Computational Modelling of Free and Moving Boundary Problems II

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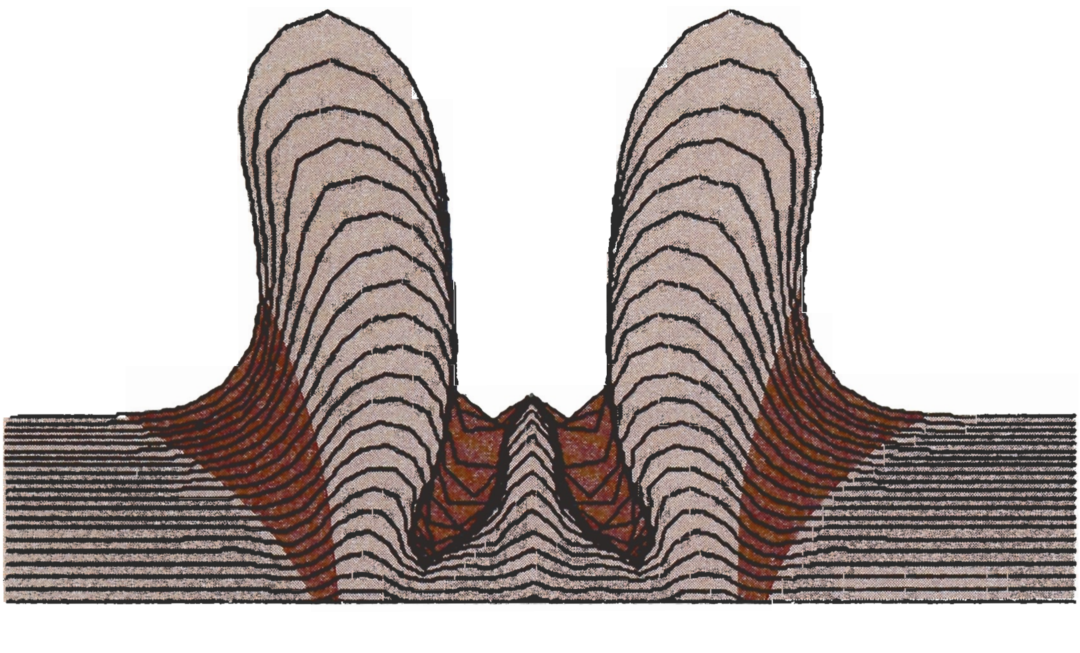

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On the determination of the unknown coefficients through phase change problems with temperature-dependent thermal conductivity

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ABSTRACT

We study the determination of unknown thermal coefficient of a semi-infinite material through a phase-change process with an overspecified condition on the fixed face with temperature-dependent thermal conductivity. We determine necessary and sufficient conditions on data in order to obtain the existence of the solution. We also give formulae for the unknown coefficients.

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 [3] with a large bibliography.

We consider the following solidification problem for a semi-infinite material with an overspecified condition on the fixed face :

$$\left|\begin{array}{ll} \rho\, c\, T_t = (\, k(T)\, T_x\,)_x \;, & 0 < x < s(t) \;, \; t > 0, \\ s(0) = 0 \;, & \qquad (1) \\ T(0,t) = T_o < T_f \;,\; t > 0 \;, & \end{array}\right.$$

$$
\begin{cases}
T(s(t),t) = T_f \ , t > 0 \ , \\
k(T_f)\, T_x(s(t),t) = \rho\, h\, \dot{s}(t) \ , \ t > 0 \ , \\
k(T_o)\, T_x(0,t) = \frac{q_o}{\sqrt{t}} \ , \ t > 0 \ ,
\end{cases}
\tag{1}
$$

where $T = T(x,t)$ is the temperature of the solid phase, $\rho > 0$ is the density of mass, $h > 0$ is the latent heat of fusion by unity of mass, $c > 0$ is the specific heat, $x = s(t)$ is the phase-change interface, T_f is the phase-change temperature (T_o is a reference temperature), $k = k(T) = k_o[1 + \beta(T - T_o)/(T_f - T_o)]$ [1,2] is the thermal conductivity, $\alpha_o = k_o/\rho c$ is the diffusion coefficient to the reference temperature $T = T_o$, and coefficients $\beta > 0, q_o > 0$.

In [4,5] one or two thermal coefficients for the case $k = k_o$ (i.e. $\beta \equiv 0$) were determined, and formulae for the unknown coefficients were given.

The goal of the present paper is to consider the general case $\beta \neq 0$. The problem consists of finding β and two other unknown elements among k_o, c, ρ, h and $s(t)$. Moreover, the coefficients $q_o > 0$ (which characterizes the heat flux at the fixed face $x = 0$) and $T_o > 0$ (which is the temperature at the fixed face $x = 0$) must be found through the experimental phase-change process.

The solution is given by :

$$
\begin{cases}
T(x,t) = T_o + (T_f - T_o)\, \frac{\Phi_\delta(\eta)}{\Phi_\delta(\lambda)} \ , \quad \eta = \frac{x}{2\sqrt{\alpha_o t}} \quad (\text{with } \delta > -1) \ , \ 0 < \eta < \lambda \\
s(t) = 2\,\sigma \sqrt{t} = 2\,\lambda \sqrt{\alpha_o t} \ , \qquad \sigma = \lambda \sqrt{\alpha_o} = \lambda \sqrt{\frac{k_o}{\rho c}} \ ,
\end{cases}
\tag{2}
$$

where the unknown coefficients must satisfy the following system of equations :

$$
\begin{cases}
\beta = \delta\, \Phi_\delta(\lambda) \ , \\
[1 + \delta\, \Phi_\delta(\lambda)]\, \frac{\Phi_\delta{}'(\lambda)}{\lambda\, \Phi_\delta(\lambda)} = \frac{2}{Ste} \ , \\
\frac{\Phi_\delta{}'(0)}{\Phi_\delta(\lambda)} = \frac{2\, q_o}{(T_f - T_o)\sqrt{k_o \rho c}} \ ,
\end{cases}
\tag{3}
$$

where $Ste = \frac{c(T_f - T_o)}{h} > 0$ is the Stefan number and $\Phi = \Phi_\delta = \Phi_\delta(x)$ is the error modified function which is the unique solution of the following value boundary problem :

$$
\begin{cases}
[(1 + \delta\, y(x))\, y'(x)]' + 2\, x\, y'(x) = 0 \\
y(0^+) = 0 \ , \ y(+\infty) = 1 \ .
\end{cases}
\tag{4}
$$

We suppose that $\delta > -1$ is a known real number. Function Φ verifies the following conditions

$$\Phi(0^+) = 0 \ , \ \Phi(+\infty) = 1 \ , \ \Phi' > 0 \text{ and } \Phi'' < 0 \, . \tag{5}$$

For $\delta = 0$, function $\Phi = \Phi_o$ is the classical error function given by

$$\Phi_o(x) = \operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-u^2)\, du \ , \tag{6}$$

which is utilized in [4, 5] for the determination of unknown thermal coefficients.

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

$$q_o = t^{1/2} k(T_o) T_x(0,t) \ (\, t^{1/2} \text{ times heat flux in } x=0 \text{ at time } t) \ \text{ for all } t>0 \ ,$$

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

through a discrete number of measurement at time $t_1, t_2, \ldots, t_n$ of the corresponding quantities.

We shall give necessary and sufficient conditions to obtain a solution of the above type and we also give formulae for the unknown thermal coefficients in ten different cases :

Case 1 : Determination of the unknown coefficients β, λ, k_o ;
Case 2 : Determination of the unknown coefficients β, λ, ρ ;
Case 3 : Determination of the unknown coefficients β, λ, h ;
Case 4 : Determination of the unknown coefficients β, λ, c ;
Case 5 : Determination of the unknown coefficients β, ρ, k_o ;
Case 6 : Determination of the unknown coefficients β, c, k_o ;
Case 7 : Determination of the unknown coefficients β, h, k_o ;
Case 8 : Determination of the unknown coefficients β, ρ, c ;
Case 9 : Determination of the unknown coefficients β, ρ, h ;
Case 10 : Determination of the unknown coefficients β, c, h .

In the Table 1 (see below) we give, case by case, the formulae for the unknown thermal coefficients and the restriction for the data to obtain the solution of the corresponding problem.

In order to simplify the building of the Table 1, let us consider the following restrictions (which is the necessary and sufficient condition for the existence and unicity of the solution) :

$$\frac{(T_f - T_o)}{2q_o}\,\Phi'(0)\,\sqrt{\rho c k_o} < 1\,, \tag{R_1}$$

$$\frac{\rho h k_o (T_f - T_o)}{2q_o^2} < 1\,, \tag{R_2}$$

$$\frac{\rho h \sigma}{q_o} < 1\,, \tag{R_3}$$

$$\frac{k_o (T_f - T_o)}{2\sigma q_o} < 1\,. \tag{R_4}$$

We also consider the following six functions, defined by $x > 0$:

$$\begin{aligned} &F_1(x) = 1 + \delta\,\Phi(x)\,, && F_2(x) = \frac{x\,\Phi(x)}{\Phi'(x)}\,, \\ &F_3(x) = [1 + \delta\,\Phi(x)]\,\Phi'(x)\,, && F_4(x) = x\,\Phi(x)\,, \\ &F_5(x) = \frac{\Phi(x)}{x}\,, && F_6(x) = \frac{x}{\Phi(x)} = \frac{1}{F_5(x)}\,, \end{aligned} \tag{7}$$

which satisfy the following conditions :

$$\begin{aligned} &F_1(0^+) = 1\,,\; F_1(+\infty) = 1+\delta\,, \\ &F_1{}' > 0 \text{ for } \delta > 0 \text{ and } F_1{}' < 0 \text{ for } -1<\delta<0, \\ &F_2(0^+) = 0\,,\; F_2(+\infty) = +\infty\,,\; F_2{}' > 0\,, \\ &F_3(0^+) = \Phi'(0) > 0\,,\; F_3(+\infty) = 0\,,\; F_3{}' < 0\,, \\ &F_4(0^+) = 0\,,\; F_4(+\infty) = +\infty\,,\; F_4{}' > 0\,, \\ &F_5(0^+) = \Phi'(0) > 0\,,\; F_5(+\infty) = 0\,,\; F_5{}' < 0\,, \\ &F_6(0) = \frac{1}{\Phi'(0)} > 0\,,\; F_6(+\infty) = +\infty\,,\; F_6{}' > 0\,, \end{aligned} \tag{8}$$

Case No.	Unknown coefficients	Restriction	Solution (In all cases β is given by $\beta = \delta\,\Phi_\delta(\lambda)$)
1	β, λ, k_o	–	$k_o = \frac{4 q_o^2}{\rho c (T_f - T_o)^2} \frac{\Phi^2(\lambda)}{\left(\Phi'(0)\right)^2}$ where λ is the unique solution of the equation $F_1(x) = \frac{2}{Ste} F_2(x)\,,\ x > 0\,.$
2	β, λ, ρ	–	$\rho = \frac{4 q_o^2}{c k_o (T_f - T_o)^2} \frac{\Phi^2(\lambda)}{\left(\Phi'(0)\right)^2}$ where λ is given as in Case 1 .
3	β, λ, h	R_1	$h = \frac{c(T_f - T_o)}{2} \frac{\Phi'(\lambda)}{\lambda\,\Phi(\lambda)} [1 + \delta\,\Phi(\lambda)]$ where λ is the unique solution of the equation $\Phi(x) = \frac{(T_f - T_o)}{2 q_o} \Phi'(0) \sqrt{\rho c k_o}\,,\ x > 0\,.$
4	β, λ, c	R_2	$c = \frac{4 q_o^2}{\rho k_o (T_f - T_o)^2} \frac{\Phi^2(\lambda)}{\left(\Phi'(0)\right)^2}$ where λ is the unique solution of the equation $F_3(x) = \frac{\rho h k_o (T_f - T_o)}{2 q_o^2} \left(\Phi'(0)\right)^2 F_6(x),\ x > 0.$
5	β, ρ, k_o	–	$\rho = \frac{2 q_o}{\sigma c (T_f - T_o)} \frac{\lambda\,\Phi(\lambda)}{\Phi'(0)}$ $k_o = \frac{2 \sigma q_o}{T_f - T_o} \frac{\Phi(\lambda)}{\lambda\,\Phi'(0)}$ where λ is given as in Case 1 .
6	β, c, k_o	R_3	k_o is given as in Case 5 $c = \frac{2 q_o}{\rho\,\sigma (T_f - T_o)} \frac{\lambda\,\Phi(\lambda)}{\Phi'(0)}$ where λ is the unique solution of the equation $F_3(x) = \frac{\rho h \sigma}{q_o} \Phi'(0)\,,\ x > 0\,.$

Case No.	Unknown coefficients	Restriction	Solution (In all cases β is given by $\beta = \delta\,\Phi_\delta(\lambda)$)
7	β, h, k_o	—	h is given as in Case 3 $k_o = \frac{\rho c \sigma^2}{\lambda^2}$ where λ is the unique solution of the equation $F_4(x) = \frac{\rho c \sigma (T_f - T_o)}{2 q_o} \Phi'(0)$, $x > 0$.
8	β, ρ, c	R_4	$c = \frac{2h}{T_f - T_o} \frac{\lambda \Phi(\lambda)}{\Phi'(\lambda)} \frac{1}{1 + \delta \Phi(\lambda)}$ $\rho = \frac{\lambda k_o (T_f - T_o)}{2 h \sigma^2} \frac{\Phi'(\lambda)\,[1 + \delta\Phi(\lambda)]}{\Phi(\lambda)}$ where λ is the unique solution of the equation $F_5(x) = \frac{k_o (T_f - T_o)}{2 \sigma q_o} \Phi'(0)$, $x > 0$.
9	β, ρ, h	R_4	h is given as in Case 3 $\rho = \frac{k_o \lambda^2}{c \sigma^2}$ where λ is given as in Case 8 .
10	β, c, h	R_4	$h = \frac{k_o (T_f - T_o)}{2 \rho \sigma^2} [1 + \delta\Phi(\lambda)] \frac{\lambda \Phi'(\lambda)}{\Phi(\lambda)}$ $c = \frac{k_o \lambda^2}{\rho \sigma^2}$ where λ is given as in Case 8 .

Table 1. Restrictions and formulae for the unknown thermal coefficients.

SOLUTION

Now we shall only prove the following properties for case 4 (determination of coefficients β, λ, c) and case 6 (determination of coefficients β, k_o, c).

Property 1.— The necessary and sufficient condition with β, λ and c unknown to obtain a unique solution is that data $q_o > 0$, $T_f > T_o$, $\delta > -1$ and coefficients $k_o > 0$, $h > 0$, $\rho > 0$ of the phase-change material verify condition (R_2). In such a case, the solution is given by (2) and

$$\beta = \delta\,\Phi(\lambda)\,, \tag{9}$$

$$c = \frac{4q_o^2}{\rho\,k_o(T_f - T_o)^2}\,\frac{\Phi^2(\lambda)}{\left(\Phi'(0)\right)^2}\,, \tag{10}$$

and $\lambda > 0$ is the unique solution of the equation :

$$F_3(x) = \frac{\rho\,h\,k_o(T_f - T_o)}{2q_o^2}\left(\Phi'(0)\right)^2 F_6(x)\ ,\ x > 0. \tag{11}$$

Proof.— The first and third equations in (3) give us the expression (9) for β and (10) for c respectively. From (10), the properties of functions F_3 and F_6 , and the second equation in (3) we obtain the equation (11) which has a unique solution $\lambda > 0$ if and only if

$$F_3(0^+) = \Phi'(0) > \frac{\rho\,h\,k_o(T_f - T_o)}{2q_o^2}\,F_6(0^+)\,, \tag{12}$$

i.e. (R_2).

Property 2.— The necessary and sufficient condition with β, k_o and c unknown to obtain a unique solution is that data $q_o > 0$, $T_f > T_o$, $\sigma > 0$, $\delta > -1$ and coefficients $h > 0$, $\rho > 0$ of the phase-change material verify condition (R_3). In such a case, the solution is given by (2), β is given by (9) and

$$k_o = \frac{2\sigma q_o}{T_f - T_o}\,\frac{\Phi(\lambda)}{\lambda\,\Phi'(0)}\,, \tag{13}$$

$$c = \frac{2q_o}{\rho\sigma(T_f - T_o)}\,\frac{\lambda\,\Phi(\lambda)}{\Phi'(0)}\,, \tag{14}$$

where $\lambda > 0$ is the unique solution of the equation :

$$F_3(x) = \frac{\rho h \sigma}{q_0} \Phi'(0) \quad , \ x > 0. \tag{15}$$

Proof.— The expression for β is given by the first equation in (3). Owing to σ is known we get

$$\lambda = \sigma \sqrt{\frac{\rho c}{k_0}} \quad , \tag{16}$$

i.e.

$$c = \frac{\lambda^2 k_0}{\rho \sigma^2} . \tag{17}$$

From (17) and the third equation in (3) we obtain the expression (12) for k_0. Then, by using (13) and (17) we have (14). Now, the second equation in (3) gives us the equation (15) for λ, which has a unique solution $\lambda > 0$ if and only if

$$F_3(0^+) = \Phi'(0) \ > \ \frac{\rho h \sigma}{q_0} \ \Phi'(0) \ , \tag{18}$$

i.e. (R_3).

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