



Determination of unknown thermal coefficients for Storm's-type materials through a phase-change process

Adriana C. Briozzo, María F. Natale, Domingo A. Tarzia*

Depto. Matemática, FCE, Univ. Austral, Paraguay 1950, (2000) Rosario, Argentina

Received 9 November 1997; received in revised form 3 January 1998

Abstract

Unknown thermal coefficients of a semi-infinite material of Storm's type through a phase-change process with an overspecified condition on the fixed face are determined. We follow the ideas developed in C. Rogers (Int. J. Non-Linear Mech. 21 (1986) 249–256) and in Tarzia (Adv. Appl. Math. 3 (1982) 74–82; Int. J. Heat Mass Transfer 26 (1983) 1151–1157). We also find formulae for the unknown coefficients and, the necessary and sufficient conditions for the existence of a similarity solution. © 1998 Elsevier Science Ltd. All rights reserved.

Keywords: Stefan problem; Free boundary problem; Moving boundary problem; Unknown thermal coefficients; Storm condition; Phase-change process; Solidification; Similarity solution

1. Introduction

The modeling of solidification systems is a problem of a great mathematical and industrial significance. Phase-change problems appear frequently in industrial processes and other problems of technological interest [1, 2, 3–11]. A large bibliography on the subject was given in [12].

Here, we consider a phase-change process (Stefan problem) for a non-linear heat conduction equation which admits a class of exact solutions analogous to the classical Lamé Clapeyron solution [13].

In this paper we consider an overspecified condition on the fixed face to the semi-infinite material,

given in [14], for a phase-change process of a Storm's-type material [15–18]. This allows us to consider some thermal coefficients as unknowns and to calculate them, under certain specified restrictions upon data.

The particular cases of determining constant thermal coefficients for a semi-infinite material were considered in [17, 18]. An analogous problem for a thermal conductivity as an affine function of the temperature was given in [19].

We suppose that the thermal coefficients $\bar{C}(T) = \rho c_p(T)$ and $\bar{k}(T)$ verify the following relation [20, 21]:

$$\frac{\bar{C}(T)}{\bar{k}(T) \left(\int_T^T \bar{C}(z) dz \right)^2} = K^* \quad (K^* > 0 \text{ constant}), \quad (1)$$

*Corresponding author: Tel: 0054 4181 4990; fax: 0054 4181 0505; e-mail: tarzia@uaufce.edu.ar.

where T_r is a reference temperature ($T_r \neq T_0, T_r < T_f$) and we shall consider the following solidification problem [16, 17, 22] with an overspecified condition (see conditions (3) and (4) below) on the fixed face $x = 0$ [14]:

$$\left. \begin{aligned} \rho c_p(T) T_t &= (\bar{k}(T) T_x)_x, & (2) \\ 0 < x < s(t), \quad t > 0, & \\ T(0, t) T_0 < T_f, \quad t > 0, & (3) \\ \bar{k}(T(0, t)) T_x(0, t) &= U(t), \quad t > 0, & (4) \\ \bar{k}(T(s(t), t)) T_x(s(t), t) &= \rho h \dot{s}(t), \quad t > 0, & (5) \\ T(s(t), t) &= T_f, \quad t > 0, & (6) \\ s(0) &= 0. & (7) \end{aligned} \right\} (P_1)$$

The heat flux $U(t)$ is given by [14]

$$U(t) = \frac{q_0}{\sqrt{t}}, \tag{4 bis}$$

where $q_0 > 0$ is a constant which characterizes the heat flux on the fixed face $x = 0$ of the phase-change material which can be determined experimentally.

We remark that if equation (1) is true then $\bar{k}(T)$ and $\bar{C}(T)$ verify the Storm’s relation [16]

$$\frac{1}{\sqrt{\bar{k}(T)\bar{C}(T)}} \frac{d}{dT} \left(\log \sqrt{\frac{\bar{C}(T)}{\bar{k}(T)}} \right) = \sqrt{K^*}. \tag{8}$$

Condition (8) was originally obtained by Storm [21] in an investigation of heat conduction in simple monoatomic metals. There, the validity of the approximation (8) was examined for aluminium, silver, sodium, cadmium, zinc, copper and lead.

The goal of this paper is to determinate the temperature $T = T(x, t)$, one or two unknown thermal coefficients chosen among $\{\rho, h, \bar{k}(T), K^*\}$, as a function of data T_0, T_f, q_0 , depending if $x = s(t)$ is a free (unknown function) or a moving (known function) boundary. We use the difference between free and moving boundary problems given in [12].

In Section 2 we consider (P_1) as a free boundary problem, that is $x = s(t)$ is unknown and we obtain it, the temperature $T(x, t)$ and one thermal coefficient chosen among $\{\rho, h, \bar{k}(T), K^*\}$. We study four cases which are summarized in Table 1 and we only give the proof of cases 1, 3 and 4.

In Section 3 we consider (P_1) as a moving boundary problem, that is $x = s(t)$ is known (given by the expression $s(t) = 2\sigma\sqrt{t}$ with $\sigma > 0$ a given constant) and we obtain the temperature $T(x, t)$ and two thermal coefficients chosen among $\{\rho, h, \bar{k}(T), K^*\}$. We study six cases which are summarized in Table 2 and we only give the proof of cases 7, 8 and 9.

In both Sections 2 and 3, we give necessary and sufficient conditions to have solutions and we also give the formulae for the unknown thermal coefficients with the restrictions for data to obtain the corresponding solutions.

In order to improve the paper we have also written two appendices A and B. Appendix A contains the definition of the functions which are used in the text with their corresponding properties. In Appendix B, we point out the restrictions upon data which became necessary and sufficient conditions for the existence of solution.

2. Unknown thermal coefficients through a free boundary problem

We consider problem (P_1) with Eqs. (1) and (4 bis). Following [16] we do several transformations in order to obtain the classical Stefan like problem (P_3) .

Let

$$Q_0^2 = K^* q_0^2, \tag{9}$$

$$k(T) = \frac{\bar{k}(T)}{q_0}, \tag{10}$$

$$C(T) = \frac{\bar{C}(T)}{q_0}. \tag{11}$$

Then, we obtain the following problem (P_2) , which is equivalent to (P_1) :

$$\begin{aligned}
 C(T)T_t &= (k(T)T_x)_x, \\
 0 < x < s(t), \quad t > 0 & \quad (12) \\
 T(0, t) &= T_0 < T_f, \quad t > 0 & \quad (13) \\
 k(T(0, t))T_x(0, t) &= \frac{1}{\sqrt{t}}, \quad t > 0 & \quad (14) \\
 k(T(s(t), t))T_x(s(t), t) &= \frac{\rho h}{q_0} \dot{s}(t), \\
 t > 0 & \quad (15) \\
 T(s(t), t) &= T_f, \quad t > 0 & \quad (16) \\
 s(0) &= 0. & \quad (17)
 \end{aligned}$$

(P₂)

$$\begin{aligned}
 T_{t^*}^* &= \frac{1}{Q_0^2} T_{x^*x^*}^*, 2\sqrt{t^*} < x^* < s^*(t^*), \\
 t^* > 0, & \quad (22) \\
 T^*(2\sqrt{t^*}, t^*) &= T_0^*, t^* > 0, & \quad (23) \\
 \frac{1}{Q_0^2} \frac{\partial T^*}{\partial x^*} (2\sqrt{t^*}, t^*) & \\
 &= -\frac{1}{\sqrt{t^*}} T^*(2\sqrt{t^*}, t^*), \quad t^* > 0, & \quad (24) \quad (P_3) \\
 \frac{1}{Q_0^2} \frac{\partial T^*}{\partial x^*} (s^*(t^*), t^*) & \\
 &= \frac{-\frac{h\rho}{q_0} \frac{ds^*}{dt^*}(t^*)}{\Phi(T_f) \left[\Phi(T_f) + \frac{h\rho}{q_0} \right]}, t^* > 0, & \quad (25) \\
 T^*(s^*(t^*), t^*) &= \frac{1}{\Phi(T_f)}, \quad t^* > 0, & \quad (26) \\
 s^*(0) &= 0. & \quad (27)
 \end{aligned}$$

Condition (1) is given now by

$$\frac{C(T)}{k(T) \left(\int_{T_r}^T C(z) dz \right)^2} = Q_0^2. \quad (1 \text{ bis})$$

Now, we define

$$\Phi(T) = \int_{T_r}^T C(\sigma) d\sigma. \quad (18)$$

Then, the non-linear equation (Eq. (12)) becomes

$$\frac{\partial}{\partial t} \Phi(T) - \frac{\partial}{\partial x} \left[k(T) \frac{\partial T}{\partial x} \right] = 0, \quad (19)$$

and condition (1) or (1 bis) is equivalent to

$$\frac{\Phi'(T)}{Q_0^2 \Phi^2(T)} = k(T). \quad (20)$$

If we define the transformation

$$x^*(x, t) = \int_0^x \Phi(T) dx + 2\sqrt{t} \quad (21a)$$

$$t^* = t \quad (21b)$$

$$T^* = \frac{1}{\Phi(T)} \quad (21c)$$

and taking into account Eqs. (1), (1 bis) or (20), problem (P₂) reduces to the following free boundary problem:

where

$$s^*(t^*) = x^*|_{x=s(t)} = \left[\Phi(T_f) + \frac{h\rho}{q_0} \right] s(t)$$

is the new free boundary and

$$T_0^* = \left(\int_{T_r}^{T_0} C(\sigma) d\sigma \right)^{-1} = \frac{1}{\Phi(T_0)}.$$

Taking into account that problem (P₃) is a classical Stefan-like problem [3, 13] with an overspecified condition, the two free boundaries conditions imply that the free boundary $s(t)$ must be of the type

$$s(t) = 2\sigma\sqrt{t}, \quad (28)$$

where σ is an unknown parameter to be determined.

Now we assume a similarity solution

$$\xi^* = \frac{x^*}{2\sqrt{t^*}}, \tag{29}$$

$$T^*(x^*, t^*) = \Phi^*(\xi^*); \tag{30}$$

then, the problem (P₃) reduces to the following problem:

$$\left. \begin{aligned} 2Q_0^2 \xi^* \frac{d\Phi^*}{d\xi^*} + \frac{d^2\Phi^*}{d\xi^{*2}} &= 0, \\ 1 < \xi^* < \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \sigma, \end{aligned} \right\} \tag{31}$$

$$\frac{d\Phi^*}{d\xi^*} = -2Q_0^2 \Phi^*, \quad \xi^* = 1, \tag{32}$$

$$\Phi^* = T_0^*, \quad \xi^* = 1, \tag{33}$$

$$\Phi^* = \frac{1}{\Phi(T_f)}, \tag{P_4}$$

$$\xi^* = \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \sigma, \tag{34}$$

$$\frac{d\Phi^*}{d\xi^*} = \frac{-2h\rho Q_0^2 \sigma}{q_0 \Phi(T_f)},$$

$$\xi^* = \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \sigma. \tag{35}$$

The solution of (31) is given by

$$\Phi^*(\xi^*) = A \operatorname{erf}[Q_0 \xi^*] + B, \tag{36}$$

where the constants A , B , σ , and the unknown coefficient (chosen among ρ , h , $k(T)$ and Q_0) are determined by conditions (32)–(35) which yield

$$A \exp(-Q_0^2) = -Q_0 \sqrt{\pi} [A \operatorname{erf}(Q_0) + B], \tag{37}$$

$$A \operatorname{erf} \left[\sigma Q_0 \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \right] + B = \frac{1}{\Phi(T_f)}, \tag{38}$$

$$\frac{A}{Q_0 \sqrt{\pi}} \exp \left[-\sigma^2 Q_0^2 \left(\Phi(T_f) + \frac{h\rho}{q_0} \right)^2 \right] = \frac{-h\rho\sigma}{q_0 \Phi(T_f)}, \tag{39}$$

$$T_0^* = A \operatorname{erf}[Q_0] + B, \tag{40}$$

and all coefficients must satisfy the condition (1) or (20) when it is available.

Finally, we invert the relations (9), (21a), (21b), (21c) and (30), and we use conditions (37)–(40), to obtain the parametric solution to the problem (P₁):

$$T = \Phi^{-1} \left[\frac{1}{A \operatorname{erf}[q_0 \sqrt{K^* \xi^*}] + B} \right] \tag{41}$$

$$\xi = \int_1^{\xi^*} \Phi^*(\xi^*) d\xi^* \tag{42}$$

where the constants A and B are given by

$$A = - \left[\Phi(T_f) \left[\frac{1}{Q_0 \sqrt{\pi}} \exp(-Q_0^2) + \operatorname{erf}(Q_0) - \operatorname{erf} \left(\sigma Q_0 \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \right) \right] \right]^{-1},$$

$$B = \frac{1}{\Phi(T_f)} - A \operatorname{erf} \left(\sigma Q_0 \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \right).$$

Then, the coefficient σ and the unknown coefficient (chosen among ρ , h , $k(T)$ and Q_0) must satisfy the following system of equations:

$$\begin{aligned} &\operatorname{erf} \left(\sigma Q_0 \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \right) + \frac{q_0}{\sqrt{\pi} h\rho} \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \\ &\times \frac{\exp(-\sigma^2 Q_0^2 (\Phi(T_f) + (h\rho/q_0))^2)}{\sigma Q_0 (\Phi(T_f) + (h\rho/q_0))} \\ &= \frac{1}{\sqrt{\pi}} \frac{\exp(-Q_0^2)}{Q_0^2} + \operatorname{erf}(Q_0), \end{aligned} \tag{43}$$

$$\begin{aligned} &\operatorname{erf} \left(\sigma Q_0 \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \right) - \operatorname{erf}(Q_0) \\ &= \left[1 - \frac{\Phi(T_0)}{\Phi(T_f)} \right] \frac{1}{\sqrt{\pi}} \frac{\exp(-Q_0^2)}{Q_0}, \end{aligned} \tag{44}$$

and conditions (1) or (20) when $k(T)$ is one of the coefficients to be determined.

If we define the dimensionless parameters:

$$\alpha = \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \frac{q_0}{h\rho\sqrt{\pi}}, \tag{45a}$$

$$\eta = \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) Q_0 \sigma, \tag{45b}$$

$$\beta = \left[1 - \frac{\Phi(T_0)}{\Phi(T_f)} \right] \frac{1}{\sqrt{\pi}}, \tag{45c}$$

the systems (43)–(44) is equivalent to

$$\operatorname{erf}(\eta) + \alpha \frac{\exp(-\eta^2)}{\eta} = \frac{1}{\sqrt{\pi}} \frac{\exp(-Q_0^2)}{Q_0} + \operatorname{erf}(Q_0), \tag{46}$$

$$\operatorname{erf}(\eta) - \operatorname{erf}(Q_0) = \beta \frac{\exp(-Q_0^2)}{Q_0}. \tag{47}$$

Now, we shall give necessary and sufficient conditions to obtain solution to above systems (46)–(47) and we also give formulae for the coefficient σ and the unknown thermal coefficients in the following four cases:

Case 1: Determination of the unknown coefficients σ, ρ .

Case 2: Determination of the unknown coefficients σ, h .

Case 3: Determination of the unknown coefficients σ, Q_0 (i.e. σ, K^*).

Case 4: Determination of the unknown coefficients $\sigma, k(T)$ (i.e. $\sigma, \bar{k}(T)$).

In Table 1 we give, case by case, the formulae for the unknown coefficients and the restriction on data to obtain the solution of the corresponding problem.

Now, we shall prove the following results for cases 1, 3 and 4.

Theorem 1 (Case 1). *If data q_0, Q_0 (i.e. K^*), T_0 and T_f verify restriction (R_1) , then there exists a unique*

similarity solution which is given by Eqs. (41), (42), (28) and

$$\sigma = \frac{\tilde{\eta}(\sqrt{\pi\tilde{\alpha}} - 1)}{Q_0\sqrt{\pi}\Phi(T_f)\tilde{\alpha}}, \quad \rho = \frac{\Phi(T_f)q_0}{h(\sqrt{\pi\tilde{\alpha}} - 1)}, \tag{48}$$

where the coefficients $\tilde{\eta}$ and $\tilde{\alpha}$ are given by

$$\tilde{\eta} = \operatorname{erf}^{-1}[g(Q_0, \beta)], \tag{49}$$

$$\tilde{\alpha} = \frac{\Phi(T_0)}{\Phi(T_f)\sqrt{\pi}} R(Q_0)V(\tilde{\eta}). \tag{50}$$

Proof. From the properties of functions $g(x, \beta)$, and $\operatorname{erf}(x)$, Eq. (47) admits a unique solution $\tilde{\eta}$ given by Eq. (49) if and only if $g(Q_0, \beta) < 1$, that is (R_1) . We obtain $\tilde{\alpha}$ from Eqs. (46), and (48) from Eq. (45). \square

Theorem 2 (Case 3). *If the coefficients σ and Q_0 (i.e. K^*) are unknown, then there exists a unique similarity solution given by Eqs. (41), (42), (28) and*

$$\sigma = \frac{\tilde{\eta}q_0}{(\Phi(T_f + (h\rho/q_0))Q_0)} \tag{51}$$

where $\tilde{\eta}$ is given by Eq. (49) and Q_0 is the unique solution of the equation

$$\operatorname{erf}^{-1}(g(x, \beta)) = R^{-1} \left(\frac{\Phi(T_0)}{\alpha\sqrt{\pi}\Phi(T_f)} R(x) \right), \tag{52}$$

$$x > Q^{-1}(\beta\sqrt{\pi}) > 0.$$

Proof. In this case, the system of Eqs. (46) and (47) is equivalent to

$$\eta = \operatorname{erf}^{-1}(g(v, \beta)), \tag{53}$$

$$\operatorname{erf}^{-1}(g(v, \beta)) = R^{-1} \left(\frac{\Phi(T_0)}{\alpha\sqrt{\pi}\Phi(T_f)} R(v) \right), \tag{54}$$

where α, β, η are defined in Eqs. (45a), (45b) and (45c) and

$$v = Q_0 > Q^{-1}(\beta\sqrt{\pi}). \tag{55}$$

Eq. (54) in variable v is equivalent to

$$F(v) = H(v), \quad v > Q^{-1}(\beta\sqrt{\pi}). \tag{56}$$

Table 1
Unknown thermal coefficients through a free boundary problem

Case no.	Unknown coefficient	Restriction	Solution
1	σ, ρ	R_1	$\sigma = \frac{\tilde{\eta}(\sqrt{\pi}\tilde{\alpha} - 1)}{Q_0\sqrt{\pi}\Phi(T_f)\tilde{\alpha}}, \quad \rho = \frac{\Phi(T_f)q_0}{h(\sqrt{\pi}\tilde{\alpha} - 1)}$ <p>where $\tilde{\eta} = \text{erf}^{-1}[g(Q_0, \beta)]$ $\tilde{\alpha} = \frac{\Phi(T_0)}{\Phi(T_f)\sqrt{\pi}} R(Q_0)V(\tilde{\eta})$</p>
2	σ, h	R_1	$\sigma \text{ is given as in Case 1, } h = \frac{\Phi(T_f)q_0}{\rho(\sqrt{\pi}\tilde{\alpha} - 1)}$ <p>where $\tilde{\eta}$ and $\tilde{\alpha}$ are given as in Case 1</p>
3	σ, Q_0	—	$Q_0 = \tilde{v}, \quad \sigma = \frac{\tilde{\eta}}{\left(\Phi(T_f) + \frac{h\rho}{q_0}\right)\tilde{v}}$ <p>with $\tilde{\eta} = \text{erf}^{-1}[g(\tilde{v}, \beta)]$ where \tilde{v} is the solution of $R(\text{erf}^{-1}(g(x, \beta))) = \frac{\Phi(T_0)}{\alpha\sqrt{\pi}\Phi(T_f)} R(x),$ $x > Q^{-1}(\beta\sqrt{\pi})$</p>
4	$\sigma, k(T)$	R_1, R_2	$\sigma = \frac{\tilde{\eta}}{\left(\Phi(T_f) + \frac{h\rho}{q_0}\right)Q_0}, \quad k(T) = \frac{C(T)}{\left[Q_0 \int_{T_f}^T C(z) dz\right]^2}$ <p>where $\tilde{\eta}$ is given as in Case 1</p>

Note: The unknown thermal coefficients can be obtained by the following transformations: $K^* = Q_0^2/q_0^2, \bar{k}(T) = q_0k(T)$.

From the properties of functions F and H , Eq. (56) has a unique solution $Q_0 > Q^{-1}(\beta\sqrt{\pi})$. Then, we obtain a unique solution for the systems (53) and (54), and from Eqs. (45a), (45b), (45c) and (55) we deduce Eq. (51). □

Theorem 3 (Case 4). *If data q_0, Q_0 (i.e. K^*), T_0, T_f, h and ρ satisfy restrictions (R_1) and (R_2) , then there exist a unique similarity solution which is given by Eqs. (41), (42), (28) and*

$$\sigma = \frac{\tilde{\eta}(\sqrt{\pi}\alpha - 1)}{Q_0\sqrt{\pi}\Phi(T_f)\alpha}, \quad k(T) = \frac{C(T)}{\left[Q_0 \int_{T_f}^T C(z) dz\right]^2}, \tag{57}$$

where $\tilde{\eta}$ is given by Eq. (49).

Proof. The systems (43) and (44) in the unknown σ is equivalent to

$$g(\eta, \alpha) = g\left(Q_0, \frac{1}{\sqrt{\pi}}\right), \tag{58}$$

$$\text{erf}(\eta) = g(Q_0, \beta). \tag{59}$$

As we have seen in Theorem 1, Eq. (59) admits a unique solution $\tilde{\eta}$, given by Eq. (49), if and only if (R_1) is satisfied.

If data satisfies (R_2) then $\tilde{\eta}$ is the solution of Eq. (58). From Eqs. (45a), (45b), (45c) and (49) we obtain expression (57) for σ and we obtain $k(T)$ from (1 bis).

3. Unknown thermal coefficients through a moving boundary problem

In order to determine two unknown thermal coefficients we must consider the moving boundary problem (P₁), where $s(t)$ is defined by $s(t) = 2\sigma\sqrt{t}$ for a given $\sigma > 0$, $U(t)$ is given by (4 bis) and the material verifies condition (1).

The temperature T of this problem is given by Eqs. (41) and (42). Then the two unknown coefficients can be chosen among $\rho, h, k(T)$ and Q_0 , which must verify Eqs. (43), (44) and the condition (1) when $k(T)$ is one of the thermal coefficients to determinate. That is, we shall consider the following cases:

Case 5: Determination of the unknown coefficients h, ρ .

Case 6: Determination of the unknown coefficients $h, k(T)$ (i.e. $h, \bar{k}(T)$).

Case 7: Determination of the unknown coefficients $\rho, k(T)$ (i.e. $\rho, \bar{k}(T)$).

Case 8: Determination of the unknown coefficients $Q_0, k(T)$ (i.e. $K^*, \bar{k}(T)$).

Case 9: Determination of the unknown coefficients Q_0, ρ (i.e. K^*, ρ).

Case 10: Determination of the unknown coefficient Q_0, h (i.e. K^*, h).

In Table 2 we give, case by case, the formulae for the two unknown thermal coefficients and the restriction for data to obtain a similarity solution of the corresponding problem.

Now, we shall only give the proof of the following results for cases 7, 8 and 9.

Theorem 4 (Case 7). *If data q_0, Q_0 (i.e. K^*), T_0, T_f and σ satisfy restrictions (R₁) and (R₃), then there exists a unique similarity solution which is given by*

Eqs. (41), (42) and

$$\rho = \left[\frac{\text{erf}^{-1}(g(Q_0, \beta))}{\sigma Q_0} - \Phi(T_f) \right] \frac{q_0}{h}, \tag{60}$$

$$k(T) = \frac{C(T)}{\left[Q_0 \int_{T_f}^T C(z) dz \right]^2}. \tag{61}$$

Proof. The equations (46) and (47) in the unknown ρ are equivalent to

$$\text{erf}(\eta) + \frac{\eta}{\sqrt{\pi}(\eta - \sigma Q_0 \Phi(T_f))} R(\eta) = g\left(Q_0, \frac{1}{\sqrt{\pi}}\right), \tag{62}$$

$$\text{erf}(\eta) = g(Q_0, \beta), \tag{63}$$

where η and β are defined in Eqs. (45a), (45b), (45c) and Eqs. (62) and (63) is a system in the unknown η .

As we have seen in Theorem 1, Eq. (63) admits a unique solution $\eta = \tilde{\eta}$, given by Eq. (49) if and only if (R₁) is satisfied.

This solution $\tilde{\eta}$ satisfies Eq. (62) whenever

$$\sigma = \frac{\text{erf}^{-1}(g(Q_0, \beta))}{Q_0 \Phi(T_f)} \times \left[1 - \frac{R(\text{erf}^{-1}(g(Q_0, \beta)))\Phi(T_f)}{R(Q_0)\Phi(T_0)} \right], \tag{64}$$

this is (R₃). On the other hand, the right-hand side member of Eq. (64) is positive because the properties of the function W_3 (see Appendix A). By using Eq. (45) we obtain ρ which is given by Eq. (60). The coefficient $k(T)$ is obtained as in Theorem 3. \square

Theorem 5 (Case 8). *If data q_0, ρ, h, T_f, T_0 and σ satisfy restrictions (R₄) and (R₅), then there exists a unique solution which is given by Eqs. (41) and (42) and*

$$Q_0 = \frac{r}{\sqrt{\varepsilon^2 - 1}}, \quad k(T) = \frac{C(T)(\varepsilon^2 - 1)}{r^2 \left(\int_{T_f}^T C(z) dz \right)^2}, \tag{65}$$

Table 2
Unknown thermal coefficients through a moving boundary problem

Case no.	Unknown coefficient	Restriction	Solution
5	h, ρ	R_1, R_3	$h = \left[\frac{\text{erf}^{-1}(g(Q_0, \beta))}{\sigma Q_0} - \Phi(T_f) \right] \frac{q_0}{\rho}$, with $\rho > 0$ arbitrary
6	$h, k(T)$	R_1, R_3	$k(T) = \frac{C(T)}{\left[Q_0 \int_{r_i}^T C(z) dz \right]^2}$ h is given as in Case 5
7	$\rho, k(T)$	R_1, R_3	$\rho = \left[\frac{\text{erf}^{-1}(g(Q_0, \beta))}{\sigma Q_0} - \Phi(T_f) \right] \frac{q_0}{h}$ $k(T)$ is given as in Case 6
8	$Q_0, k(T)$	R_4, R_5	$Q_0 = \frac{r}{\sqrt{\varepsilon^2 - 1}}$ $k(T)$ is given as in Case 6
9	Q_0, ρ	R_6	$Q_0 = \tilde{v}, \rho = \frac{q_0}{h} \left(\frac{\tilde{\eta}}{\sigma \tilde{v}} - \Phi(T_f) \right)$ where $\tilde{\eta} = \text{erf}^{-1}[g(\tilde{v}, \beta)]$ with \tilde{v} is the solution of $P\left(x, \frac{1}{\sigma \Phi(T_f)}\right) = Z_2(x)$, with $x > Q^{-1}(\beta\sqrt{\pi})$
10	Q_0, h	R_6	Q_0 is given as in Case 9, $h = \frac{q_0}{\rho} \left(\frac{\tilde{\eta}}{\sigma \tilde{v}} - \Phi(T_f) \right)$, where $\tilde{\eta}$ and \tilde{v} are given as in Case 9.

Note: The unknown thermal coefficients can be obtained by the following transformations: $K^* = Q_0^2/q_0^2$, $\bar{k}(T) = q_0 k(T)$.

where

$$\varepsilon = \sigma \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) > 1,$$

$$r = \sqrt{\log \left(\frac{q_0 \Phi(T_f)}{\sigma h \rho \Phi(T_0)} \right)} > 0. \tag{66}$$

Proof. The systems (46) and (47) in the unknown Q_0 is equivalent to

$$\text{erf}(\varepsilon v) + \frac{\varepsilon q_0}{\sigma h \rho \sqrt{v}} R(\varepsilon v) = \frac{1}{\sqrt{\pi}} R(v) + \text{erf}(v), \tag{67}$$

$$\text{erf}(\varepsilon v) - \text{erf}(v) = \beta R(v), \tag{68}$$

where v, β and ε are defined in Eqs. (55), (45a), (45b), (45c) and (66), respectively.

The systems (67) and (68) is equivalent to

$$\text{erf}(\varepsilon v) - \text{erf}(v) = \beta R(v), \tag{69}$$

$$R(\varepsilon v) \frac{\varepsilon q_0}{\sigma h \rho \sqrt{\pi}} = \left(\frac{1}{\sqrt{\pi}} - \beta \right) R(v). \tag{70}$$

Eq. (70) in variable v admits a unique solution

$$\tilde{v} = \frac{r}{\sqrt{\varepsilon^2 - 1}} \quad \text{with} \quad r = \sqrt{\log \left(\frac{q_0 \Phi(T_f)}{\sigma h \rho \Phi(T_0)} \right)} \tag{71}$$

if and only if

$$\frac{q_0 \Phi(T_f)}{\sigma h \rho \Phi(T_0)} > 1 \quad \text{and} \quad \sigma \left(\Phi(T_f) + \frac{h \rho}{q_0} \right) > 1. \quad (72)$$

The solution \tilde{v} also solves Eq. (69) if (R_1) is satisfied and if the data verify the condition

$$\begin{aligned} & \operatorname{erf}\left(\frac{r}{\sqrt{\varepsilon^2 - 1}}\right) + \beta R\left(\frac{r}{\sqrt{\varepsilon^2 - 1}}\right) \\ & - \operatorname{erf}\left(\frac{r\varepsilon}{\sqrt{\varepsilon^2 - 1}}\right) = 0, \end{aligned} \quad (73)$$

when

$$\frac{q_0}{\sigma h \rho} > 1 \quad (74)$$

is provided. Then, \tilde{v} solves Eqs. (69) and (70) if the conditions (72), (74), (R_1) (which are equivalent to (R_5)), and (R_4) are satisfied. Moreover, if (R_4) and (R_5) are verified then there exists a unique solution $Q_0 = \tilde{v}$ given by Eq. (65). The coefficient $k(T)$ is obtained as in the Theorem 3.

Theorem 6 (Case 9). *If data q_0, ρ and T_f satisfy the restriction (R_6) , then there exists a unique similarity solution which is given by Eqs. (41), (42) and Q_0, ρ are given by*

$$\rho = \frac{q_0}{h} \left(\frac{\tilde{\eta}}{\sigma Q_0} - \Phi(T_f) \right), \quad (75)$$

where $\tilde{\eta}$ is given by Eq. (49) and Q_0 is the solution of the equation

$$P\left(x, \frac{1}{\sigma \Phi(T_f)}\right) = Z_2(x) \quad \text{with} \quad x > Q^{-1}(\beta \sqrt{\pi}). \quad (76)$$

Proof. The systems (46) and (47) in the unknowns Q_0, ρ is equivalent to

$$\operatorname{erf}(\eta) - \operatorname{erf}(v) = \beta R(v), \quad (77)$$

$$\begin{aligned} & R(\eta) \left(1 + \frac{1}{\eta / (\sigma \Phi(T_f) v) - 1} \right) \frac{1}{\sqrt{\pi}} \\ & = \left(\frac{1}{\sqrt{\pi}} - \beta \right) R(v) \end{aligned} \quad (78)$$

in the unknowns η and v , which were defined by Eqs. (45a), (45b), (45c) and (55).

From Eq. (77) we have

$$\eta = \operatorname{erf}^{-1}(g(v, \beta)) \quad \text{for} \quad v > Q^{-1}(\beta \sqrt{\pi}). \quad (79)$$

If we replace Eq. (79) into Eq. (78) we obtain

$$1 + \frac{1}{\frac{q_0}{\sigma \Phi(T_f)} Z_1(v) - 1} = \frac{\Phi(T_0)}{\Phi(T_f)} \frac{R(v)}{R(\operatorname{erf}^{-1}(g(v, \beta)))} \quad (80)$$

which is equivalent to Eq. (76). This equation has a unique solution $x = \tilde{v}$ if and only if $\sigma \Phi(T_f) \leq 1$, that is (R_6) . In this case we obtain one solution $\tilde{\eta} = \operatorname{erf}^{-1}(g(\tilde{v}, \beta))$ and $Q_0 = \tilde{v}$. Therefore, there exist a unique solution Q_0, ρ given by Eqs. (75), (49) and (76). \square

4. Conclusion

We determine unknown thermal coefficients of a semi-infinite material that verifies the Storm condition through a phase-change process for a non-linear heat conduction equation with an overspecified condition on the fixed face. We also give necessary and sufficient conditions for the existence of a solution and we give the corresponding formulae.

Nomenclature

$T(x, t)$	distribution of temperature in the semi-infinite material $x > 0$ at time t
x	spatial variable
t	temporal variable
$s(t)$	free boundary
h	heat latent of fusion by unit of mass
ρ	density of mass of the material
$c_p = c_p(T)$	specific heat per unit of mass (constant pressure)
$\bar{C}(T) = \rho c_p(T)$	specific heat per unit of volume
$\bar{k}(T)$	thermal conductivity
T_f	change-phase temperature
T_r	reference temperature ($T_r < T_f$)
q_0, T_0, σ	constants ($T_0 \neq T_r$).

Appendix A

Consider the following parameters:

$$\alpha = \left(\Phi(T_f) + \frac{h\rho}{q_0} \right) \frac{q_0}{h\rho\sqrt{\pi}},$$

$$\beta = \left[1 - \frac{\Phi(T_0)}{\Phi(T_f)} \right] \frac{1}{\sqrt{\pi}} < \frac{1}{\sqrt{\pi}},$$

$$r = \sqrt{\log \left(\frac{q_0\Phi(T_f)}{\sigma h\rho\Phi(T_0)} \right)}.$$

We define the following real functions which have been used in the text and in the tables:

$$R(x) = \frac{\exp(-x^2)}{x}, \quad V(x) = x \exp(x^2),$$

$$Q(x) = \sqrt{\pi}x \exp(x^2) \operatorname{erfc}(x), \quad x > 0,$$

$$g(x, p) = \operatorname{erf}(x) + pR(x), \quad p > 0, \quad x > 0,$$

$$F(x) = \operatorname{erf}^{-1}(g(x, \beta)) \quad \text{for } x > Q^{-1}(\beta\sqrt{\pi}),$$

$$H(x) = R^{-1} \left(\frac{(1/\sqrt{\pi}) - \beta}{\alpha} R(x) \right), \quad x > 0.$$

$$W_1(x) = R^{-1}((1 - \sqrt{\pi}\beta)R(x)),$$

$$W_2(x) = \operatorname{erf}(W_1(x)) - \beta R(x),$$

$$W_3(x) = \operatorname{erf}(x) - W_2(x), \quad x > 0,$$

$$h_1(x) = \frac{1}{\sqrt{x^2 - 1}}, \quad h_2(x) = xh_1(x), \quad x > 1,$$

$$H_1(x) = g(rh_1(x), \beta), \quad H_2(x) = \operatorname{erf}(rh_2(x)), \quad x > 1,$$

$$Z_1(x) = \frac{F(x)}{x}, \quad x > Q^{-1}(\beta\sqrt{\pi}),$$

$$\begin{aligned} Z_2(x) &= \frac{\Phi(T_0)}{\Phi(T_f)} \frac{R(x)}{R(F(x))} \\ &= \frac{\Phi(T_0)}{\Phi(T_f)} \exp(x^2(Z_1^2(x) - 1))Z_1(x), \end{aligned}$$

$$x > Q^{-1}(\beta\sqrt{\pi}),$$

$$\begin{aligned} P \left(x, \frac{1}{\sigma\Phi(T_f)} \right) &= 1 + \frac{1}{\frac{1}{\sigma\Phi(T_f)} Z_1(x) - 1}, \\ & \quad x > Q^{-1}(\beta\sqrt{\pi}), \end{aligned}$$

which satisfy the following properties:

$$R(0^+) = +\infty, \quad R(+\infty) = 0,$$

$$R'(x) < 0, \quad \forall x > 0,$$

$$V(0) = 0, \quad V(+\infty) = +\infty,$$

$$V'(x) > 0, \quad \forall x > 0,$$

$$Q(0) = 0, \quad Q(+\infty) = 1, \quad Q'(x) > 0, \quad \forall x > 0,$$

$$\begin{aligned} g(0^+, p) &= +\infty, \quad \forall p > 0, \quad g(Q^{-1}(p\sqrt{\pi}), p) = 1 \\ & \quad \text{for } 0 < p < 1/\sqrt{\pi}, \end{aligned}$$

$$g(+\infty, p) = \begin{cases} 1^+ & \text{for } p \geq 1/\sqrt{\pi}, \\ 1^- & \text{for } 0 < p < 1/\sqrt{\pi}, \end{cases}$$

$$\frac{\partial g}{\partial x}(x, p) =$$

$$\begin{cases} < 0, \forall x > 0 & \text{for } p \geq 1/\sqrt{\pi}, \\ < 0, 0 < x < \sqrt{\frac{p}{2((1/\sqrt{\pi}) - p)}} & \text{for } 0 < p < 1/\sqrt{\pi}, \\ = 0, x = \sqrt{\frac{p}{2((1/\sqrt{\pi}) - p)}} & \text{for } 0 < p < 1/\sqrt{\pi}, \\ > 0, x > \sqrt{\frac{p}{2((1/\sqrt{\pi}) - p)}} & \text{for } 0 < p < 1/\sqrt{\pi}, \end{cases}$$

$$F(Q^{-1}(\beta\sqrt{\pi})) = +\infty, \quad F(+\infty) = +\infty,$$

$$F'(x)$$

$$\begin{cases} < 0 & \text{if } Q^{-1}(\beta\sqrt{\pi}) < x < \sqrt{\frac{\beta}{2((1/\sqrt{\pi}) - \beta)}}, \\ = 0 & \text{if } x = \sqrt{\frac{\beta}{2((1/\sqrt{\pi}) - \beta)}}, \\ > 0 & \text{if } x > \sqrt{\frac{\beta}{2((1/\sqrt{\pi}) - \beta)}}, \end{cases}$$

$$F(x) \cong \sqrt{\log\left(\frac{x \exp(x^2)}{\sqrt{\pi}((1/\sqrt{\pi}) - \beta)}\right)}$$

when $x \rightarrow +\infty$,

$$H(0) = 0, \quad H(+\infty) = +\infty, \quad H'(x) > 0,$$

$$H(x) \cong \sqrt{\log\left(\frac{\alpha x \exp(x^2)}{((1/\sqrt{\pi}) - \beta)}\right)} \quad \text{when } x \rightarrow +\infty,$$

$$W_1(0) = 0, \quad W_1(+\infty) = +\infty,$$

$$W'_1(x) > 0, \quad \forall x > 0,$$

$$W_1(x) \cong \sqrt{\log\left(\frac{x \exp(x^2)}{\sqrt{\pi}((1/\sqrt{\pi}) - \beta)}\right)}$$

when $x \rightarrow +\infty$,

$$h_1(1^+) = +\infty, \quad h_1(+\infty) = 0, \quad h'_1(x) < 0,$$

$$h_2(1^+) = +\infty, \quad h_2(+\infty) = 1^+, \quad h'_2(x) < 0,$$

$$H_1(1^+) = 1, \quad H_1(+\infty) = +\infty,$$

$$H_1(\varepsilon_1) = g(rh_1(\varepsilon_1), \beta) = g(x_1, \beta) = \min_{x \in \mathbb{R}} g(x, \beta),$$

$$x_1 = \sqrt{\frac{\beta}{2((1/\sqrt{\pi}) - \beta)}}, \quad \varepsilon_1 = h_1^{-1}\left(\frac{x_1}{r}\right) > 1,$$

$$H'_1(x) = \begin{cases} < 0 & \text{if } 1 < x < \varepsilon_1 \\ = 0 & \text{if } x = \varepsilon_1 \\ > 0 & \text{if } x > \varepsilon_1 \end{cases}, \quad H'_1(1^+) = 0^-,$$

$$H_2(1^+) = 1, \quad H_2(+\infty) = \text{erf}(r) < 1,$$

$$H'_2(x) < 0, \quad H'_2(1^+) = 0^-,$$

$$W_2(0^+) = -\infty, \quad W_2(+\infty) = 1,$$

$$W'_2(x) > 0, \quad \forall x > 0,$$

$$W_3(0^+) = +\infty, \quad W_3(+\infty) = 0,$$

$$W'_3(x) < 0, \quad \forall x > 0,$$

$$Z_1(Q^{-1}(\beta\sqrt{\pi})) = +\infty, \quad Z_1(+\infty) = 1,$$

$$Z_1(x) < 0, \quad \forall x > Q^{-1}(\beta\sqrt{\pi}),$$

$$Z_1(x) > 1, \quad \forall x > Q^{-1}(\beta\sqrt{\pi}),$$

$$Z_2(Q^{-1}(\beta\sqrt{\pi})) = +\infty, \quad Z_2(+\infty) = 1,$$

$$Z'_2(x) < 0, \quad \forall x > Q^{-1}(\beta\sqrt{\pi}),$$

$$\lim_{x \rightarrow +\infty} \exp(x^2(Z'_1(x) - 1)) = \frac{1}{1 - \beta\sqrt{\pi}},$$

$$P(Q^{-1}(\beta\sqrt{\pi}), \eta) = 1 \quad \forall \eta > 0,$$

$$P(+\infty, \eta) = \begin{cases} 1 + \frac{1}{\eta - 1} & \text{if } \eta \neq 1 \\ +\infty & \text{if } \eta = 1 \end{cases},$$

$$\frac{\partial P}{\partial x}(x, \eta) = \begin{cases} > 0 & \text{if } \eta \geq 1 \\ < 0 & \eta < 1 \end{cases}.$$

Appendix B

Let

$$\alpha = \left(\Phi(T_f) + \frac{h\rho}{q_0}\right) \frac{q_0}{h\rho\sqrt{\pi}},$$

$$\beta = \left[1 - \frac{\Phi(T_0)}{\Phi(T_f)}\right] \frac{1}{\sqrt{\pi}} < \frac{1}{\sqrt{\pi}},$$

$$r = \sqrt{\log\left(\frac{q_0\Phi(T_f)}{\sigma h\rho\Phi(T_0)}\right)}, \quad \varepsilon = \sigma\left(\Phi(T_f) + \frac{h\rho}{q_0}\right).$$

We define the following conditions for data which have been used as restrictions in the text and in the tables:

$$(R_1) \quad Q_0 > Q^{-1}(\beta\sqrt{\pi}).$$

$$(R_2) \quad R(\text{erf}^{-1}(g(Q_0, \beta))) = \frac{\Phi(T_0)}{\alpha\sqrt{\pi}\Phi(T_f)} R(Q_0).$$

$$(R_3) \quad \sigma = \frac{\text{erf}^{-1}(g(Q_0, \beta))}{Q_0\Phi(T_f)} \times \left[1 - \frac{R(\text{erf}^{-1}(g(Q_0, \beta)))\Phi(T_f)}{R(Q_0)\Phi(T_0)}\right].$$

$$(R_4) \quad \sigma\left(\Phi(T_f) + \frac{h\rho}{q_0}\right) > 1$$

and

$$\operatorname{erf}\left(\frac{r}{\sqrt{\varepsilon^2 - 1}}\right) + \beta R \left(\frac{r}{\sqrt{\varepsilon^2 - 1}}\right) - \operatorname{erf}\left(\frac{r\varepsilon}{\sqrt{\varepsilon^2 - 1}}\right) = 0.$$

$$(R_5) \quad 1 - \frac{q_0}{\sigma h \rho} < 0 < 1 - \frac{\Phi(T_0)}{\Phi(T_f)} < Q \left(\frac{r}{\sqrt{\varepsilon^2 - 1}}\right).$$

$$(R_6) \quad \sigma \Phi(T_f) \leq 1.$$

Acknowledgements

This paper has been partially sponsored by the project #4798/96 “Free Boundary Problems for the Heat-Diffusion Equation” from CONICET-UA, Rosario (Argentina). We thank the anonymous referee whose detailed comments helped us to improve the organization and content of the paper.

References

- [1] V. Alexiades, A.D. Solomon, *Mathematical Modeling of Melting and Freezing Processes*, Hemisphere, Washington, DC, Taylor & Francis, Washington, 1993.
- [2] S.N. Antontsev, K.H. Hoffmann, A.M. Khludev (Eds.), *Free Boundary Problems in Continuum Mechanics*, ISNM 106, Birkhäuser, Basel, 1992.
- [3] H.S. Carslaw, J.C. Jaeger, *Conduction of Heat in Solids*. Oxford University Press, London, 1959.
- [4] J.M. Chadam, H. Rasmussen (Eds.), *Free Boundary Problems Involving Solids*, Pitman Research Notes in Mathematics Series, vol. 281, Longman, Essex, 1993.
- [5] J. Crank, *Free and Moving Boundary Problems*, Clarendon Press, Oxford, 1984.
- [6] J.I. Diaz, M.A. Herrero, A. Liñan, J.L. Vazquez (Eds), *Free Boundary Problems: Theory and Applications*, Pitman Research Notes in Mathematics Series, vol. 323, Longman, Essex, 1995.
- [7] K.H. Hoffmann, J. Sprekels (Eds.), *Free Boundary Value Problems*, ISNM 95, Birkhäuser, Basel, 1990.
- [8] V.J. Lunardini, *Heat Transfer with Freezing and Thawing*. Elsevier, Amsterdam, 1991.
- [9] P. Neittaanmäki (Ed.), *Numerical Methods for Free Boundary Problems*, ISNM, vol. 99, Birkhäuser, Basel, 1991.
- [10] L.C. Wrobel, C.A. Brebbia (Ed.), *Computational Methods for Free and Moving Boundary Problems in Heat and Fluid-flow*. Computational Mechanics Publications, Southampton, 1993.
- [11] L.C. Wrobel, B. Sarler, C.A. Brebbia (Eds), *Computational Modelling of Free and Moving Boundary Problems III*, Computational Mechanics Publications, Southampton, 1995.
- [12] D.A. Tarzia, A bibliography on moving-free boundary problems for the heat diffusion equation. The Stefan problem. Progetto Nazionale M.P.I.: Equazioni di Evoluzione e Applicazioni Fisco—matematiche. Firenze (1988) (with 2528 references). An up-dated one will be given in 1997 with more than 4500 titles on the subject.
- [13] G. Lamé, B.P. Clapeyron, Memoire sur la solidification par refroidissement d'un globe liquide, *Ann. Chim. Phys.* 47 (1831).
- [14] D.A. Tarzia, An Inequality for the Coefficient σ of the Free Boundary $s(t) = 2\sigma\sqrt{t}$ of the Neumann Solution for the Two-Phase Stefan Problems. *Quart. Appl. Math.* 39 (1981) 491.
- [15] J.R. Cannon, *The One-Dimensional Heat Equation*. Addison-Wesley, Menlo Park, CA, 1984.
- [16] C. Rogers, On a Class of Moving Boundary Problems in Non-Linear Heat Conduction: Application of a Bäcklund Transformation, *Int. J. Non-Linear Mech.* 21 (1986) 249.
- [17] D.A. Tarzia, Determination of the unknown coefficients in the Lamé-Clapeyron problem (or one-phase Stefan problem). *Adv. Appl. Math.* 3 (1982) 74.
- [18] D.A. Tarzia, Simultaneous determination of two unknown thermal coefficients through an inverse one-phase Lamé-Clapeyron (Stefan) Problem with an overspecified condition on the fixed face. *Int. J. Heat Mass Transfer* 26 (1983) 1151.
- [19] D.A. Tarzia, The determination of unknown thermal coefficients through phase change process with temperature-dependent thermal conductivity, *Int. Comm. Heat Mass Transfer*, 25 (1998) 139.
- [20] J.H. Knight and J.R. Philip, Exact solutions in nonlinear diffusion, *J. Engng Math.* 8 (1974) 219.
- [21] M.L. Storm, Heat equations in simple metals. *J. Appl. Phys.* 22 (1951) 940.
- [22] J.G. Kingston and C. Rogers, Reciprocal Bäcklund transformations of conservation laws. *Phys. Lett A92*, (1982) 261.