Applied Mathematics and Computation 468 (2024) 128524

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Full Length Article

Relationship between two solidification problems in order to determine unknown thermal coefficients when the heat transfer coefficient is very large

N.N. Salva [a,b,*], D.A. Tarzia [c,d]

[a] CONICET-CNEA, Centro Atómico Bariloche, San Carlos de Bariloche, Argentina
[b] Universidad Nacional del Comahue, Quintral 1250, San Carlos de Bariloche, Argentina
[c] Departamento de Matemática, Facultad de Ciencias Empresariales, Universidad Austral, Paraguay 1950, Rosario S2000FZF, Argentina
[d] CONICET, Buenos Aires, Argentina

A R T I C L E I N F O

Keywords:
Phase-change processes
Unknown thermal coefficient
Free boundary problem
Moving boundary problem
Convective boundary conditions
Asymptotic analysis

A B S T R A C T

The phase-change processes are found in a wide variety of dynamic systems, for example in the study of snow avalanches. When a thermal property of the material is unknown, we can add a boundary condition to formulate an Inverse Stefan Problem, and determine this property. In this paper we study a heat conduction phase-change problem with Robin and Neumann boundary condition at a fixed face. This overspecified condition allows to simultaneously determine two unknown thermal coefficients through a moving boundary problem or a free boundary problem. Formulae for different cases where obtained by Ceretani and Tarzia (2015) [6]. The formulation with these type of boundary conditions is a more realistic one than the heat conduction phase-change problems with Dirichlet and Neumann boundary condition at the fixed face, considered by Tarzia, (1982-1983). Therefore we propose to study the relationship between the problems with Robin-Neumann conditions, and the problems with Dirichlet-Neumann conditions. The main result of this work is the convergence analysis of these problems, when the heat transfer coefficient h of the Robin condition is very large. We present for each case of the free and moving boundary problems, an upper bound for the error of the two unknown parameters, obtaining in every case a bound of order $o(\frac{1}{h})$. Finally we show a numerical example of the convergence, for a phase change material commonly used in heating or cooling processes.

1. Introduction

The phase-change processes occur when a material changes of phase, for example, from liquid to solid. They are presented in a wide variety of dynamic systems: in the solidification process in the metal industry [11,3,12], in building applications [25] or in the study of snow avalanches [1,4,17]. The heat conduction problems with phase change are called Stefan Problems. When the initial and boundary conditions, as well as the thermal properties of the material, are known, we have a Direct Stefan Problems, which involves solving the temperature and the moving free surface (for free boundary problems), or only the temperature, when the moving surface is already known (moving boundary problems). In contrast, when we need to determine some initial temperature and/or boundary

* Corresponding author at: CONICET-CNEA, Centro Atómico Bariloche, San Carlos de Bariloche, Argentina.
E-mail address: natalia.salva@yahoo.com.ar (N.N. Salva).

https://doi.org/10.1016/j.amc.2023.128524
Received 15 August 2023; Received in revised form 23 October 2023; Accepted 25 December 2023

conditions, and/or thermal properties from additional information, we have an Inverse Stefan Problem [13]. For example, in the process of ironmaking, a one-dimensional inverse Stefan problem is defined, where the phase-change surface is identified, based on data from internal measurement of temperature and heat flux [11]. We refer the reader to [7,23] and the references therein for a recent survey in applications in Stefan problems.

In this article we study a phase-change process modeling the solidification of an homogeneous material, with Robin and Neumann (or flux) condition at the fixed face $x = 0$. We consider the following problem with an overspecified condition:

$$(1)\begin{cases} \rho c T_t(x,t) = kT_{xx}(x,t), & 0 < x < s(t),\ t > 0, & \text{(1a)}\\ s(0) = 0, & & \text{(1b)}\\ T(s(t),t) = T_f, & t > 0, & \text{(1c)}\\ kT_x(s(t),t) = \rho l \dot{s}(t), & t > 0, & \text{(1d)}\\ kT_x(0,t) = \dfrac{h}{\sqrt{t}}(T(0,t) - T_0), & t > 0, & \text{(1e)}\\ kT_x(0,t) = \dfrac{q}{\sqrt{t}}, & t > 0, & \text{(1f)} \end{cases}$$

where $T(x,t)$ is the temperature of the solid phase, $k > 0$ is the thermal conductivity, $\rho > 0$ is the density of mass, $l > 0$ 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_0 is the external temperature at the fixed face $x = 0$ ($T_0 < T_f$), h is the coefficient that characterizes the heat transfer at $x = 0$ for the Robin condition (1e), and q is the coefficient that characterizes the heat flux at $x = 0$ given by (1f) which must be obtained experimentally through a phase-change process. The thermal parameters mentioned before are all positive constant.

This Stefan problem, with an overspecified condition at the fixed face $x = 0$, allows us to determine some thermal coefficients. For the free boundary problems, considering a similarity solution, the phase-change interface $s(t)$ is assumed to be proportional to $\sqrt{t}$, e.g. $s(t) = 2\lambda\sqrt{\alpha t}$, where α is the diffusion coefficient and λ is an unknown parameter that should be determine as part of the solution [8]. We can formulate free boundary problems, stating four different cases, which consist in the determination of λ and one thermal coefficient chosen among $\{k, l, c, \rho\}$. We can also formulate moving boundary problems for the simultaneous determination of two thermal coefficient chosen among: density (ρ), latent heat (l), specific heat (c) and thermal conductivity (k). In these problems the phase-change interface is already known and is related to a parameter σ obtained experimentally through a phase-change process [22]. We remark that the idea to use an overspecified condition to determine thermal coefficients was introduced in [5] and the reference within. Other methods to determine thermal coefficients are, for example, inverse heat transfer, optimization problems and experimental methods [2,9,10,14–16,18–20,24,26].

In [6] a semi-infinite material under a solidification process with the Solomon-Wilson-Alexiades mushy zone model with a heat flux condition at a fixed boundary was considered. The problem was also overspecified through a convective boundary condition, formulating several free boundary and moving boundary problems. If the mushy zone collapses into the phase change interface, this problem reduces to the Stefan problems (1). Therefore the formulae obtained for the unknown thermal coefficients in [6] can be used for the free and moving boundary problems associated to (1).

When we consider a Robin or convective conditions Eq. (1e), we have a more realistic case, in contrast to the classical Dirichlet boundary condition, where the external temperature is assumed to be instantaneously transferred to the material. In [21] and [22], the author considered the same Stefan problem with the difference that the convective condition was replaced with a Dirichlet condition, formulating free and moving boundary problems for the simultaneous determination of two unknown parameters in [21] and [22], respectively. In this article we will analyze the convergence of problem (1) to the Stefan problems considered in [21] and [22], when the heat transfer coefficient h tends to $+\infty$ (that is, h very large). Although this convergence between problems was briefly discussed in [6], we give in this article a more exhaustive analysis, presenting for each case of the free and moving boundary problems, an upper bound for the parameter error, obtaining in every case a bound of order $o(\frac{1}{h})$.

In Section 2 we summarize the formulae for the unknown thermal coefficients corresponding to four cases for free boundary problem and six cases for moving boundary problem, and present the similarity type solution to problem (1). In Section 3 we present the formulae for the unknown thermal coefficients corresponding to four cases for free boundary problem considered in [21] and six cases for moving boundary problem considered in [22]. Next we analyze case by case, the convergence between the two Stefan problems, when the heat transfer coefficient h tends to $+\infty$. Finally, in Section 4 we show a numerical example of the convergence, for a phase change material, Paraffin C_{18}, which is a useful substance in heating or cooling processes.

2. Formulae for the unknown thermal coefficients

In order to give, case by case, the formulae for the unknown thermal coefficients, let us consider the following real functions and parameters A_i ($i = 0, .., 4$), which help us to obtain simple mathematical expressions for the unknown thermal coefficients:

$$E_0(x) = \mathrm{erf}(x), \qquad E_0(x,h) = \mathrm{erf}(x) + \frac{\sqrt{k\rho c}}{\sqrt{\pi}}\frac{1}{h}, \qquad A_0 = \frac{\sqrt{k\rho c}(T_f - T_0)}{q\sqrt{\pi}},$$

$$E_1(x) = xe^{x^2}\,\mathrm{erf}(x), \qquad E_1(x,h) = xe^{x^2}\,\mathrm{erf}(x) + \frac{qc}{l\sqrt{\pi}}\frac{1}{h}, \qquad A_1 = \frac{c(T_f - T_0)}{l\sqrt{\pi}},$$

$$E_2(x) = \frac{\mathrm{erf}(x)}{xe^{x^2}}, \qquad E_2(x,h) = \frac{\mathrm{erf}(x)}{xe^{x^2}} + \frac{lk\rho}{q\sqrt{\pi}}\frac{1}{h}, \qquad A_2 = \frac{lk\rho(T_f - T_0)}{q^2\sqrt{\pi}},$$

$$E_3(x) = \frac{\mathrm{erf}(x)}{x}, \qquad E_3(x,h) = \frac{\mathrm{erf}(x)}{x} + \frac{k}{\sigma\sqrt{\pi}}\frac{1}{h}, \qquad A_3 = \frac{k(T_f - T_0)}{q\sigma\sqrt{\pi}},$$

$$E_4(x) = x\,\mathrm{erf}(x), \qquad E_4(x,h) = x\,\mathrm{erf}(x) + \frac{\sigma\rho c}{\sqrt{\pi}}\frac{1}{h}, \qquad A_4 = \frac{\sigma\rho c(T_f - T_0)}{q\sqrt{\pi}}.$$

Proposition 1. *The error function* erf *and the functions* E_i $(i = 0, .., 4)$ *have the following properties:*

$$0 < \mathrm{erf}(x) < 1, \quad \mathrm{erf}(+\infty) = 1, \quad \mathrm{erf}(0^+) = 0, \quad \mathrm{erf}'(x) > 0, \quad \mathrm{erf}''(x) < 0. \tag{2}$$

$$E_1(x) > 0, \quad E_1(+\infty) = +\infty, \quad E_1(0^+) = 0, \quad E_1'(x) > 0. \tag{3}$$

$$0 < E_2(x) < \frac{2}{\sqrt{\pi}}, \quad E_2(+\infty) = 0, \quad E_2(0^+) = \frac{2}{\sqrt{\pi}}, \quad E_2'(x) < 0. \tag{4}$$

$$0 < E_3(x) < \frac{2}{\sqrt{\pi}}, \quad E_3(+\infty) = 0, \quad E_3(0^+) = \frac{2}{\sqrt{\pi}}, \quad E_3'(x) < 0. \tag{5}$$

$$E_4(x) > 0, \quad E_4(+\infty) = +\infty, \quad E_4(0^+) = 0, \quad E_4'(x) > 0. \tag{6}$$

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):

$$0 < \frac{\sqrt{k\rho c}(T_f - T_0)}{q\sqrt{\pi}} - \frac{\sqrt{k\rho c}}{\sqrt{\pi}}\frac{1}{h} < 1 \tag{R_1}$$

$$\frac{(T_f - T_0)}{q} - \frac{1}{h} > 0 \tag{R_2}$$

$$0 < \frac{lk\rho(T_f - T_0)}{2q^2} - \frac{lk\rho}{2q}\frac{1}{h} < 1 \tag{R_3}$$

$$0 < \frac{k(T_f - T_0)}{2q\sigma} - \frac{k}{2\sigma}\frac{1}{h} < 1 \tag{R_4}$$

$$\frac{q}{\sigma\rho l} > 1 \tag{R_5}$$

$$0 < \frac{(T_f - T_0)}{q}\frac{\sqrt{k\rho c}}{\sqrt{\pi}} < 1 \tag{$R_{1\infty}$}$$

$$0 < \frac{(T_f - T_0)}{q^2}\frac{lk\rho}{2} < 1 \tag{$R_{3\infty}$}$$

$$0 < (T_f - T_0)\frac{k}{2\sigma q} < 1 \tag{$R_{4\infty}$}$$

Remark 1. Note that if the restriction (R_1) holds, as $\sqrt{k\rho c}/\sqrt{\pi} > 0$, then the restriction ($R_2$) holds too. In a similar way, if (R_3) holds then (R_2) holds, and if (R_4) holds then (R_2) also holds. The restrictions with subindex ∞ are the ones corresponding to the limit problem (1_∞) defined in the next section.

2.1. Free boundary problems

We consider the following four cases for the free boundary problem (1), where we determine the temperature $T(x,t)$, the free boundary interface $s(t)$ (i.e., the coefficient λ is defined below in (7b)) and one thermal coefficient:

FB: (1) λ, l, (2) λ, k, (3) λ, ρ, (4) λ, c.

Table 1
Formulae and restrictions for the unknown thermal coefficients for the four cases with free boundary formulation with the corresponding restrictions.

Case N°	Unknown coeff.	Restrictions	Solution
FB-1	λ, l	R_1	$l = q\sqrt{\frac{c}{k\rho}}\frac{e^{-\lambda^2}}{\lambda}$, and $\lambda > 0 /\ E_0(\lambda, h) = A_0$
FB-2	λ, k	R_2	$k = \frac{cq^2}{\rho l^2}\frac{e^{-2\lambda^2}}{\lambda^2}$, and $\lambda > 0 /\ E_1(\lambda, h) = A_1$
FB-3	λ, ρ	R_2	$\rho = \frac{cq^2}{kl^2}\frac{e^{-2\lambda^2}}{\lambda^2}$, and $\lambda > 0 /\ E_1(\lambda, h) = A_1$
FB-4	λ, c	R_3	$c = \frac{\rho k l^2}{q^2}\lambda^2 e^{2\lambda^2}$, and $\lambda > 0 /\ E_2(\lambda, h) = A_2$

Theorem 1. *The Stefan problem* (1) *has the similarity solution* (T, s) *given by:*

$$\begin{cases} T(x,t) = (T_f - T_0)\varphi\left(\dfrac{x}{2\sqrt{\alpha t}}\right) + T_0, & \text{if } 0 < x < s(t), t > 0, \quad (7a) \\ s(t) = 2\lambda\sqrt{\alpha t}, & \text{if } t > 0, \quad (7b) \end{cases}$$

if and only if the parameter $\lambda > 0$ *and the thermal coefficient satisfy the following conditions:*

$$\begin{cases} \lambda e^{\lambda^2} = \dfrac{q}{l}\sqrt{\dfrac{c}{k\rho}}, & (8a) \\ 1 + \sqrt{\pi}\dfrac{h}{\sqrt{k\rho c}}\,\mathrm{erf}(\lambda) = \dfrac{h}{q}(T_f - T_0), & (8b) \end{cases}$$

where $B_i = h\sqrt{\alpha}/k$ *(Biot number),* erf *is the error function and* φ *is defined by:*

$$\varphi(\eta) = \frac{1 + \sqrt{\pi}B_i erf(\eta)}{1 + \sqrt{\pi}B_i erf(\lambda)}. \tag{9}$$

Proof 1. When we look for a similarity solution to problem, the temperature $T(x,t)$ is a function of the single variable $\eta = \dfrac{x}{2\sqrt{\alpha t}}$, where $\alpha = \dfrac{k}{\rho c}$ is the diffusion coefficient. Through Eq. (1a), (1c) and (1e), we obtain the following differential problem for the function φ:

$$\begin{cases} \varphi''(\eta) + 2\eta\varphi'(\eta) = 0, \quad 0 < \eta < \lambda, & (10a) \\ \varphi'(0) - 2B_i\varphi(0) = 0, & (10b) \\ \varphi(\lambda) = 1\,. & (10c) \end{cases}$$

Solving problem (10), we obtain (9). Using the rest of the equations in problem (1), the following conditions must be satisfy:

$$\begin{cases} \varphi'(\lambda) = \lambda\dfrac{2l}{c(T_f - T_0)}\,, & (11a) \\ \sqrt{k\rho c}\varphi'(0)(T_f - T_0) = 2q\,, & (11b) \end{cases}$$

which is equivalent to (8), by using the expression (9).

Table 1 summarizes the formulae for the unknown thermal coefficients corresponding to the four cases for the free boundary problem (1) following [6]. In some cases, the formulae are not identical to the ones in [6], but it can be obtained using the parameter equations (8).

2.2. Moving boundary problems

For the moving boundary formulation, the phase change interface is already known, given by:

$$s(t) = 2\sigma\sqrt{t}\,, \tag{12}$$

where σ must be obtained experimentally ($\sigma = \lambda\sqrt{\alpha}$) through a phase-change process [22]. We consider the six cases for a moving boundary problem, where we determine the temperature $T(x,t)$ and the following parameters (here $\sigma > 0$ is a known coefficient):

MB: (1) l, ρ, (2) l, k, (3) l, c, (4) ρ, k, (5) ρ, c, (6) k, c.

Table 2
Formulae for the unknown thermal coefficients for the six cases with moving boundary formulation with the corresponding restrictions.

Case N°	Unknown coeff.	Restrictions	Solution
MB-1	l, ρ	R_4	$l = \dfrac{cq\sigma}{k}\dfrac{e^{-\xi^2}}{\xi^2}$, $\rho = \left(\frac{\xi}{\sigma}\right)^2 \frac{k}{c}$, where $\xi > 0 /\ E_3(\xi, h) = A_3$.
MB-2	k, l	R_2	$k = \dfrac{\rho c \sigma^2}{\xi^2}$, $l = \dfrac{q}{\rho\sigma} e^{-\xi^2}$, where $\xi > 0 / E_4(\xi, h) = A_4$.
MB-3	l, c	R_4	$l = \frac{q}{\rho\sigma} e^{-\xi^2}$, $c = \left(\frac{\xi}{\sigma}\right)^2 \frac{k}{\rho}$, where $\xi > 0 /\ E_3(\xi, h) = A_3$.
MB-4	ρ, k	R_2	$\rho = \frac{q}{l\sigma} e^{-\xi^2}$, $k = \frac{\sigma c q}{l}\frac{e^{-\xi^2}}{\xi^2}$, where $\xi > 0 /\ E_1(\xi, h) = A_1$.
MB-5	c, ρ	R_4	$\rho = \frac{q}{l\sigma} e^{-\xi^2}$, $c = \frac{lk}{\sigma q}\xi^2 e^{\xi^2}$, where $\xi > 0 /\ E_3(\xi, h) = A_3$.
MB-6	k, c	R_2, R_5	$c = \dfrac{q\sqrt{\pi}}{\sigma\rho}\dfrac{E_4(\xi)}{(T_f - T_0) - \frac{q}{h}}$, $k = \dfrac{q\sigma\sqrt{\pi}}{(T_f - T_0) - \frac{q}{h}} E_3(\xi)$, where $\xi = \sqrt{\ln\left(\frac{q}{\rho l \sigma}\right)}$.

Next we present the similarity solution to the Stefan problem (1).

Theorem 2. *If the moving boundary is given by (12), with $\sigma > 0$, then the Stefan problem (1) has the similarity solution T given by:*

$$T(x,t) = (T_f - T_0)\phi\left(\frac{x}{2\sqrt{\alpha t}}\right) + T_0, \qquad \text{if } 0 < x < s(t), t > 0, \tag{13}$$

if and only if the thermal coefficients satisfy the following conditions:

$$\begin{cases} \sigma e^{\sigma^2 \rho c/k} = \dfrac{q}{l\rho}, & (14a) \\ 1 + \sqrt{\pi}\dfrac{h}{\sqrt{k\rho c}} \operatorname{erf}\left(\sigma\sqrt{\dfrac{\rho c}{k}}\right) = \dfrac{h}{q}(T_f - T_0), & (14b) \end{cases}$$

where ϕ is defined by:

$$\phi(\eta) = \frac{1 + \sqrt{\pi} B_i erf(\eta)}{1 + \sqrt{\pi} B_i \operatorname{erf}\left(\sigma\sqrt{\frac{\rho c}{k}}\right)}. \tag{15}$$

Proof 2. Similar to Proof 1.

Table 2 summarizes the formulae for the unknown thermal coefficients corresponding to the six cases for the moving boundary problem (1), following [6].

3. Convergence analysis when *h* tends to infinity

In this section we will analyze the convergence of problem (1) when the heat transfer coefficient in the Robin condition (1e), h goes to infinity. If for each $h > 0$ the solution to problem (1) is such that $T(0,\cdot)$ and $T_x(0,\cdot)$ admit bounds independent of h (what actually happens in the most common physical situations), then, we get that $T(0,t)$ goes to T_0. In other words, if we were able to consider an infinite value for the heat transfer coefficient, then the temperature function given through problem (1) would satisfy the temperature boundary condition:

$$T(0,t) = T_0, \qquad \forall t > 0. \tag{1e$_\infty$}$$

Let us note as (1_∞) the problem (1) with the condition (1e) modified by ($1e_\infty$). This problem is also over-specified, and therefore, for free boundary problems, we can formulate four cases of simulation determination of coefficients. This was studied in [21], giving the formulae for the coefficients in each case and the restrictions for the data. For moving boundary problems, we can formulate six cases of simulation determination of coefficients, which was studied in [22].

We will show that, when h goes to infinity, the solutions given in this paper in each case tend to the solutions in [21] and [22], for free boundary problems and moving problems, respectively.

Table 3
Formulae and restrictions for the unknown thermal coefficients for the four cases with free boundary formulation in [21], with the corresponding restrictions.

Case N°	Unknown coeff.	Restrictions	Solution
FB-1	λ_∞, l_∞	$R_{1\infty}$	$l_\infty = q\sqrt{\frac{c}{k\rho}}\frac{e^{-\lambda_\infty^2}}{\lambda_\infty}$, and $\lambda_\infty > 0 /\ E_0(\lambda_\infty) = A_0$.
FB-2	λ_∞, k_∞		$k_\infty = \frac{cq^2}{\rho l^2}\frac{e^{-2\lambda_\infty^2}}{\lambda_\infty^2}$, and $\lambda_\infty > 0 /\ E_1(\lambda_\infty) = A_1$.
FB-3	$\lambda_\infty, \rho_\infty$		$\rho_\infty = \frac{cq^2}{kl^2}\frac{e^{-2\lambda_\infty^2}}{\lambda_\infty^2}$, and $\lambda_\infty > 0 /\ E_1(\lambda_\infty) = A_1$.
FB-4	λ_∞, c_∞	$R_{3\infty}$	$c_\infty = \frac{\rho k l^2}{q^2}\lambda_\infty^2 e^{2\lambda_\infty^2}$, and $\lambda_\infty > 0 /\ E_2(\lambda_\infty) = A_2$.

3.1. Free boundary problems

The next theorem is one of the main results in [21], which presents the similarity type solution for the free boundary problem (1_∞):

Theorem 3. *The Stefan problem (1_∞) has the similarity solution $\tilde{T}, \tilde{s}$ given by:*

$$\begin{cases} \tilde{T}(x,t) = \dfrac{(T_f - T_0)}{\operatorname{erf}(\lambda_\infty)}\operatorname{erf}\left(\dfrac{x}{2\sqrt{\alpha t}}\right) + T_0, & \text{if } 0 < x < \tilde{s}(t), t > 0, \quad (16a)\\ \tilde{s}(t) = 2\lambda_\infty\sqrt{\alpha t}, & \text{if } t > 0, \quad (16b)\end{cases}$$

if and only if the parameter $\lambda_\infty > 0$ and the thermal coefficients satisfy the following conditions:

$$\begin{cases} \lambda_\infty e^{\lambda_\infty^2} = \dfrac{q}{l}\sqrt{\dfrac{c}{k\rho}}, & (17a)\\ \operatorname{erf}(\lambda_\infty) = \sqrt{k\rho c}\,\dfrac{(T_f - T_0)}{q\sqrt{\pi}}. & (17b)\end{cases}$$

We summarize, in Table 3, the results for the four cases with free boundary in problem (1_∞).

Note that the coefficient's expressions for $k_\infty, c_\infty, \rho_\infty$ have been slightly modified, from the ones presented in [21], using the following equation:

$$\operatorname{erf}(\lambda_\infty) = \frac{c(T_f - T_0)}{l\sqrt{\pi}}\frac{e^{-\lambda_\infty^2}}{\lambda_\infty}.$$

Remark 2. Note that if $h \to \infty$, the conditions in (8) converge to the conditions in (17), by the unicity of positive solutions for λ and λ_∞, we have that $\lambda = \lambda(h) \to \lambda_\infty$. Rewriting φ as:

$$\varphi(\eta) = \frac{\frac{1}{\sqrt{\pi}B_i} + \operatorname{erf}(\eta)}{\frac{1}{\sqrt{\pi}B_i} + \operatorname{erf}(\lambda)},$$

we have that $1/B_i \to 0$, therefore $\varphi(x) \to \operatorname{erf}(x)/\operatorname{erf}(\lambda_\infty)$, and finally we get that $T = T(h) \to \tilde{T}$ and $s = s(h) \to \tilde{s}$.

Next we prove some properties for the auxiliary functions, that analyze mainly the convergence of λ to λ_∞. Next we prove only Proposition 5 for the Case 1, and state that the proof of Propositions 6 to 8 are similar to the Case 1 using the properties of the corresponding auxiliary functions.

Proposition 2. *Let us define, for each fixed $h > 0$, $\lambda = \lambda(h)$ as the unique positive solution of the equation:*

$$E_0(x,h) = A_0, \tag{18}$$

and λ_∞ as the unique positive solution of the equation:

$$E_0(x) = A_0, \tag{19}$$

then:

1. *$\lambda < \lambda_\infty$, $\forall h > 0$,*
2. *$\{\lambda\}_h$ is an increasing sequence, that is: $h_i < h_j \Rightarrow \lambda(h_i) < \lambda(h_j)$,*
3. *and the difference between λ_∞ and λ is bounded by $o(1/h)$, that is:*

$$0 < \lambda_\infty - \lambda < \frac{\sqrt{k\rho c}}{\sqrt{\pi} E_0'(\lambda_\infty)} \frac{1}{h}, \qquad \forall h > 0. \tag{20}$$

Proof 3. First we note that:

$$E_0(x,h) = E_0(x) + \frac{\sqrt{k\rho c}}{\sqrt{\pi}} \frac{1}{h} > E_0(x), \quad \forall x > 0,$$

resulting in:

$$A_0 = E_0(\lambda, h) > E_0(\lambda), \quad \forall \lambda > 0.$$

Noting that $A_0 = E_0(\lambda_\infty)$, we have that $E_0(\lambda_\infty) > E_0(\lambda)$, $\forall \lambda > 0$. Using the property of E_0 being an increasing function, we get $\lambda < \lambda_\infty$, $\forall h > 0$.

The second property of this proposition comes directly from the definition of $\lambda(h)$ and the fact that E_0 is increasing. For the third property of this proposition, we use the mean value theorem, obtaining:

$$|\lambda - \lambda_\infty| = \frac{|E_0(\lambda,h) - E_0(\lambda_\infty,h)|}{|E_0'(x)|}, \quad \text{for some } x \text{ between } \lambda \text{ and } \lambda_\infty \ . \tag{21}$$

Using the definition of λ and λ_∞, we have:

$$|E_0(\lambda,h) - E_0(\lambda_\infty,h)| = \frac{\sqrt{k\rho c}}{\sqrt{\pi}} \frac{1}{h}.$$

Using the fact that E_0' is positive and decreasing, then $|E_0'(x)| \geq E_0'(\lambda_\infty)$, $\forall x < \lambda_\infty$. From this bound and (21), we get (20).

Proposition 3. *Let us define, for each fixed $h > 0$, $\lambda = \lambda(h)$ as the unique positive solution of the equation:*

$$E_1(x,h) = A_1\,, \tag{22}$$

and λ_∞ as the unique positive solution of the equation:

$$E_1(x) = A_1\,, \tag{23}$$

then:

1. *$\lambda < \lambda_\infty$, $\forall h > 0$,*
2. *$\{\lambda\}_h$ is an increasing sequence, that is: $h_i < h_j \Rightarrow \lambda(h_i) < \lambda(h_j)$,*
3. *and the difference between λ_∞ and λ is bounded by $o(1/h)$, that is exists $h_1 > 0$ such that:*

$$0 < \lambda_\infty - \lambda < \frac{qc}{\sqrt{\pi} l E_1'(\lambda(h_1))} \frac{1}{h}, \qquad \forall h > h_1. \tag{24}$$

Proof 4. The proof of the first and second properties is similar to Proposition 2, using the fact that E_1 is an increasing function.

For the third property of this proposition, we use the mean value theorem, obtaining:

$$|\lambda - \lambda_\infty| = \frac{|E_1(\lambda,h) - E_1(\lambda_\infty,h)|}{|E_1'(x)|}\,, \quad \text{for some } x \text{ between } \lambda \text{ and } \lambda_\infty \ . \tag{25}$$

Using the definition of λ and λ_∞, we have:

$$|E_1(\lambda,h) - E_1(\lambda_\infty,h)| = \frac{qc}{l\sqrt{\pi}} \frac{1}{h}.$$

Using the fact that E_1' is positive and increasing, and that $\{\lambda\}_h$ is an increasing sequence, there exists $h_1 > 0$ such that: $|E_1'(x)| \geq E_1'(\lambda(h_1))$, $\forall x > \lambda(h_1)$. From this bound and (25), we get (24).

Proposition 4. *Let us define, for each fixed $h > 0$, $\lambda = \lambda(h)$ as the unique positive solution of the equation:*

$$E_2(x,h) = A_2\,, \tag{26}$$

and λ_∞ as the unique positive solution of the equation:

$$E_2(x) = A_2, \tag{27}$$

then:

1. $\lambda > \lambda_\infty, \qquad \forall h > 0,$
2. $\{\lambda\}_h$ *is a decreasing sequence, that is:* $h_i < h_j \Rightarrow \lambda(h_i) > \lambda(h_j)$,
3. *and the difference between* λ_∞ *and* λ *is bounded by* $o(1/h)$*, that is exists* $h_2 > 0$ *such that:*

$$|\lambda_\infty - \lambda| < \frac{k\rho l}{q\sqrt{\pi}|E_2'(\lambda(h_2))|}\frac{1}{h}, \qquad \forall h > h_2. \tag{28}$$

Proof 5. First we note that:

$$E_2(\lambda) + \frac{lk\rho}{q\sqrt{\pi}}\frac{1}{h} = E_2(\lambda_\infty), \quad \forall \lambda > 0,$$

resulting in $E_2(\lambda_\infty) > E_2(\lambda)$, $\forall \lambda > 0$. Using the decreasing character of E_2, we get $\lambda > \lambda_\infty$, $\forall h > 0$.

The second property of this proposition comes directly from the definition of $\lambda(h)$ and the fact that E_2 is decreasing.

For the third property of this proposition, we use the mean value theorem, obtaining:

$$|\lambda - \lambda_\infty| = \frac{|E_2(\lambda, h) - E_2(\lambda_\infty, h)|}{|E_2'(x)|}, \qquad \text{for some } x \text{ between } \lambda \text{ and } \lambda_\infty. \tag{29}$$

Using the definition of λ and λ_∞, we have:

$$|E_2(\lambda, h) - E_2(\lambda_\infty, h)| = \frac{lk\rho}{q\sqrt{\pi}}\frac{1}{h}.$$

Using the fact that E_2' is bounded and $E_2'(+\infty) = 0$, there exists h_2 such that: $|E_2'(x)| \geq E_2'(\lambda(h_2))$, $\forall x \in (\lambda_\infty, \lambda(h_2))$. From this bound and (29), we get (28).

We consider now the four cases for the unknown thermal coefficients for the corresponding free boundary problem (1).

3.1.1. Case 1: simultaneous determination of $\{\lambda, l\}$

Proposition 5. *Let* λ *and* l *be the unknown parameters in Problem (1) for certain* h*, and let* λ_∞ *and* l_∞ *be the unknown parameters in Problem (*1_∞*). Then:*

1. $\{\lambda\}_h$ *is an increasing sequence that goes to* λ_∞ *with order* $o(1/h)$*, that is Eq. (20) is satisfied.*
2. $\{l\}_h$ *is a sequence that goes to* l_∞ *with order* $o(1/h)$*, that is exists* $h^* > 0$ *such that:*

$$|l_\infty - l| < \frac{qc}{\sqrt{\pi}E_0'(\lambda_\infty)}\left(\frac{1 + 2\lambda_\infty^2}{\lambda^{*2}\exp(\lambda^{*2})}\right)\frac{1}{h}, \qquad \forall h > h^*, \tag{30}$$

where $\lambda^* = \lambda(h^*)$.

Proof 6. The first property of this proposition is given by Proposition 2. For the second property, observe that:

$$|l_\infty - l| = q\sqrt{\frac{c}{k\rho}}\left|\frac{e^{-\lambda^2}}{\lambda} - \frac{e^{-\lambda_\infty^2}}{\lambda_\infty}\right|.$$

Using the mean value theorem for the function $f(x) = \dfrac{e^{-x^2}}{x}$, we have that exists $h^* > 0$ such that:

$$\left|\frac{e^{-\lambda^2}}{\lambda} - \frac{e^{-\lambda_\infty^2}}{\lambda_\infty}\right| \leq \left(\frac{1 + 2\lambda_\infty^2}{\lambda^{*2}\exp(\lambda^{*2})}\right)|\lambda_\infty - \lambda|, \qquad \forall \lambda \in (\lambda^*, \lambda_\infty).$$

From this bound and Eq. (20) we get Eq. (30).

3.1.2. Case 2: simultaneous determination of $\{\lambda, k\}$

Proposition 6. *Let* λ *and* k *be the unknown parameters in Problem (1) for certain* h*, and let* λ_∞ *and* k_∞ *be the unknown parameters in Problem (*1_∞*). Then:*

1. $\{\lambda\}_h$ *is an increasing sequence that goes to* λ_∞ *with order* $o(1/h)$*, that is Eq. (24) is satisfied.*

Table 4
Formulae for the unknown thermal coefficients for the six cases with moving boundary formulation in [22] with the corresponding restrictions.

Case N°	Unknown coeff.	Restrictions	Solution
MB-1	l_∞, ρ_∞	$R_{4\infty}$	$l_\infty = \frac{cq\sigma}{k}\frac{e^{-\xi_\infty^2}}{\xi_\infty^2}$, $\rho_\infty = \left(\frac{\xi_\infty}{\sigma}\right)^2 \frac{k}{c}$, where $\xi_\infty > 0 /\ E_3(\xi_\infty) = A_3$.
MB-2	l_∞, k_∞		$l_\infty = \frac{q}{\rho\sigma} e^{-\xi_\infty^2}$, $k_\infty = \frac{\rho c \sigma^2}{\xi_\infty^2}$, where $\xi_\infty > 0 / E_4(\xi_\infty) = A_4$.
MB-3	l_∞, c_∞	$R_{4\infty}$	$l_\infty = \frac{q}{\rho\sigma} e^{-\xi_\infty^2}$, $c_\infty = \left(\frac{\xi_\infty}{\sigma}\right)^2 \frac{k}{\rho}$, where $\xi_\infty > 0 /\ E_3(\xi_\infty) = A_3$.
MB-4	ρ_∞, k_∞		$\rho = \frac{q}{l\sigma} e^{-\xi_\infty^2}$, $k = \frac{\sigma c q}{l} \frac{e^{-\xi_\infty^2}}{\xi_\infty^2}$, where $\xi_\infty > 0 /\ E_1(\xi_\infty) = A_1$.
MB-5	ρ_∞, c_∞	$R_{4\infty}$	$\rho_\infty = \frac{q}{l\sigma} e^{-\xi_\infty^2}$, $c_\infty = \frac{lk}{\sigma q}\xi_\infty^2 e^{\xi_\infty^2}$, where $\xi_\infty > 0 /\ E_3(\xi_\infty) = A_3$.
MB-6	k_∞, c_∞	R_5	$c_\infty = \frac{q\sqrt{\pi}}{\sigma\rho}\frac{E_4(\xi_\infty)}{(T_f - T_0)}$, $k_\infty = \frac{q\sigma\sqrt{\pi}}{(T_f - T_0)} E_3(\xi_\infty)$, where $\xi_\infty = \sqrt{\ln\left(\frac{q}{\rho l \sigma}\right)}$.

2. *$\{k\}_h$ is a sequence that goes to k_∞ with order $o(1/h)$, that is*

$$|k_\infty - k| < \frac{q^3 c^2}{\rho l^3 \sqrt{\pi} E_1'(\lambda_1)} \left(\frac{2 + 4\lambda_\infty^2}{\lambda_1^3 \exp(2\lambda_1^2)}\right) \frac{1}{h}, \qquad \forall h > h_1, \tag{31}$$

where $\lambda_1 = \lambda(h_1)$ and h_1 is the one given by Proposition 3.

3.1.3. Case 3: simultaneous determination of $\{\lambda, \rho\}$

Proposition 7. *Let λ and ρ be the unknown parameters in Problem (1) for certain h, and let λ_∞ and ρ_∞ be the unknown parameters in Problem (1_∞). Then:*

1. *$\{\lambda\}_h$ is an increasing sequence that goes to λ_∞ with order $o(1/h)$, that is Eq. (24) is satisfied.*
2. *$\{\rho\}_h$ is a sequence that goes to ρ_∞ with order $o(1/h)$, that is*

$$|\rho_\infty - \rho| < \frac{q^3 c^2}{k l^3 \sqrt{\pi} E_1'(\lambda_1)} \left(\frac{2 + 4\lambda_\infty^2}{\lambda_1^3 \exp(2\lambda_1^2)}\right) \frac{1}{h}, \qquad \forall h > h_1, \tag{32}$$

where $\lambda_1 = \lambda(h_1)$ and h_1 is the one given by Proposition 3.

3.1.4. Case 4: simultaneous determination of $\{\lambda, c\}$

Proposition 8. *Let λ and c be the unknown parameters in Problem (1) for certain h, and let λ_∞ and c_∞ be the unknown parameters in Problem (1_∞). Then:*

1. *$\{\lambda\}_h$ is a decreasing sequence that goes to λ_∞ with order $o(1/h)$, that is Eq. (28) is satisfied.*
2. *$\{c\}_h$ is a sequence that goes to c_∞ with order $o(1/h)$, that is*

$$|c_\infty - c| < \frac{k^2 \rho^2 l^3}{q^3 \sqrt{\pi} |E_2'(\lambda_2)|} (2\lambda_2 + 4\lambda_2^3) \exp(2\lambda_2^2) \frac{1}{h}, \qquad \forall h > h_2, \tag{33}$$

where $\lambda_2 = \lambda(h_2)$ and h_2 is the one given by Proposition 4.

3.2. Moving boundary problems

In the moving boundary formulation, the phase change interface is already known, given by (12). In Table 4 summarizes the results in [22], for moving boundary problems.

The next theorem is one of the main results in [22]:

Theorem 4. *If the moving boundary $\tilde{s}$ is given by (12), with $\sigma > 0$, then the Stefan problem (1_∞) has the similarity solution $\tilde{T}$ given by:*

$$\tilde{T}(x,t) = \frac{(T_f - T_0)}{\operatorname{erf}(\sigma/\sqrt{\alpha})} \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right) + T_0, \quad \text{if } 0 < x < \tilde{s}(t), t > 0, \tag{34}$$

if and only if the thermal coefficients satisfy the following conditions:

$$\begin{cases} \sigma e^{\sigma^2 \rho c/k} = \dfrac{q}{l\rho}\,, & (35a) \\ \operatorname{erf}\left(\sigma\sqrt{\dfrac{\rho c}{k}}\right) = \sqrt{k\rho c}\dfrac{(T_f - T_0)}{q\sqrt{\pi}}\,, & (35b) \end{cases}$$

Remark 3. Note that if $h \to \infty$, the conditions in (14) converge to the conditions in (35). Rewriting ϕ as:

$$\phi(\eta) = \frac{\frac{1}{\sqrt{\pi}B_i} + \operatorname{erf}(\eta)}{\frac{1}{\sqrt{\pi}B_i} + \operatorname{erf}(\sigma/\sqrt{\alpha})}\,,$$

we have that $1/B_i \to 0$, therefore $\phi(x) \to \operatorname{erf}(x)/\operatorname{erf}(\sigma/\sqrt{\alpha})$, and finally we get that $T = T(h) \to \tilde{T}$.

Next we prove some properties for the last auxiliary functions, that analyze mainly the convergence of ξ to ξ_∞. The proof of Propositions 11 to 15 are similar to proof of Proposition 5. In this section we only prove Proposition 16 for Case 6 that is different from the rest.

Proposition 9. *Let us define, for each fixed $h > 0$, $\xi = \xi(h)$ as the unique positive solution of the equation:*

$$E_3(x,h) = A_3\,, \tag{36}$$

and ξ_∞ as the unique positive solution of the equation:

$$E_3(x) = A_3\,, \tag{37}$$

then:

1. $\xi > \xi_\infty, \qquad \forall h > 0,$
2. $\{\xi\}_h$ *is a decreasing sequence, that is:* $h_i < h_j \Rightarrow \xi(h_i) > \xi(h_j)$,
3. *and the difference between ξ_∞ and ξ is bounded by $o(1/h)$, that is exists $h_3 > 0$ such that:*

$$|\xi_\infty - \xi| < \frac{k}{\sigma\sqrt{\pi}|E_3'(\xi(h_3))|}\frac{1}{h}, \qquad \forall h > h_3. \tag{38}$$

Proof 7. Similar to the proof of Proposition 4.

Proposition 10. *Let us define, for each fixed $h > 0$, $\xi = \xi(h)$ as the unique positive solution of the equation:*

$$E_4(x,h) = A_4\,, \tag{39}$$

and ξ_∞ as the unique positive solution of the equation:

$$E_4(x) = A_4\,, \tag{40}$$

then:

1. $\xi > \xi_\infty, \qquad \forall h > 0,$
2. $\{\xi\}_h$ *is an increasing sequence, that is:* $h_i < h_j \Rightarrow \xi(h_i) < \xi(h_j)$,
3. *and the difference between ξ_∞ and ξ is bounded by $o(1/h)$, that is exists $h_4 > 0$ such that:*

$$|\xi_\infty - \xi| < \frac{\rho c\sigma}{\sqrt{\pi}|E_4'(\xi(h_4))|}\frac{1}{h}, \qquad \forall h > h_4. \tag{41}$$

Proof 8. Similar to the proof of Proposition 3.

Now, we consider the six cases for the two unknown thermal coefficients for the corresponding moving boundary problem (1) with data (12).

3.2.1. Case 1: simultaneous determination of $\{l, \rho\}$

Proposition 11. *Let l and ρ be the unknown parameters in the moving formulation of Problem (1) for certain h, and let l_∞ and ρ_∞ be the unknown parameters in the moving formulation of Problem (1_∞). Then:*

1. $\{\xi\}_h$ *is a decreasing sequence that goes to* ξ_∞ *with order* $o(1/h)$*, that is Eq. (38) is satisfied.*
2. $\{l\}_h$ *is a sequence that goes to* l_∞ *with order* $o(1/h)$*, that is exists* $h_6 > 0$ *such that:*

$$|l_\infty - l| < \frac{cq}{\sqrt{\pi}|E_3'(\xi_3)|}\left(\frac{2\xi_6^2+1}{\xi_\infty^2\exp(\xi_\infty^2)}\right)\frac{1}{h}, \qquad \forall h > h_6, \tag{42}$$

   where $\xi_6 = \xi(h_6)$.
3. $\{\rho\}_h$ *is a sequence that goes to* ρ_∞ *with order* $o(1/h)$*, that is*

$$|\rho_\infty - \rho| < \frac{k^2 2\xi_4}{\sigma^3 c|E_3'(\xi_4)|}\frac{1}{h}, \qquad \forall h > h_3, \tag{43}$$

   where $\xi_4 = \xi(h_3)$ *and* h_3 *is the one given by Proposition 9.*

3.2.2. Case 2: simultaneous determination of $\{l, k\}$

Proposition 12. *Let* $l = l(h)$ *and* $k = k(h)$ *be the unknown parameters in the moving formulation of Problem (1) for certain* h*, and let* l_∞ *and* k_∞ *be the unknown parameters in the moving formulation of Problem* (1_∞)*. Then:*

1. $\{\xi\}_h$ *is an increasing sequence that goes to* ξ_∞ *with order* $o(1/h)$*, that is Eq. (41) is satisfied.*
2. $\{l\}_h$ *is a sequence that goes to* l_∞ *with order* $o(1/h)$*, that is exists* $h^* > 0$ *such that:*

$$|l_\infty - l| < \frac{2cq\xi_\infty}{\sqrt{\pi}E_4'(\xi^*)}\exp(-\xi^{*2})\frac{1}{h}, \qquad \forall h > h^*, \tag{44}$$

   where $\xi^* = \xi(h^*)$.
3. $\{k\}_h$ *is a sequence that goes to* k_∞ *with order* $o(1/h)$*, that is exists* $h^* > 0$ *such that:*

$$|k_\infty - k| < \frac{2\rho^2 c^2\sigma^3}{\xi^{*3}\sqrt{\pi}|E_4'(\xi^*)|}\frac{1}{h}, \qquad \forall h > h^*. \tag{45}$$

3.2.3. Case 3: simultaneous determination of $\{l, c\}$

Proposition 13. *Let* $l = l(h)$ *and* $c = c(h)$ *be the unknown parameters in the moving formulation of Problem (1) for certain* h*, and let* l_∞ *and* c_∞ *be the unknown parameters in the moving formulation of Problem* (1_∞)*. Then:*

1. $\{\xi\}_h$ *is a decreasing sequence that goes to* ξ_∞ *with order* $o(1/h)$*, that is Eq. (38) is satisfied.*
2. $\{l\}_h$ *is a sequence that goes to* l_∞ *with order* $o(1/h)$*, that is exists* $h^* > 0$ *such that:*

$$|l_\infty - l| < \frac{2kq\xi^*}{\sigma^2\rho\sqrt{\pi}|E_3'(\xi^*)|}\exp(-\xi_\infty^2)\frac{1}{h}, \qquad \forall h > h^*, \tag{46}$$

   where $\xi^* = \xi(h^*)$.
3. $\{c\}_h$ *is a sequence that goes to* c_∞ *with order* $o(1/h)$*, that is exists* $h^* > 0$ *such that:*

$$|c_\infty - c| < \frac{2k^2\xi^*}{\sigma^3\rho\sqrt{\pi}|E_3'(\xi^*)|}\frac{1}{h}, \qquad \forall h > h^*. \tag{47}$$

3.2.4. Case 4: simultaneous determination of $\{\rho, k\}$

Proposition 14. *Let* $\rho = \rho(h)$ *and* $k = k(h)$ *be the unknown parameters in the moving formulation of Problem (1) for certain* h*, and let* ρ_∞ *and* k_∞ *be the unknown parameters in the moving formulation of Problem* (1_∞)*. Then:*

1. $\{\xi\}_h$ *is an increasing sequence that goes to* ξ_∞ *with order* $o(1/h)$*, that is:*

$$0 < \xi_\infty - \xi < \frac{qc}{\sqrt{\pi}lE_1'(\xi(h_1))}\frac{1}{h}, \qquad \forall h > h_1.$$

2. $\{\rho\}_h$ *is a sequence that goes to* ρ_∞ *with order* $o(1/h)$*, that is*

$$|\rho_\infty - \rho| < \frac{2cq^2\xi_\infty}{l^2\sigma\sqrt{\pi}E_1'(\xi_1)}\exp(-\xi_1^2)\frac{1}{h}, \qquad \forall h > h_1, \tag{48}$$

   where $\xi_1 = \xi(h_1)$.

3. $\{k\}_h$ *is a sequence that goes to* k_∞ *with order* $o(1/h)$*, that is*

$$|k_\infty - k| < \frac{q^2 c^2 \sigma (2\xi_\infty^2 + 1)}{l^2 \xi_1^2 \exp(\xi_1^2)\sqrt{\pi} E_1'(\xi_1)} \frac{1}{h}, \qquad \forall h > h_1. \tag{49}$$

3.2.5. Case 5: simultaneous determination of $\{\rho, c\}$

Proposition 15. *Let* $\rho = \rho(h)$ *and* $c = c(h)$ *be the unknown parameters in the moving formulation of Problem (1) for certain* h*, and let* ρ_∞ *and* c_∞ *be the unknown parameters in the moving formulation of Problem* (1_∞)*. Then:*

1. $\{\xi\}_h$ *is a decreasing sequence that goes to* ξ_∞ *with order* $o(1/h)$*, that is Eq. (38) is satisfied.*
2. $\{\rho\}_h$ *is a sequence that goes to* ρ_∞ *with order* $o(1/h)$*, that is*

$$|\rho_\infty - \rho| < \frac{2kq\xi_4}{l\sigma^2\sqrt{\pi}|E_3'(\xi_4)|} \exp(-\xi_\infty^2) \frac{1}{h}, \qquad \forall h > h_3, \tag{50}$$

where $\xi_4 = \xi(h_3)$.

3. $\{c\}_h$ *is a sequence that goes to* c_∞ *with order* $o(1/h)$*, that is*

$$|c_\infty - c| < \frac{k^2 l (2\xi_4 + 2\xi_4^3)\exp(\xi_4^3)}{\sigma^2 q \sqrt{\pi}|E_4'(\xi_4)|} \frac{1}{h}, \qquad \forall h > h_3. \tag{51}$$

3.2.6. Case 6: simultaneous determination of $\{k, c\}$

Proposition 16. *Let* $k = k(h)$ *and* $c = c(h)$ *be the unknown parameters in the moving formulation of Problem (1) for certain* h*, and let* k_∞ *and* c_∞ *be the unknown parameters in the moving formulation of Problem* (1_∞)*. Then:*

1. $\{\xi\}_h$ *is a constant sequence and* $\xi = \xi_\infty$.
2. $\{k\}_h$ *is a sequence that goes to* k_∞ *with order* $o(1/h)$*, that is exists* $h^* > 0$ *such that:*

$$|k_\infty - k| < \frac{\operatorname{erf}(\xi_\infty)\sigma\sqrt{\pi}q^2}{\xi_\infty (T_f - T_0)(T_f - T_0 - q/h^*)} \frac{1}{h}, \qquad \forall h > h^*. \tag{52}$$

3. $\{c\}_h$ *is a sequence that goes to* c_∞ *with order* $o(1/h)$*, that is exists* $h^* > 0$ *such that:*

$$|c_\infty - c| < \frac{\xi_\infty \operatorname{erf}(\xi_\infty)\sqrt{\pi}q^2}{\sigma\rho(T_f - T_0)(T_f - T_0 - q/h^*)} \frac{1}{h}, \qquad \forall h > h^*. \tag{53}$$

Proof 9. First we note that $\xi = \xi_\infty$ for every $h > 0$. Using the corresponding expressions for each coefficient, we have:

$$\begin{aligned} |k_\infty - k| &= q\sigma\sqrt{\pi}E_3(\xi_\infty)\left|\frac{1}{(T_f - T_0)} - \frac{1}{(T_f - T_0 - q/h)}\right|, \\ |c_\infty - c| &= \frac{q\sqrt{\pi}}{\sigma\rho}E_4(\xi_\infty)\left|\frac{1}{(T_f - T_0)} - \frac{1}{(T_f - T_0 - q/h)}\right|. \end{aligned} \tag{54}$$

Using Restriction R_2 and algebraic operations, we have that for $h > h^*$:

$$\left|\frac{1}{(T_f - T_0)} - \frac{1}{(T_f - T_0) - q/h}\right| \le \frac{q}{(T_f - T_0)(T_f - T_0 - q/h^*)} \frac{1}{h}, \tag{55}$$

where h^* is any positive fixed value. From these bounds, the proposition holds.

4. Numerical example

We analyzed the convergence for Paraffin C_{18}, a phase change material which is a substance that releases or absorbs sufficient energy at the phase transition (from liquid to solid or vice versa) to provide useful heat or cooling. The thermal data in Table 5 was obtained from [25], and calculated from (8). In Table 6 we show the values of each restriction for the thermal parameters considered, in each case the restriction is satisfied.

Table 5
Thermal coefficients for Paraffin C_{18}.

Parameter	Units	Paraffin
k	J/s m °C	0.15
ρ	kg/m^3	900
c	J/kg °C	2160
l	J/kg	244000
T_0	°C	0
T_f	°C	28
h	kg/∘C s$^{5/2}$	62170.7
λ	adim.	0.33664961
σ	m/s$^{1/2}$	0.000093513781
q	kg/s$^{5/2}$	23000
B_i	adim.	115.13092944

Table 6
Restrictions for Paraffin C_{18}.

Restriction	Variable condition	Value
R_1	$0 < R < 1$	0.3681285
$R_{1\infty}$	$0 < R < 1$	0.37089332
R_2	$0 < R$	0.00120130
R_3	$0 < R < 1$	0.86023995
$R_{3\infty}$	$0 < R < 1$	0.87175803
R_4	$0 < R < 1$	0.96347287
$R_{4\infty}$	$0 < R < 1$	0.97637317
R_5	$R > 1$	1.12000479

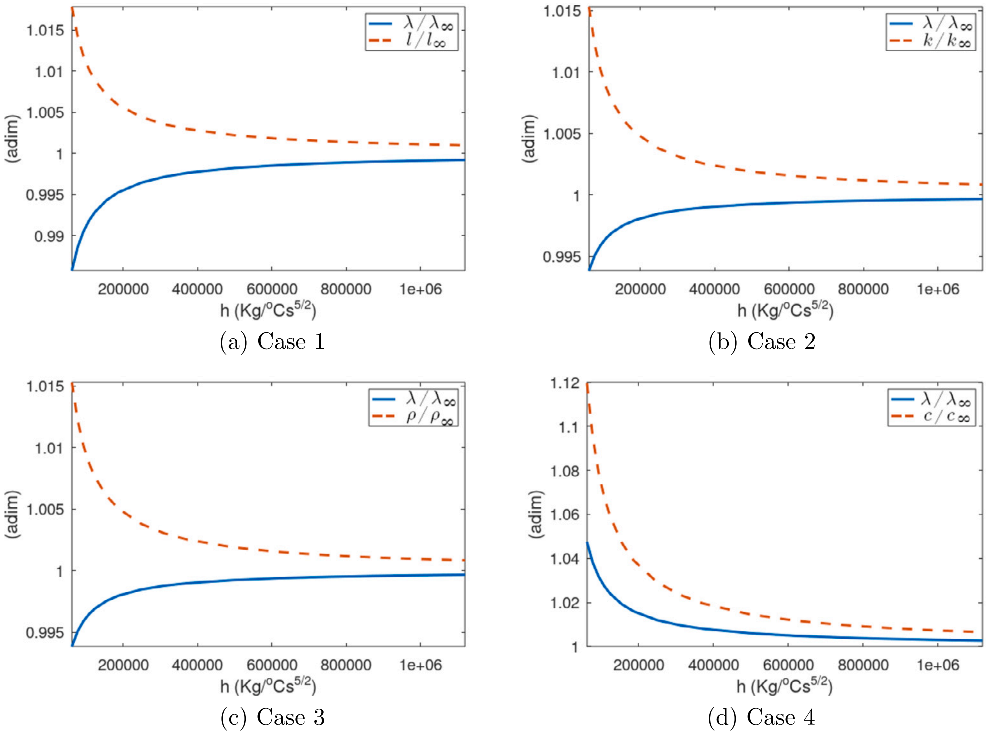
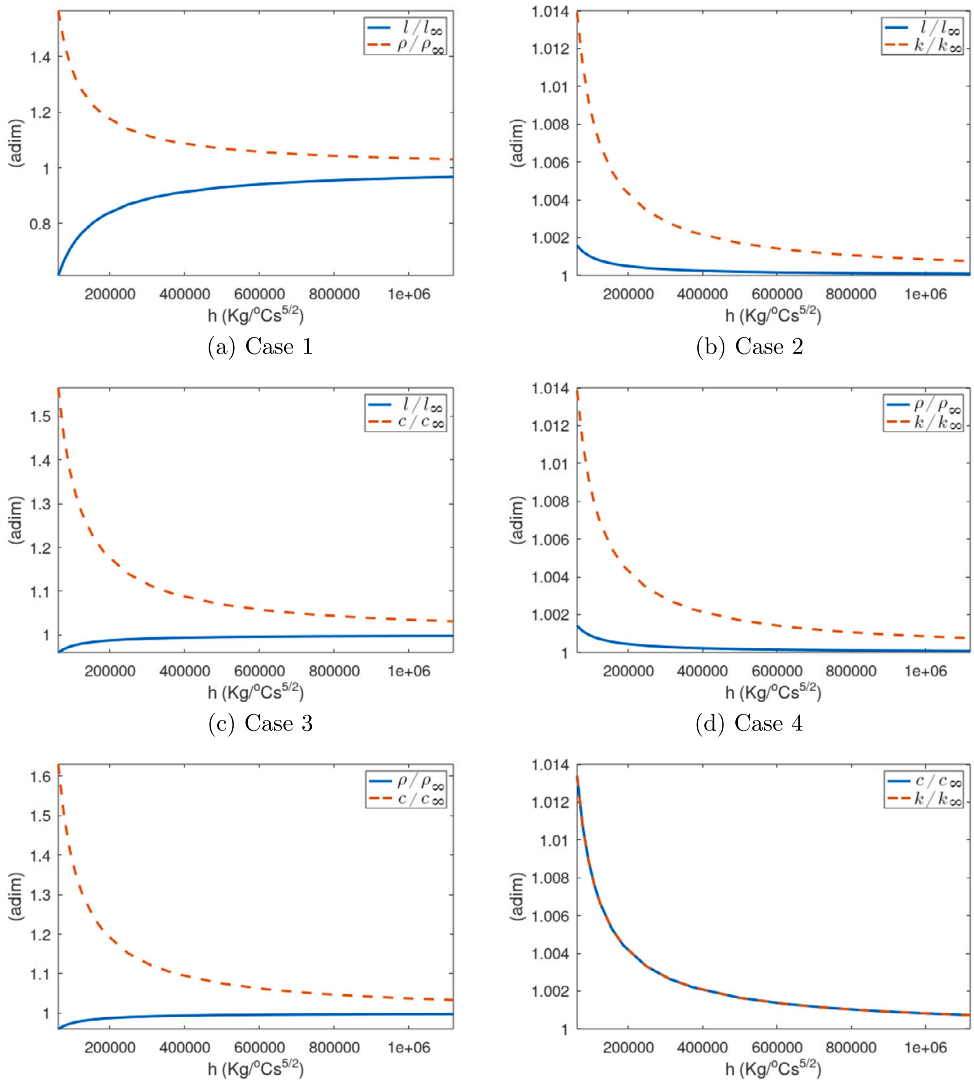


Fig. 1. Convergence for each unknown parameter, for the four cases of free boundary problems.

4.1. Free boundary problems

In Fig. 1 we plot, for each case, the convergence of each parameter normalized by the parameter of the limit problem (1_∞), for example, in Case 1, we plot $\frac{\lambda}{\lambda_\infty}$ and $\frac{l}{l_\infty}$. Note that from this normalization, we can deduce the relative error between the parameters, for example, if $\lambda/\lambda_\infty = 1.10$, then the relative error e_r is:



(a) Case 1 (b) Case 2
(c) Case 3 (d) Case 4
(e) Case 5 (f) Case 6

Fig. 2. Convergence for each unknown parameter, for the six cases of moving boundary problems.

$$e_r = \frac{\lambda - \lambda_\infty}{\lambda_\infty} = 0.10 = 10\%\,.$$

From Fig. 1, we observe that the case with the slowest convergence is Case 4, which needs values of $h \approx 3.7 \times 10^5$ to reach a relative error lower than 2% in both parameters. The rest of the cases have similar behavior of convergence, beginning with a relative error lower than 2% in both parameters, where $h \approx 6.2 \times 10^4$.

4.2. Moving boundary problems

In Fig. 2 we plot, for each case, the convergence of each thermal coefficient normalized by the parameter of the limit problem (1_∞).

We observe that the case with the slowest convergence is Case 1, with a similar behavior for both parameters, reaching a relative error lower than 4% for $h > 9 \times 10^5$. Next we have Case 3 and 5, where for both cases the parameter c has a slower convergence compared to the parameter l or ρ, for cases 3 and 5, respectively. Here, for both cases, the relative error for the specific heat is lower than 4% for $h > 9 \times 10^5$. Instead, the latent heat of fusion and the density starts with a relative error lower than 4%, for cases 3 and 5, respectively. Finally, the cases 2, 4 and 6 have the fastest convergence. In Cases 2 and 4, we have a similar situation as the one described before, where the conductivity k has a slower convergence compared to the parameter l and ρ, for Cases 2 and 4, respectively.

Note that Case 6 is the only case where the converging curves for the two coefficients coincide. Analyzing the corresponding equations, we observe that $\xi_\infty = \xi$, and when we compute k/k_∞ and c/c_∞ we get same result:

$$k/k_\infty = c/c_\infty = \frac{T_f - T_0}{(T_f - T_0) - \frac{q}{h}}.$$

5. Conclusions

We considered a phase-change process with two conditions at the boundary $x = 0$, a Robin and a Neumann type conditions. This overspecified condition allowed us to obtain formulae for the simultaneous determination of two unknown thermal coefficients. We state four cases of free boundary problems (the solid-liquid interface is unknown), and six cases of moving boundary problems (the solid-liquid interface is known a priori), where the formulae for the different cases where obtained by [6]. We analyzed the convergence of these problems to a solidification problem with Dirichlet and Neumann boundary conditions at the fixed face given in [21,22], when the heat transfer coefficient at this face goes to infinity.

For each case of the free and moving boundary problems, we present an upper bound for the parameter error, obtaining in every case a bound of order $o(\frac{1}{h})$. To prove these bounds, we had to study the dependence of auxiliary functions of the parameters h and x, given in Section 2.

Finally, at the numerical example we had that for the free boundary problems, Case 4 presents the slowest convergence, corresponding to the unknown parameters λ and c. For the moving boundary problems, Cases 1, 3 and 5 present similar convergence rate, which is overall slower than Cases 2, 4 and 6. We could justify analytically that in Case 6, corresponding to the unknown parameters k and c, the normalized curves coincide for both parameters.

Data availability

No data was used for the research described in the article.

Acknowledgements

The authors have been supported by CONICET, Argentina within the project PIP 0275, Universidad Austral, Rosario, Argentina, by the European Union's Horizon 2020 Research and Innovation Programme within the Marie Sklodowska-Curie grant agreement 823731 CONMECH, and by the research project 04/B251 of Universidad Nacional del Comahue.

References

[1] M.P. Akimov, S.D. Mordovskoy, N.P. Starostin, Calculating thermal insulation thickness and embedment depth of undergoing heat supply pipeline for permafrost soils, Mag. Civ. Eng. 46 (2) (2014) 14–23.
[2] S. Alpar, B. Rysbaiuly, Determination of thermophysical characteristics in a nonlinear inverse heat transfer problem, Appl. Math. Comput. 440 (2023) 127656.
[3] A. Borodin, A. Ivanova, Modeling of the temperature field of a continuously cast ingot with determination of the position of the phase-transition boundary, J. Eng. Phys. Thermophys. 87 (2) (2014) 507–512.
[4] B. Calusi, L. Fusi, A. Farina, On a free boundary problem arising in snow avalanche dynamics, ZAMM J. Appl. Math. Mech. 96 (4) (2016) 453–465.
[5] J.R. Cannon, The One-Dimensional Heat Equation, Addison-Wesley, Menlo Park, California, 1984.
[6] A. Ceretani, D. Tarzia, Determination of one unknown thermal coefficient through a mushy zone model with a convective overspecified boundary condition, Math. Probl. Eng. 2015 (2015) 1–8.
[7] G. Chen, H. Shahgholian, J.L. Vazquez, Free boundary problems: the forefront of current and future developments, Philos. Trans. R. Soc. A, Math. Phys. Eng. Sci. 373 (2015) 20140285.
[8] S.H. Cho, J.E. Suderland, Phase change problems with temperature-dependent thermal conductivity, Trans. Am. Soc. Mech. Eng. 96 (1974).
[9] Z.C. Deng, L. Yang, J.N. Yu, G.W. Luo, Identifying the diffusion coefficient by optimization from the final observation, Appl. Math. Comput. 219 (2013) 4410–4422.
[10] F. Erdoğdu, A review on simultaneous determination of thermal diffusivity and heat transfer coefficient, J. Food Eng. 86 (2008) 453–459.
[11] T.P. Fredman, A boundary identification method for an inverse heat conduction problem with an application in ironmaking, Heat Mass Transf. 41 (2004) 95–103.
[12] M. Gaudiano, G.A. Torres, C. Turner, On a convective condition in the diffusion of a solvent into a polymer with non- constant conductivity coefficient, Math. Comput. Simul. 80 (2009) 479–489.
[13] N.L. Gol'dman, Inverse Stefan problems, J. Eng. Phys. Thermophys. 65 (1993).
[14] T.C. Hou, S.J. Huang, C. Hsu, A new approach for determination of the coefficient of thermal expansion of asphalt concrete, Measurement 85 (2016) 222–231.
[15] M.J. Huntul, D. Lesnic, M.S. Hussein, Reconstruction of time-dependent coefficients from heat moments, Appl. Math. Comput. 301 (2017) 233–253.
[16] V. Kumar, U.S. Dixit, J. Zhang, Determination of thermal conductivity, absorptivity and heat transfer coefficient during laser-based manufacturing, Measurement 131 (2019) 319–328.
[17] B.L. Kurylyk, M. Hayashi, Improved Stefan equation correction factors to accommodate sensible heat storage during soil freezeng or thawing, Permafr. Periglac. Process. 27 (2) (2016) 189–203.
[18] I.O. Mohamed, Determination of an effective heat transfer coefficients for can headspace during thermal sterilization process, J. Food Eng. 79 (2007) 1166–1171.
[19] M. Pons, P. Dantzer, Determination transfer of thermal coefficient conductivity of hydrogen and storage wall heat materials, Int. J. Hydrog. Energy 19 (7) (1994) 611–616.
[20] R. Ramsaroop, P. Persad, Determination of the heat transfer coefficient and thermal conductivity for coconut kernels using an inverse method with a developed hemispherical shell model, J. Food Eng. 110 (2012) 141–157.
[21] D.A. Tarzia, Determination of the unknown coefficients in the Lamé-Clapeyron problem (or one-phase Stefan problem), Adv. Appl. Math. 3 (1982) 74–82.
[22] 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 Transf. 26 (1983) 1151–1158.

[23] D.A. Tarzia, Explicit and approximated solutions for heat and mass transfer problems with a moving interface, in: Mohamed El-Amin (Ed.), Advanced Topics in Mass Transfer, InTech Open Acces, Publishers, Rijeka (Croacia), 2011, pp. 439–484, Chapter 20.
[24] Y. Yu, D. Xu, On the inverse problem of thermal conductivity determination in nonlinear heat and moisture transfer model within textiles, Appl. Math. Comput. 264 (2015) 284–299.
[25] D. Zhou, C.Y. Zhao, Y. Tian, Review on thermal energy storage with phase change materials (PCMs) in building applications, Appl. Energy 92 (2012) 593–605.
[26] T. Zhou, J. Yuan, M. Li, Simultaneously estimate solid- and liquid-phase thermal conductivities, Int. Commun. Heat Mass Transf. 119 (2020) 104959.