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THE DETERMINATION OF UNKNOWN THERMAL COEFFICIENTS THROUGH PHASE CHANGE PROCESS 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 due to 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 [8] with a large bibliography.

We consider the following solidification problem for a semi-infinite material with an overspecified condition on the fixed face [1, 3, 4, 6]:

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

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), $k = k(T) = k_o\,[1 + \beta\,(T - T_o)/(T_f - T_o)]$ [5, 7] is the thermal conductivity, $\alpha_o = k_o/\rho c$ is the diffusion coefficient to the reference temperature $T = T_o$, and coefficients $\beta > 0$, $q_o > 0$.

The phase-change process with temperature dependent thermal conductivity was firstly studied in [5]. In [9, 10] 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 in 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 [2].

The solution is given by :

$$T(x,t) = T_o + (T_f - T_o)\frac{\Phi_\delta(\eta)}{\Phi_\delta(\lambda)}\ , \quad \eta = \frac{x}{2\sqrt{\alpha_o t}} \quad (\text{with } \delta > -1)\ , \quad 0 < \eta < \lambda \tag{2}$$

$$s(t) = 2\,\sigma\,\sqrt{t} = 2\,\lambda\,\sqrt{\alpha_o t}\ , \qquad \sigma = \lambda\,\sqrt{\alpha_o} = \lambda\,\sqrt{\frac{k_o}{\rho c}}\ , \tag{3}$$

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

$$\beta = \delta\,\Phi_\delta(\lambda)\ , \tag{4}$$

$$[1 + \delta\,\Phi_\delta(\lambda)]\,\frac{\Phi'_\delta(\lambda)}{\lambda\,\Phi_\delta(\lambda)} = \frac{2}{\mathrm{Ste}}\ , \tag{5}$$

$$\frac{\Phi'_\delta(0)}{\Phi_\delta(\lambda)} = \frac{2\,q_o}{(T_f - T_o)\,\sqrt{k_o \rho c}}\ , \tag{6}$$

where $\mathrm{Ste} = \dfrac{c(T_f - T_o)}{h} > 0$ 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 :

$$\begin{cases} [(1 + \delta\,y(x))\,y'(x)]' + 2\,x\,y'(x) = 0 \\ y(0^+) = 0\ ,\ \ y(+\infty) = 1\ . \end{cases} \tag{7}$$

From now on we suppose that $\delta > -1$ is a given real number. Function Φ verifies the following conditions

$$\Phi(0^+) = 0\ ,\ \ \Phi(+\infty) = 1\ ,\ \ \Phi' > 0 \ \text{ and } \ \Phi'' < 0\ . \tag{8}$$

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

$$\Phi_o(x) = \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-u^2)\,du\ , \tag{9}$$

which was utilized in [9, 10] 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 :

$q_o = t^{1/2}\,k(T_o)\,T_x(0,t)$ ($t^{1/2}$ times heat flux in $x = 0$ at time t) 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 $t_1, t_2, \dots, t_n$ of the corresponding quantities. In [2] this method was indicated in order to apply the formulae obtained in [9, 10].

We shall give necessary and sufficient conditions to obtain a solution of the above type (2), (3) 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 .

We remark that cases 1 to 4 correspond to a free boundary problem (the phase-change interface, i.e. coefficient λ, is unknown) and cases 5 to 10 correspond to a moving boundary problem (the phase-change interface is given by $s(t) = 2\sigma\sqrt{t}$ with $\sigma > 0$ [6, 8]).

In order to 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, let us consider the following restrictions (which can be considered as the necessary and sufficient condition for the existence and uniqueness of the solution for some particular cases):

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

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

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

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

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

$$\left| \begin{array}{lll} F_1(x) = 1 + \delta\Phi(x) \ , & F_2(x) = \dfrac{x\Phi(x)}{\Phi'(x)} \ , & F_3(x) = [1 + \delta\Phi(x)]\,\Phi'(x) \ , \\ F_4(x) = x\Phi(x) \ , & F_5(x) = \dfrac{\Phi(x)}{x} \ , & F_6(x) = \dfrac{x}{\Phi(x)} = \dfrac{1}{F_5(x)} \ , \end{array} \right. \tag{10}$$

which satisfy the following properties :

$$
\begin{array}{l}
F_1(0^+) = 1 \ , \ F_1(+\infty) = 1+\delta \ , \qquad F_1' > 0 \text{ for } \delta > 0 \text{ and } F_1' < 0 \text{ for } -1 < \delta < 0 , \\
F_2(0^+) = 0 \ , \ F_2(+\infty) = +\infty \ , \ F_2' > 0 \ ; \quad F_3(0^+) = \Phi'(0) > 0 \ , \ F_3(+\infty) = 0 \ , \ F_3' < 0 \ , \\
F_4(0^+) = 0 \ , \ F_4(+\infty) = +\infty \ , \ F_4' > 0 \ ; \quad F_5(0^+) = \Phi'(0) > 0 \ , \ F_5(+\infty) = 0 \ , \ F_5' < 0 \ , \\
F_6(0) = \dfrac{1}{\Phi'(0)} > 0 \ , \ F_6(+\infty) = +\infty \ , \ F_6' > 0 \ .
\end{array} \tag{11}
$$

Solution

Now we shall only prove the following properties corresponding to cases 1 (determination of coefficients β, λ, k_o), 3 (determination of coefficients β, λ, h), 4 (determination of coefficients β, λ, c), 6 (determination of coefficients β, c, k_o), 7 (determination of coefficients β, h, k_o), and 8 (determination of coefficients β, ρ, c).

Property 1 (Case 1).– For any data $q_o > 0$, $T_f > T_o$, $\delta > -1$ and coefficients $\rho > 0$, $h > 0$, $c > 0$ of the phase-change material the problem of determining the unknown coefficients β, λ and k_o has always a solution which is given by (2), (3) and

$$\beta = \delta\, \Phi(\lambda) \ , \tag{12}$$

$$k_o = \frac{4\, q_o^2}{\rho\, c\, (T_f - T_o)^2} \frac{\Phi^2(\lambda)}{\left(\Phi'(0)\right)^2} \tag{13}$$

where λ is the unique solution of the equation

$$F_1(x) = \frac{2}{\text{Ste}} F_2(x) \ , \quad x > 0 \ . \tag{14}$$

Proof.– The equations (4) and (6) give us the expression (12) for β and (13) for k_o. From equation (5), we obtain the equation (14) which has a unique solution $\lambda > 0$ taking into account the properties (11) corresponding to the functions F_1 and F_2.

Property 2 (Case 3).– The necessary and sufficient condition with β, λ and h unknowns to obtain a unique solution is that data $q_o > 0$, $T_f > T_o$, $\delta > -1$ and coefficients $k_o > 0$, $\rho > 0$, $c > 0$ of the phase-change material verify condition (R_1). In such a case, the solution is given by (2), (3), β is given by (12) and

$$h = \frac{c\,(T_f - T_o)}{2} \frac{\Phi'(\lambda)}{\lambda\, \Phi(\lambda)} \left[1 + \delta\, \Phi(\lambda)\right] \tag{15}$$

where λ is the unique solution of the equation

$$\Phi(x) = \frac{(T_f - T_o)}{2\, q_o} \Phi'(0) \sqrt{\rho\, c\, k_o} \ , \quad x > 0 \ . \tag{16}$$

Proof.– The equations (4) and (5) give us the expression (12) for β and (15) for h. From equation (6) and properties (11) for the function Φ, we obtain for λ the equation (16) which has a unique solution $\lambda > 0$ if and only if

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

that is condition (R_1).

Property 3 (Case 4).– The necessary and sufficient condition with β, λ and c unknowns 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), (3), β is given by (12), and

$$c = \frac{4 q_o^2}{\rho\, k_o (T_f - T_o)^2} \frac{\Phi^2(\lambda)}{\left(\Phi'(0)\right)^2}, \tag{17}$$

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

$$F_3(x) = \frac{\rho h k_o (T_f - T_o)}{2 q_o^2} \left(\Phi'(0)\right)^2 F_6(x) \quad , \quad x > 0. \tag{18}$$

Proof.– The equations (4) and (6) give us the expression (12) for β and (17) for c respectively. From (5), (17), the properties of functions F_3 and F_6, given in (11), we obtain the equation (18) which has a unique solution $\lambda > 0$ if and only if

$$F_3(0^+) = \Phi'(0) \quad > \quad \frac{\rho h k_o (T_f - T_o)}{2 q_o^2} F_6(0^+), \tag{19}$$

i.e. condition (R_2) .

Property 4 (Case 6).– The necessary and sufficient condition with β, k_o and c unknowns 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 (12) and

$$k_o = \frac{2 \sigma q_o}{T_f - T_o} \frac{\Phi(\lambda)}{\lambda \Phi'(0)}, \tag{20}$$

$$c = \frac{2 q_o}{\rho \sigma (T_f - T_o)} \frac{\lambda \Phi(\lambda)}{\Phi'(0)}, \tag{21}$$

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

$$F_3(x) = \frac{\rho h \sigma}{q_o} \Phi'(0) \quad , \quad x > 0. \tag{22}$$

Proof.– The expression for β is given from equation (4). Owing to σ is known we get

$$\lambda = \sigma \sqrt{\frac{\rho c}{k_o}} , \tag{23}$$

i.e.

$$c = \frac{\lambda^2 k_o}{\rho \sigma^2} . \tag{24}$$

From (24) and the equation (6) we obtain the expression (20) for k_o. Then, by using (20) and (24) we have (21). Now, taking into account the properties of the functions F_3 and Φ in (11), the equation (5) gives us the equation (22) for λ, which has a unique solution $\lambda > 0$ if and only if

$$F_3(0^+) = \Phi'(0) > \frac{\rho h \sigma}{q_o} \Phi'(0) , \tag{25}$$

i.e. condition (R_3).

Property 5 (Case 7).– For any data $q_o > 0$, $T_f > T_o$, $\sigma > 0$, $\delta > -1$ and coefficients $\rho > 0$, $c > 0$ of the phase-change material the problem of determining the unknown coefficients β, k_o and h has always a solution which is given by (2), β is given by (12), h is given by (15), and

$$k_o = \frac{\rho c \sigma^2}{\lambda^2} \tag{26}$$

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

$$F_4(x) = \frac{\rho c \sigma (T_f - T_o)}{2 q_o} \Phi'(0) \quad , \quad x > 0 . \tag{27}$$

Proof.– The equations (4) and (5) give us the expression (12) for β and (15) for h. From (3) we obtain the expression (26) for k_o. From equation (6), we obtain for λ the equation (27) which has a unique solution $\lambda > 0$ taking into account the properties corresponding to the functions F_4 and Φ, given in (11).

Property 6 (Case 8).– The necessary and sufficient condition with β, ρ and c unknowns to obtain a unique solution is that data $q_o > 0$, $T_f > T_o$, $\sigma > 0$, $\delta > -1$ and coefficients $k_o > 0$, $h > 0$ of the phase-change material verify condition (R_4). In such a case, the solution is given by (2), β is given by (12) and

$$c = \frac{2h}{T_f - T_o} \frac{\lambda \Phi(\lambda)}{\Phi'(\lambda)} \frac{1}{1 + \delta \Phi(\lambda)} \tag{28}$$

$$\rho = \frac{\lambda k_o (T_f - T_o)}{2 h \sigma^2} \frac{\Phi'(\lambda)\,[1 + \delta \Phi(\lambda)]}{\Phi(\lambda)} \tag{29}$$

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

$$F_5(x) = \frac{k_o (T_f - T_o)}{2 \sigma q_o} \Phi'(0) \quad , \quad x > 0 . \tag{30}$$

Proof.– The expression for β is given (12) from equation (4). From (5), we obtain the expression (27). Owing to (23) and (28) we deduce (29). Then, from equation (6) we have, for λ, the equation (30) which has a unique solution $\lambda > 0$ if and only if $k_o (T_f - T_o) \Phi'(0) / 2 \sigma q_o < \Phi'(0)$, that is condition ($R_4$).

Now, we shall give in Table 1, case by case, the formulae of the unknown thermal coefficients and the restriction for data in order to obtain the solution of the corresponding problem.

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

TABLE 1. Restrictions and formulae for the unknown thermal coefficients for the ten cases.

Table continued.

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 $k_o = \dfrac{\rho c \sigma^2}{\lambda^2}$ where λ is the unique solution of the equation $F_4(x) = \dfrac{\rho c \sigma (T_f - T_o)}{2 q_o} \Phi'(0)$, $x > 0$.
8	β, ρ, c	R_4	$c = \dfrac{2h}{T_f - T_o} \dfrac{\lambda \Phi(\lambda)}{\Phi'(\lambda)} \dfrac{1}{1 + \delta\Phi(\lambda)}$ $\rho = \dfrac{\lambda k_o (T_f - T_o)}{2 h \sigma^2} \dfrac{\Phi'(\lambda)[1 + \delta\Phi(\lambda)]}{\Phi(\lambda)}$ where λ is the unique solution of the equation $F_5(x) = \dfrac{k_o (T_f - T_o)}{2 \sigma q_o} \Phi'(0)$, $x > 0$.
9	β, ρ, h	R_4	h is given as in Case 3 $\rho = \dfrac{k_o \lambda^2}{c \sigma^2}$ where λ is given as in Case 8 .
10	β, c, h	R_4	$h = \dfrac{k_o (T_f - T_o)}{2 \rho \sigma^2} [1 + \delta\Phi(\lambda)] \dfrac{\lambda \Phi'(\lambda)}{\Phi(\lambda)}$ $c = \dfrac{k_o \lambda^2}{\rho \sigma^2}$ where λ is given as in Case 8 .

TABLE 1. *(Continued)*

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Nomenclature

c	specific heat , [J/Kg °K] ,
erf	error function
F_i	real function (i = 1, ..., 6)
h	latent heat of fusion, [J/Kg] ,
k	thermal conductivity, [W m/(m^2 °K)] , $k_o = k(T_o)$ reference thermal conductivity,
q_o	coefficient which characterizes the heat flux on the fixed face x=0, [Ws/m^2] ,
s	position of phase change location , [m] ,
Ste	Stefan number, $\frac{c\,(T_f - T_o)}{h}$,
t	time variable , [s] ,
T	temperature of the solid phase, [°K] , T_o (temperature on the fixed face x=0),
T_f	phase–change temperature, [°K] ,
x	spatial variable , [m] ,
	Greek symbols :
α_o	reference thermal diffusivity , $\frac{k_o}{\rho c}$, [m^2/s] ,
β	coefficient in $k(T) = k_o[1 + \beta(T - T_o)/(T_f - T_o)]$,
δ, λ	dimensionless parameters
Φ	error modified function
σ	coefficient which characterizes the moving boundary, [m/$\sqrt{s}$] ,
ρ	mass density, [Kg/m^3] ,

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