varepsilon} \left[\frac{cah_0}{k\ell} \exp(-\xi^2) - \xi \right]$$

where ξ is the unique solution of the equation

$$(48) \quad f(x) = \frac{B}{h_0} \frac{\sqrt{k\rho c}}{\sqrt{\pi}} , \quad x > 0 .$$

Moreover, for the other case with ε unknown we have analogous results.

A longer version of this paper can be requested to the author.

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Nomenclature

$a = \frac{k}{\rho c}$	thermal diffusivity
B	temperature on the fixed face $x=0$
c	specific heat
$-C < 0$	initial temperature
h_0	coefficient defined by (3)
H_0	coefficient defined by (3bis)
k	thermal conductivity
l	latent heat of fusion
r	mushy zone-solid interface
s	mushy zone-liquid interface
t	time variable
x	spatial variable

Greek Symbols

γ	coefficient defined by (2)
ϵ	coefficient defined by (1)
σ	coefficient which characterizes the boundary s by (20) or (36)
μ	coefficient which characterizes the boundary r by (10)
ρ	mass density
θ	temperature
$\xi = \frac{\sigma}{a}$	dimensionless parametre defined by (21) and the coefficient which characterizes the boundary s by (9)
ω	coefficient which characterizes the boundary r by (20)

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