MODELLING THERMAL PARAMETER ESTIMATION WITH AN INVERSE PHASE-CHANGE PROBLEM WITH TEMPERATURE-DEPENDENT CONDUCTIVITY

by

Natalia N. SALVA[a,b], Mara ROSSANI[c,d], and Domingo A. TARZIA[c,d]*

[a] CNEA-CONICET, Bariloche Atomic Center, Bariloche, Argentina
[b] National University of Comahue, Bariloche, Argentina
[c] Department of Mathematics, Austral University, Rosario, Argentina
[d] CONICET, Buenos Aires, Argentina

Original scientific paper
https://doi.org/10.2298/TSCI2604927S

Formulae are derived for the simultaneous determination of two unknown thermal coefficients in a semi-infinite material with temperature-dependent thermal conductivity. This is achieved through a phase-change process involving an over-specified condition on the fixed face (flux and convective boundary conditions) via a moving boundary problem (inverse Stefan problem). We perform a sensitivity analysis of the identified coefficients regarding variations in the remaining thermal parameters. This study is applied to ten different materials, representing distinct cases, considering both positive and negative slopes of thermal conductivity.

Keywords*: phase-change processes, unknown thermal coefficient, error function, moving boundary problem, convective boundary conditions, non-linear second order ordinary differential equation*

Introduction

In this work, we analyse a 1-D phase-change process describing the solidification of a homogeneous material, where the heat exchange at the fixed boundary is controlled by a convective (Robin) condition. This modelling choice provides a more realistic representation of the physical process compared to the classical Dirichlet condition, which implicitly assumes instantaneous transfer of external temperature to the material [1, 2].

Furthermore, while many studies assume constant thermophysical properties, experimental evidence shows that near the fusion temperature the thermal conductivity of several materials can be accurately modeled as a linear function of temperature [3]. Motivated by this observation, we consider a temperature-dependent thermal conductivity, resulting in a non-linear phase-change model. This class of problems appears in a wide variety of natural and industrial processes, including metal solidification, glass manufacturing, permafrost dynamics and snow avalanches, among many others [4]. Such processes are often modeled using free or moving boundary problems, whose mathematical analysis remains an active area of research due to both their theoretical complexity and their relevance in applications. We refer the reader to [5, 6] and the references therein for a survey on recent developments and open challenges in this field.

* Corresponding author, e-mail: dtarzia@austral.edu.ar

The development of exact similarity solutions for Stefan-type problems with temperature-dependent thermal conductivity traces back to the seminal work of Cho and Sunderland [7], who introduced the modified error function in the context of prescribed boundary temperature conditions. Subsequent research expanded this approach to include convective boundary conditions, leading to the creation of the generalized modified error function [8]. This research path offers a systematic method to derive similarity-type solutions by means of auxiliary non-linear ODE.

Determining thermophysical coefficients such as thermal conductivity, latent heat, specific heat, and density of mass is a key aspect of modelling phase-change processes. A common approach involves imposing additional boundary information, such as a prescribed flux boundary condition, resulting in overspecified Stefan problems that can help identify unknown coefficients. Several contributions in this area can be found in [9-12], where different combinations of boundary data are used to recover thermal parameters.

Recently, in [13], we introduced a new auxiliary function, the similar generalized modified error (SGME) function, and analyzed its analytical properties. This function allowed the development of similarity solutions for a class of free boundary Stefan problems with temperature-dependent thermal conductivity and convective boundary conditions. In this article, we expand this framework to a family of inverse Stefan problems involving a prescribed moving boundary of the form:

$$s(t) = 2\sigma\sqrt{t} \tag{1}$$

where the coefficient $\sigma > 0$ is determined throught experiments.

The main contribution of this work is the analytical determination of thermal coefficients in ten different moving boundary problems cases, where two unknown parameters are identified simultaneously along with the temperature distribution. Additionally, since inverse problems of this type are usually ill-posed [14, 15], we complement the theoretical results with a sensitivity analysis of the estimated parameters. Although numerous studies address the identification of thermal coefficients, sensitivity analyses are still relatively scarce in [14, 16]. Here, we conduct a case-by-case sensitivity analysis for ten different materials, including five with a positive thermal conductivity slope and five with a negative slope to evaluate the robustness of the identification process.

In section *Formulation fot the inverse moving phase problem*, we provide the mathematical formulation for determining one or two unknown thermal coefficients, with the expressions for these coefficients summarized in tab. 1. Finally, in section *Sensitivity analysis*, we present the sensitivity analysis.

Formulation for the inverse moving phase problem

We examine the following solidification problem for a semi-infinite material with two simultaneous boundary conditions at the fixed face $x = 0$, including a convective condition and a prescribed heat flux. This is modeled by the equations and conditions:

$$\rho c T_t(x,t) = \left[k\left(T(x,t)\right) T_x(x,t) \right]_x, \quad 0 < x < s(t), \quad t > 0 \tag{2a}$$

$$s(0) = 0 \tag{2b}$$

$$T(x,0) = T(+\infty,t) = T_f, \quad x > 0, \quad t > 0 \tag{2c}$$

$$T[s(t),t] = T_f, \quad t > 0 \tag{2d}$$

$$k(T_f)T_x[s(t),t] = \rho l\dot{s}(t),\ t > 0 \tag{2e}$$

$$k[T(x,t)]T_x(0,t) = \frac{h_0}{\sqrt{t}}[T(0,t) - T_\infty],\ t > 0 \tag{2f}$$

$$k[T(0,t)]T_x(0,t) = \frac{q_0}{\sqrt{t}},\ t > 0 \tag{2g}$$

where $T(x, t)$ is the temperature of the solid phase, $\rho > 0$ – the density of mass, $l > 0$ – the latent heat of fusion by unity of mass, $c > 0$ – the specific heat, $x = s(t)$ – the phase-change interface, T_f – the phase-change temperature, T_∞ – the external temperature at the fixed face $x = 0$ ($T_\infty < T_f$), h_0 – the coefficient characterizing the heat transfer coefficient at $x = 0$ given by eq. (2f), and q_0 – the coefficient characterizing the heat flux at $x = 0$ given by eq. (2g) which must be obtained experimentally through a phase-change process. The parameters mentioned earlier are all constant. We assume that the thermal conductivity is temperature-dependent and has the expression:

$$k(T) = k_0\left(1 + \beta\frac{T - T_\infty}{T_f - T_\infty}\right) \tag{3}$$

where $k_0 > 0$ and $\beta > -1$ are the given constants [7].

We note that the phase-change problem (2) with conditions eqs. (2a)-(2f) is a classical Stefan problem [2, 17]. We consider that the condition eq. (2g) is an overspecified condition at the fixed face $x = 0$, of the type described in [18]. We observe that if $\beta = 0$, then the problem (2) reduced to the classical one-phase Stefan problem with an overspecified condition at the fixed face $x = 0$ and the corresponding simultaneous determination of thermal coefficients for this problem was recently studied in [19]. In [13] we recently examined five instances of free boundary problems for this same phase-change problem (2), where the interface is also unknown. In this paper, we focus on moving boundary problems, where the interface is defined by the expression (1), characterized by a known coefficient $\sigma > 0$. We determine the temperature $T(x, t)$ and two thermal parameters for a moving boundary problem across the ten cases:

$$\begin{aligned} &\text{Case 1: } (\rho,l) \quad \text{Case 2: } (k_0,l) \quad \text{Case 3: } (c,l) \quad \text{Case 4: } (k_0,\rho) \quad \text{Case 5: } (\rho,c) \\ &\text{Case 6: } (k_0,c) \quad \text{Case 7: } (\beta,l) \quad \text{Case 8: } (\beta,k_0) \quad \text{Case 9: } (\beta,\rho) \quad \text{Case 10: } (\beta,c) \end{aligned} \tag{4}$$

As in [13], we can obtain a similarity solution to problem (2), where the temperature $T(x, t)$ can be written as a function of the single variable

$$\eta = \frac{x}{2\sqrt{\alpha_0 t}} \text{ and } \alpha_0 = \frac{k_0}{\rho c}$$

is the thermal diffusivity.

Proposition 1. If the moving boundary $s(t)$ is given by eq. (1), with $\sigma > 0$, then the inverse Stefan problem (2) has the similarity solution T given by:

$$T(x,t) = (T_f - T_\infty)\,\varphi\left(\frac{x}{2\sqrt{\alpha_0 t}}\right) + T_\infty,\ \text{if}\ \ 0 < x < s(t),\ t > 0 \tag{5}$$

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

$$\varphi'(0) = \frac{2h_0}{\sqrt{k_0 \rho c}} \frac{\varepsilon_0}{(1+\varepsilon_0 \beta)} \tag{6a}$$

$$\varphi'\left(\sigma\sqrt{\frac{\rho c}{k_0}}\right) = \sigma\sqrt{\frac{\rho c}{k_0}} \frac{2l}{(1+\beta)c(T_f - T_\infty)} \tag{6b}$$

where φ is the SGME function, defined in [13], that satisfies the ordinary differential problem:

$$\begin{gathered} \left\{\left[1+\beta\varphi(\eta)\right]\varphi'(\eta)\right\}' + 2\eta\varphi'(\eta) = 0, \quad 0 < \eta < \zeta \\ \varphi(0) = \varepsilon_0 \\ \varphi(\zeta) = 1 \end{gathered} \tag{7}$$

and the additional parameter $\zeta > 0$ satisfies:

$$\zeta = \sigma\sqrt{\frac{\rho c}{k_0}} \tag{8}$$

assuming that

$$\varepsilon_0 = \frac{q_0}{h_0(T_f - T_\infty)}$$

satisfies the condition $\varepsilon_0 < 1$.

Proof 1. When we look for a similarity solution problem, the temperature $T(x, t)$ is a function of the single variable

$$\eta = \frac{x}{2\sqrt{\alpha_0 t}}$$

Through eqs. (2a), (2d), (2f), and (2g) we obtain the differential problem (7) for the SGME function. Using the rest of the equations in problem (2), we obtain that the equations in eq. (6) must be satisfy for the thermal coefficients.

Considering that the solution φ of the problem (7) depends on the parameters $\beta > 0$ and $\zeta > 0$, and that ζ depends on k_0, ρ, and c, we should note that whenever we need to calculate φ, there is an iterative process involved, because it depends on the unknown parameters being determined.

We remark that the solution of the ordinary differential problem (7) is similar to the generalized modified error function defined in [8], and presents some characteristic features of the classical error function, such as monotony, concavity, and boundedness [13]. For simplicity in the presented formulae, we define an auxiliary real function:

$$F_1(x) = \frac{\varphi'(x)}{x} \tag{9}$$

which properties were analyzed in [13].

The following proposition derives the formulae for Case 1. The remaining nine cases are summarized in tab. 1 due to space limitations and their derivations are similar to the case presented.

Table 1. Formulae for the unknown thermal coefficients for the ten cases with moving boundary formulation

Case number	Unknown coefficient	Solution
1	ρ, l	$l=\frac{c(1+\beta)(T_f-T_\infty)}{2}F_1(\zeta),\ \rho=\frac{\zeta^2}{\sigma^2}\frac{k_0}{c}$ where ζ is the unique solution of eq. (11)
2	k_0, l	$l=\frac{c(1+\beta)(T_f-T_\infty)}{2}F_1(\zeta),\ k_0=\frac{\sigma^2}{\zeta^2}\rho c$ where ζ is the unique solution of: $\frac{\varphi'_\zeta(0)}{\zeta}=\frac{2h_0\varepsilon_0}{\sigma\rho c(1+\varepsilon_0\beta)},\ \zeta>0$
3	c, l	$l=\frac{\zeta^2}{\sigma^2}\frac{k_0}{\rho}\frac{(1+\beta)(T_f-T_\infty)}{2}F_1(\zeta),\ c=\frac{\zeta^2}{\sigma^2}\frac{k_0}{\rho}$ where ζ is the unique solution of eq. (11)
4	k_0, ρ	$k_0=\frac{2h_0\varepsilon_0}{1+\beta\varepsilon_0}\frac{\sigma}{\zeta\varphi'_\zeta(0)},\ \rho=\frac{2h_0\varepsilon_0}{\sigma c(1+\beta\varepsilon_0)}\frac{\zeta}{\varphi'_\zeta(0)}$ where ζ is the unique solution of: $F_1(\zeta)=\frac{2l}{(1+\beta)c(T_f-T_\infty)}$
5	ρ, c	$c=\frac{2l}{(1+\beta)(T_f-T_\infty)}\frac{1}{F_1(\zeta)},\ \rho=\frac{k_0(1+\beta)(T_f-T_\infty)}{2l\sigma^2}\zeta^2F_1(\zeta)$ where ζ is the unique solution of eq. (11)
6	k_0, c	$c=\frac{2l}{(1+\beta)(T_f-T_\infty)F_1(\zeta)},\ k_0=\frac{2\rho l\sigma^2}{(1+\beta)(T_f-T_\infty)}\frac{1}{\zeta\varphi'(\zeta)}$ where ζ is the unique solution of: $\frac{\varphi'_\zeta(0)}{\zeta}=\frac{(1+\beta)(T_f-T_\infty)h_0\varepsilon_0}{\rho l\sigma(1+\beta\varepsilon_0)}F_1(\zeta),\ \zeta>0$
7	β, l	$\beta=\frac{1}{\varepsilon_0}\left(\frac{2h_0\varepsilon_0}{\varphi'(0)\sqrt{k_0\rho c}}-1\right),\ l=\frac{F_1(\zeta)c(T_f-T_\infty)}{2\varepsilon_0}\left[\frac{2h_0\varepsilon_0}{\varphi'(0)\sqrt{k_0\rho c}}-(1-\varepsilon_0)\right]$ where ζ is given by eq. (8), with the data restriction $\varphi'_\beta(0)<\frac{2h_0\varepsilon_0}{\sqrt{\rho c k_0}}$
8	β, k_0	$\beta=\frac{2l}{c(T_f-T_\infty)F_1(\zeta)}-1,\ k_0=\frac{\rho c\sigma^2}{\zeta^2}$ where ζ is the unique solution of: $\frac{\zeta}{\varphi'_\zeta(0)}=\frac{\rho c\sigma}{2h_0\varepsilon_0}\left[(1-\varepsilon_0)+\frac{2l\varepsilon_0}{c(T_f-T_\infty)F_1(\zeta)}\right],\ \zeta>0$

→

Table 1. Continuation

9	β, ρ	$\beta = \dfrac{2l}{c(T_f - T_\infty)F_1(\zeta)} - 1,\ \rho = \dfrac{\zeta^2}{\sigma^2}\dfrac{k_0}{c}$ where ζ is the unique solution of: $\zeta\varphi'_\zeta(0)\left[(1-\varepsilon_0) + \dfrac{2l\varepsilon_0}{c(T_f - T_\infty)F_1(\zeta)}\right] = \dfrac{2\sigma\varepsilon_0 h_0}{k_0},\ \zeta > 0$
10	β, c	$c = \dfrac{\zeta^2}{\sigma^2}\dfrac{k_0}{\rho},\ \beta = \dfrac{2l\rho\sigma^2}{(T_f - T_\infty)k_0}\dfrac{1}{\zeta^2 F_1(\zeta)} - 1$ where ζ is the unique solution of: $\zeta\varphi'_\zeta(0)\left[(1-\varepsilon_0) + \dfrac{2l\rho\varepsilon_0\sigma^2}{(T_f - T_\infty)k_0}\dfrac{1}{\zeta\varphi'(\zeta)}\right] = \dfrac{2\sigma\varepsilon_0 h_0}{k_0},\ \zeta > 0$

Proposition 2. If the moving boundary is given by eq. (1), then the temperature of problem (2) with unknown thermal coefficients $\{\rho, l\}$ is given by eq. (5), and ρ, and l are given by the following expressions:

$$l = \frac{c(1+\beta)(T_f - T_\infty)}{2} F_1(\zeta) \tag{10a}$$

$$\rho = \frac{\zeta^2}{\sigma^2}\frac{k_0}{c} \tag{10b}$$

where ζ is the solution of the equation:

$$\zeta\varphi'_\zeta(0) = \frac{2\varepsilon_0 h_0 \sigma}{(1+\varepsilon_0\beta)k_0},\ \zeta > 0 \tag{11}$$

Proof 2. Recall that the differential system for the similar generalized modified error function depends on the variable ζ defined in eq. (8), from which expression (10b) immediately follows. From the eq. (6b) the expression (10a) is also obtained. Substituting eq. (10b) into (6a), we arrive at the non-linear eq. (11) which determines the parameter ζ. We note that the right-hand side of eq. (11) is a positive constant depending only on the given data. Moreover, for $\zeta > 0$, the left-hand side of eq. (11) is a continuous and strictly increasing function of ζ, since $\varphi'_\zeta(0) > 0$ and tends to zero as $\zeta \to 0^+$. Therefore, by the intermediate value theorem, there exists a unique solution $\zeta > 0$ of eq. (11).

Consequently, the thermal coefficients ρ and l are uniquely determined by eq. (10).

Sensitivity analysis

In this section we analyze the sensitivity of the parameters involved in the identification process, specifically, how small perturbations in the input data affect the parameters being determined. We present a case-by-case sensitivity analysis for ten different materials: five with a positive thermal conductivity slope β (Fe, Se, U, Ni, and Nb), and five with a negative slope (Al, Cu, Sn, Li, and Ag). The thermal data was obtained from [3].

In tab. 2 we show all the parameters used for each material. Note that some parameters in these tables are obtained directly from [3, 20] (k_0, β, ρ, c, l, T_f), others are assumed (h_0, T_∞), and others are determined (ζ, ε_0, q_0) solving the whole problem (2).

For the sensitivity analysis, we compute the sensitivity of a coefficient A relative to another parameter B, which is the partial derivative of A with respect to B. To assess how known parameters influence unknown coefficients, and to enable comparison of sensitivities, we define the dimensionless normalized sensitivity [21]:

$$S(A,B) := \frac{B}{A}\frac{\partial A}{\partial B} \tag{12}$$

Due to its dimensionless nature, we can compare the sensitivities of parameters with different magnitudes. The normalized sensitivity indicates the percentage change in the value of parameter A when variable B increases or decreases by 1% of its value [22, 23]. This definition is similar to what is called elasticity in economics. In each case of moving boundary problems, the coefficient A is one of the thermal coefficients determined simultaneously, and the coefficient B chosen from the set of thermal coefficients used as data.

Table 2. Thermal coefficients for materials with positive and negative conductivity slope

Parameter	Units	Materials				
		Fe	Se	U	Ni	Nb
k_0	[$Js^{-1}m^{-1}°C^{-1}$]	31.83	6.4954	48.417	81.128	82.156
β	adim.	0.087043	0.10829	0.11929	0.076647	0.076212
ρ	[kgm^{-3}]	7874	4819	19050	8908	8570
c	[$Jkg^{-1}°C^{-1}$]	449.41	321.17	116.37	444.7	264.77
l	[Jkg^{-1}]	247090	68389	58816	293063	288451
h_0	[$kg°C^{-1}s^{-5/2}$]	1e+05	1e+05	1e+05	1e+05	1e+05
T_∞	[°C]	1229.5	173.64	905.96	1162.3	1974.3
T_f	[°C]	1536.8	217.05	1132.5	1452.8	2467.8
ζ	adim.	0.47511	0.3101	0.43312	0.40868	0.42324
q_0	[$kgs^{-5/2}$]	3428312.7	228953.0	2695502.7	5654695.5	7459668.9
		Al	Cu	Sn	Li	Ag
k_0	[$Js^{-1}m^{-1}°C^{-1}$]	219.38	346.41	67.743	71.897	370.62
β	adim.	–0.036594	–0.047061	–0.025527	–0.021984	–0.041758
ρ	[kgm^{-3}]	2700	8920	7310	535	10498
c	[$Jkg^{-1}°C^{-1}$]	904.37	384.42	217.33	3573.5	235.46
l	[Jkg^{-1}]	396590	206137	58967	432276	104756
h_0	[$kg°C^{-1}s^{-5/2}$]	$1{\cdot}10^{05}$	$1{\cdot}10^{05}$	$1{\cdot}10^{05}$	$1{\cdot}10^{05}$	$1{\cdot}10^{05}$
T_∞	[°C]	528.04	866.28	185.53	144.44	768.68
T_f	[°C]	660.05	1082.8	231.91	180.55	960.85
ζ	adim.	0.3165	0.34602	0.25868	0.34015	0.36707
q_0	[$kgs^{-5/2}$]	3560956.5	7241494.4	779500.5	542592.4	5681390.7

We will approximate $S(A, B)$ by the following central difference quotient of the derivative:

$$S(A,B) \approx \frac{B}{A(B)}\frac{A(B^+) - A(B^-)}{B^+ - B^-} \tag{13}$$

where $B^+ = B + \epsilon|B|$, $B^- = B - \epsilon|B|$, $\epsilon > 0$ and $A(B)$, $A(B^+)$, and $A(B^-)$ represents the determination of parameter A, considering as data the parameter B, B^+, or B^-, respectively.

We used the free software SCILAB* for the numerical analysis. For each case, the parameters depend on a additional variable ζ, which is the solution of certain equation, for example in Case 1 ζ is the solution of eq. (11). Note that this equation involves the SGME function. To find the solution of the equation, we used the Levenberg-Marquardt algorithm, for non-linear equations. The command bvodeS was used to solve the differential problem (7), which allowed us to evaluate the SGME function at the necessary points. Finally, using the calculated value of ζ, we evaluated the unknown thermal coefficients.

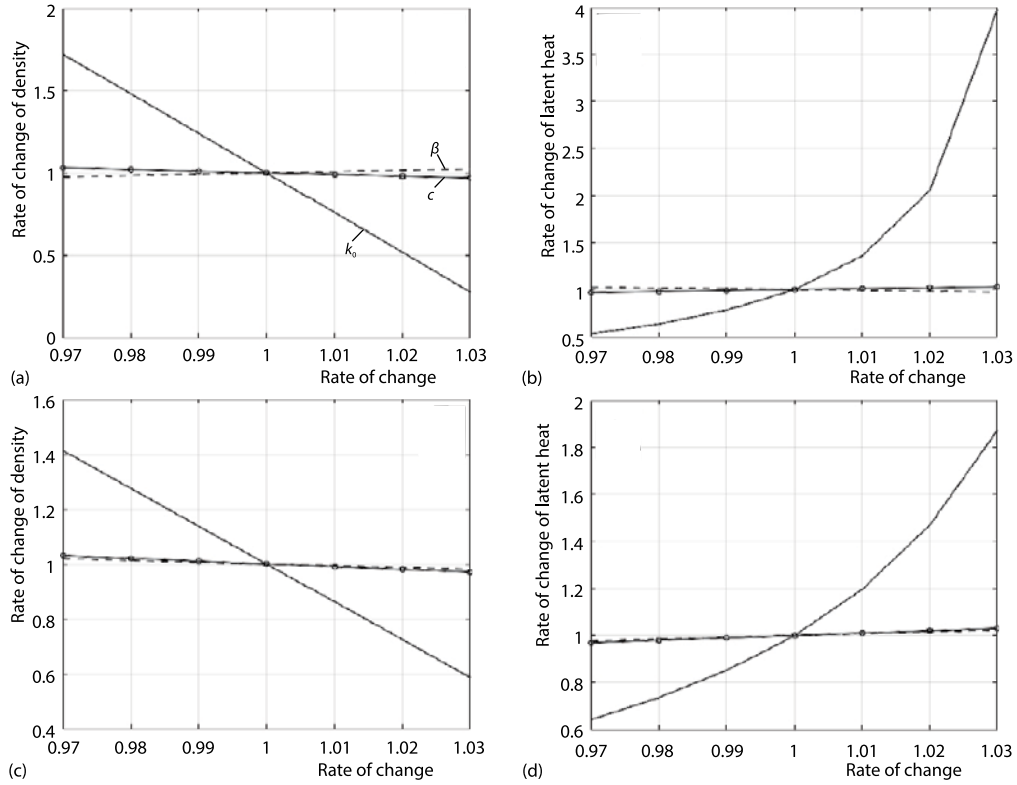


Figure 1. Variation of the normalized parameters for Case 1; (a) and (b) correspond to ρ and l, respectively, for Cu, and (c) and (d) correspond to ρ and l, respectively, for Fe

Firstly, we show the sensitivity plots, for Case 1, for two materials: Cu and Fe. In fig. 1 we plot the normalized values of the parameter ρ and l, *vs.* the normalized values of the data coefficients (k_0, β, and c), that is $A(B^*)/A(B)$ as a function of B^*/B, where $A(B^*)$ represents the determination of parameter A, considering the parameter B as data. For example, in fig. 1(a), for Cu, we show on the x-axis the relative change of the three parameters k_0, β, and, c, and on the y-axis the relative change of the density. When $x = 1.01$, this means that, for example, $k_0^+/k_0 = 1.01$, which implies that $k_0^+ = 1.01k_0 = k_0 + 1\%k_0$. The new value of k_0 represents an increment of 1% of the original value of k_0. That is, instead of being 346.41 J/sm°C, we take 349.87 J/sm°C. Then we compute the density value using the corresponding formula in tab. 1. This new value of the density corresponds to a decrement of around 25% of the original value. In the plot, we have $y = 0.759$, that is, $\rho^+/\rho = 0.759$, which implies that $\rho^+ = \rho - 0.241\rho$.

* https://www.scilab.org

In other words, the value of ρ decreases by 24.1%. Instead of being 8920 kg/m^3, it is equal to 6769.5 kg/m^3 when k_0 = 349.87 J/sm°C.

Note that the scales on the x- and y-axes are not identical: while the x-axis ranges from 0.97-1.03, the y-axis spams from 0.2-1.8. This can be slightly misleading, because although the parameters on the x-axis change by up to 3%, the density varies by up to 80% of its value. The slope of the line corresponding to k_0 at $x = 1$ equals the normalized sensitivity, which in this case is –24.07. The sign of the normalized sensitivity relates to the relationship between the parameters; here, the sensitivity is negative, indicating that ρ is inversely proportional to k_0. In other words, when k_0 increases, ρ decreases.

Another interesting feature observed in fig. 1 is the parabolic shape of the curves corresponding to k_0 in the plots for the determination of the latent heat, l. In almost all cases, these curves are linear. The parabolic shape on the right-hand side of $x = 1$ indicates that sensitivity increases as the error in the data parameter k_0 increases. Note that on the left-hand side of $x = 1$ the curves are also slightly parabolic. However, in this region, sensitivity decreases as the value of k_0 decreases. Therefore, in this case, sensitivity is not symmetric with respect to increases and decreases in the data parameter.

Secondly, we want to point out that all parameters are positive, except for the one related to the slope of the thermal conductivity, namely β. In fig. 1(a), the line corresponding to β has a positive slope, which means, the normalized sensitivity is positive. Recall that $\beta < 0$ for Cu. Therefore, if we increase its value by 1%, we get

$$\beta^+ = \beta + \frac{1}{100}\beta = \beta - 0.01|\beta| = -0.046590$$

compared to –0.047061 (value given for Cu in 2). Note that the magnitude of β^+ is smaller than that of β. For this new value of β, the density is slightly higher, because it is multiplied by 1.007. On the other hand, for Iron, in fig. 1(c), we see a negative normalized sensitivity for the parameter β. Recall that $\beta > 0$ for Fe. This opposite behavior between materials with positive and negative thermal conductivity slopes occurs whenever the parameter β is involved.

Table 3. Sensitivity of the parameter β in Case 7 for different materials

Material	Al	Cu	Sn	Li	Ag
k_0	96.977	60.059	226.95	290.33	76.449
ρ	3.3372	2.4944	5.1614	11.425	3.5603
c	3.3372	2.4944	5.1614	11.425	3.5603
Material	Fe	Se	U	Ni	Nb
k_0	–96.982	–170.89	–67.462	–64.582	–83.035
ρ	–7.0295	–5.2031	–3.9844	–3.4658	–4.7901
c	–7.0295	–5.2031	–3.9844	–3.4658	–4.7901

To illustrate this behavior, we show in tab. 3 the sensitivity of the parameter β for Case 7, covering all the materials considered. For materials with a negative thermal conductivity slope, the sensitivities concerning the data (k_0, ρ, c) are all positive, in contrast, for the other materials, the sensitivities are all negative. This fact can be explained by the definition of sensitivity: in eq. (13), the values are normalized by multiplying or dividing by the unaltered parameters. Therefore, the sign of the parameters influences the calculation of the normalized sensitivity, and it is expected that changing in the sign of a parameter results in a change in the sign of the sensitivity.

We also choose Case 7 because it shows the highest normalized sensitivities among all the cases. In tab. 3, we highlight in orange sensitivities above than 10%, and in red those above than 40%. Here, we observe that the most sensitive materials are Sn, Li, and Se, a behavior that is also observed in almost all the other cases.

Thirdly, in fig. 2(a) we show the relationship between the specific heat and the parameter ρ for Case 6. Here, we observe that Sn is the most sensitive material, as it exhibits the greatest relative change with the steepest slope (the curve with black circles). Conversely, the material with the smallest slope is Fe, identified by the gray circles. This figure highlights the dependence of the sensitivities on the material considered. Conducting this type of analysis is crucial because the inverse problems related to moving boundary Stefan problems do not behave the same across different materials. In fig. 2(b) we show, for the same case, the relationship between the specific heat and the parameter k_0. In this case, the sensitivities are very similar, which is why a zoomed-in section of the graph is presented. If a statistical analysis were performed on the values plotted in this figure, the resulting standard deviation would be close to zero.

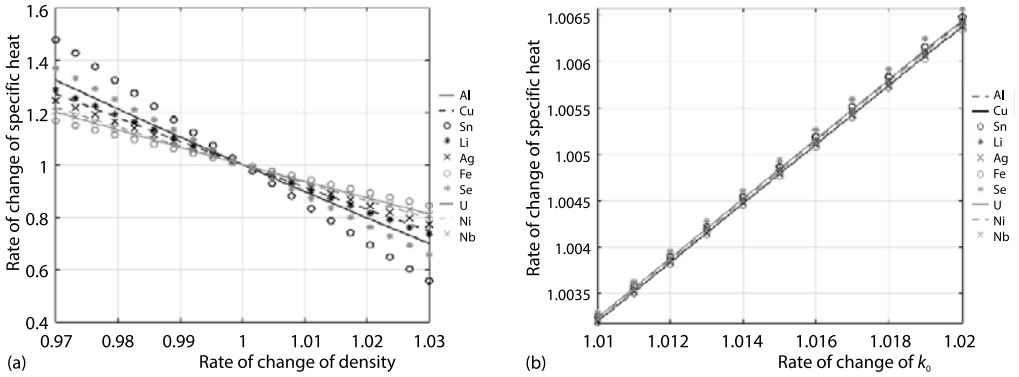


Figure 2. Parametric change of c in Case 6 for different materials; (a) *vs.* the relative change of ρ and (b) *vs.* the relative change of k_0

Finally, in tab. 4 we present, case-by-case, the sign, minimum, maximum, mean, and standard deviation of the normalized sensitivities given by eq. (13), analyzing the ten materials as data. Note that the sign of the sensitivity is sometimes multiplied by the sign of β, $sg(\beta)$, because of the opposite behavior between materials with positive and negative thermal conductivity slopes as explained earlier in fig. 1. In this tab. 4 we colored with yellow the mean sensitivities higher than 5%, with orange the ones higher than 10%, and with red the ones higher than 40%.

There are two cases where the sensitivities and the standard deviation are generally low, which measures how spread out the data points are from the mean sensitivity; these are Cases 2 and 4. The highest sensitivity in these cases appears in Case 2, with a value of 1.22% for the parameter l relative to the density ρ. This indicates that when ρ increases by 1%, the latent heat of fusion l also increases by 1.22%. The next case in order of increasing sensitivity is Case 6, which has a maximum sensitivity of 15.3% for the specific heat with respect to ρ.

In Cases 1, 3, and 5, the unknown parameters tend to have higher sensitivities relative to the parameter associated with the initial thermal conductivity, k_0. For the remaining known parameters, the sensitivities are less than 5%. We can state that for all the analyzed materials, k_0 is the most sensitive parameter, that is when k_0 is a data, the unknown parameters are sensible to k_0. A small perturbation in k_0 causes a large change in the value of the parameters being esti-

Table 4. Statistics in sensitivities for the ten different cases

Case	Parametre	Sign	Minimum	Maximum	Mean	Standard deviation	Sign	Minimum	Maximum	Mean	Standard deviation
				ρ					l		
1	k_0	–	13.7	43.9	24.3	9.048	+	17.2	58.4	30.04	12.2
	β	–sg(β)	0.32	1.7	0.806	0.38	+sg(β)	0.36	1.93	0.91	0.421
	c	–	0.99	1	1	0.0002	+	0.99	1	0.99	0.0002
				k_0					l		
2	β	–sg(β)	0.012	0.062	0.035	0.016	+sg(β)	0.0002	0.0029	0.0013	0.0009
	ρ	–	0.022	0.072	0.045	0.015	–	1.06	1.22	1.14	0.047
	c	–	0.022	0.072	0.045	0.015	–	0.069	0.22	0.14	0.047
3				c					l		
	k_0	–	13.7	43.9	24.3	9.048	+	3.02	3.13	3.09	0.032
	β	–sg(β)	0.32	1.7	0.806	0.385	+sg(β)	0.0401	0.196	0.112	0.051
	ρ	–	0.99	1	1	0.0002	–	1	1	1	0.00003
4				k_0					ρ		
	β	–sg(β)	0.012	0.062	0.036	0.016	+sg(β)	0.0002	0.0024	0.0011	0.0008
	c	–	0.021	0.059	0.039	0.011	–	0.065	0.18	0.12	0.036
	l	+	0.021	0.059	0.039	0.011	–	0.43	0.47	0.45	0.012
5				ρ					c		
	k_0	+	3.02	3.13	3.09	0.032	–	16.9	47.06	27.4	9.03
	β	+sg(β)	0.0401	0.19	0.112	0.051	–sg(β)	0.36	1.93	0.91	0.42
	l	–	1	1	1	0.00003	+	0.99	1	1	0.0002
6				k_0					c		
	β	–sg(β)	0.012	0.063	0.036	0.016	+sg(β)	0.003	0.016	0.0087	0.0048
	ρ	+	0.31	0.33	0.32	0.003	–	5.39	15.3	8.88	2.99
	l	+	0.31	0.33	0.32	0.003	–	4.39	14.3	7.87	2.99
7				β					l		
	k_0	–sg(β)	60.05	290.3	123.3	79.3	–	1.88	15.6	5.36	3.96
	ρ	–sg(β)	2.49	11.4	5.04	2.58	–	1.18	1.71	1.37	0.18
	c	–sg(β)	2.49	11.4	5.04	2.58	–	0.18	0.71	0.37	0.18
8				β					k_0		
	ρ	+sg(β)	11.9	59.8	31.08	16.3	–	0.1002	0.64	0.34	0.16
	c	+sg(β)	1.01	6.51	3.53	1.51	–	0.036	0.11	0.082	0.028
	l	+sg(β)	10.9	53.3	27.5	15.1	–	0.063	0.53	0.26	0.14
9				β					ρ		
	k_0	–sg(β)	51.7	243.7	102.8	67.7	–	1.55	9.97	3.73	2.39
	c	–sg(β)	2.06	8.54	3.64	1.86	–	0.15	0.41	0.26	0.092
	l	+sg(β)	2.06	8.54	3.64	1.86	–	0.58	0.84	0.73	0.092
10				β					c		
	k_0	–sg(β)	22.7	105.4	47.2	27.6	–	8.94	27.51	14.2	7.1
	ρ	+sg(β)	7.3	33.9	15.2	8.93	–	2.41	6.52	4.24	1.5
	l	+sg(β)	7.3	33.9	15.2	8.93	–	1.41	5.51	3.24	1.5

mated. In contrast, there are cases where the mean sensitivity is higher than 50%, namely Cases 7-10. These mentioned high sensitivities appear when calculating the parameter β. For example, in Case 7 we have the highest sensitivity, of 290% when calculating β and analyzing k_0, for Li, see tab. 3. The mean sensitivity for this specific set of parameters is 123.3%. Case 9 also shows a very high sensitivity, when calculating β and analyzing k_0, with a mean sensitivity of 102.3%.

Conclusion

We examined a phase-change process with two conditions at the fixed boundary $x = 0$, a Robin and a Neumann conditions. This overspecified condition enabled us to derive formulae for simultaneously determining two unknown thermal coefficients in moving boundary problems. Although, in theory, ten different cases can be defined for parameter determination, the sensitivity analysis shows that some of these cases are not suitable for estimating certain parameters due to excessively high sensitivities, especifically Cases 7-10. It is important to conduct this type of analysis because the inverse problems considered for moving boundary Stefan problems do not behave the same way for all materials.

Acknowledgment

The authors have been supported by Projects O06-25CI2002 and O06-25CI2004 from Austral University, Rosario, Argentina, and by the Research Project 04/B251 of Universidad Nacional del Comahue.

References

[1] Alexiades, V., Solomon, A. D., *Mathematical Modelling of Melting and Freezing Processes*, Hemisphere Publishing Corp., Washington, USA, 1993
[2] Carslaw, H. S., Jaeger, C. J., *Conduction of Heat in Solids*, Clarendon Press, Oxford, UK, 1959
[3] Touloukian, Y. S., *et al*., *Thermal conductivity of Metallic Elements and Alloys*, IFI/PLENUM, New York-Washington, USA, 1970
[4] Lunardini, V. J., *Heat Transfer with Freezing and Thawing*, Elsevier, Amsterdam, The Netherlands, 1991
[5] Chen, G., *et al*., Free Boundary Problems: The Forefront of Current and Future Developments, *Phil. Trans. R. Soc*., *373A* (2015), 20140285
[6] Tarzia, D. A., Explicit and Approximated Solutions for Heat and Mass Transfer Problems with a Moving Interface, (Ed. El-Amin, M.), in: *Advanced Topics in Mass Transfer*, InTech Open Acces Publishers, Rijeka, Croacia, 2011, Chapter 20, pp. 439-484
[7] Cho, S. H., Suderland, J. E., Phase Change Problems Wwth Temperature-Dependent Thermal Conductivity, *Transactions of the ASME, J. Heat Transfer*, *96C* (1974), 2, pp. 214-217
[8] Ceretani, A. M., *et al*., An Exact Solution for A Stefan Problem with Variable Thermal Conductivity and a Robin Boundary Condition, Non-Linear Analysis, *Real World Applications*, *40* (2018), Apr., pp. 243-259
[9] Inatomi, Y., *et al.*, Density and Thermal Conductivity Measurements for Silicon Melt by Electromagnetic Levitation under a Static Magnetic Field, *Int. J. Thermophysics*, *28* (2007), Feb., pp. 44-59
[10] Lamvik, M., Zhou, J. M., A Novel Technique for Measuring the Thermal Conductivity of Metallic Materials during Meeting And Solidification, *Meas. Sci. Technol*., *6* (1995), 7, pp. 880-887
[11] Salva, N. N., Tarzia, D. A., Simultaneous determination of Unknown Coefficients through Phase-Change Process with Temperature-Dependent Thermal Conductivity, *JP Journal of Heat and Mass Transfer*, *5* (2011), 1, pp. 11-39
[12] Tarzia, D. A., The Determination of Unknown Thermal Coefficients Through Phase Change Process with Temperature-Dependent Thermal Conductivity, *Int. Comm. Heat Mass Transfer*, *25* (1998), 1, pp. 139-147
[13] Salva, N. N., *et al*., Determination of One Thermal Coefficient through an Overspecified Stefan Problem with Temperature-Dependent Thermal Conductivity, Considering Flux And Convective Boundary Conditions, *Int. J. App. and Comp. Math*., *12* (2026), 31, pp. 1-19
[14] Blackwell, B. F., Dowding, K. J., Handbook of Numerical Heat Transfer, in: *Sensitivity Analysis ans Uncertainty Propagation of Computational Models*, Kluwer Academic, Amsterdam, The Netherlands, 1989, Chapter 14

[15] Deng, Z. C., *et al.*, Optimization Method for an Evolutional Type Inverse Heat Conduction Problem, *J. Phys. A: Math. Theor*, *41* (2008), 035201
[16] Benke, K. K., *et al*., Parameter Uncertainty, Sensitivity Analysis and Prediction Error in A Water-Balance Hydrological Model, *Mathematical and Computer Modelling*, *47* (2008), 11-12, pp. 1134-1149
[17] Tarzia, D. A., Relationship between Neumann Solution for the Two-Phase Lame-Clapeyron-Stefan Problem with Convective and Boundary Conditions, *Thermal Science*, *21* (2017), 1A, pp. 187-197
[18] Tarzia, D. A., An Inequality for the Coefficient σ of the free boundary $s(t) = 2\sigma(t)^{1/2}$ of the Neumann Solution for the Two-Phase Stefan Problem, *Quart. Appl . Math*., *39* (1981), 4, pp. 491-497
[19] Salva, N. N., Tarzia, D. A., Relationship between Two Solidification Problems in Order to Determine Unknown Thermal Coefficients When the Heat Transfer Coefficient Is Very Large, *Applied Mathematics and Computation*, *468* (2024), 128524
[20] Lide, D. R., *The CRC Handbook of Chemistry and Physics*, 82nd ed., CRC Press, Boca Raton, Fla., USA, 2001
[21] Marinetti, S., Vavilov, V., Sensitivity Analysis of Classical Heat Conduction Solutions Applied to Materials Characterization, *Heat Transfer Engineering*, *26* (2005), 9, pp. 50-60
[22] Colin, E., *et al*., A General Sensitivity Equation Formulation for Turbulent Heat Transfer, *Numerical Heat Transfer*, *49* (2006), 2, pp. 125-153
[23] Imani, A., *et al*., Simultaneous Estimation of Temperature- Dependent Thermal Conductivity and Heat Capacity Based on Modified Genetic Algorithm., *Inverse Probl. Sci. Eng*., *14* (2006), 7, pp. 767-783

Paper submitted: December 20, 2025
Paper revised: February 15, 2026
Paper accepted: March 10, 2026

2026 Published by the Vinča Institute of Nuclear Sciences, Belgrade, Serbia.
This is an open access article distributed under the CC BY 4.0 terms and conditions.