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ORIGINAL PAPER

Determination of One Thermal Coefficient Through an Overspecified Stefan Problem with Temperature-Dependent Thermal Conductivity, Considering Flux and Convective Boundary Conditions

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Abstract

Formulae are obtained for the determination of one unknown thermal coefficient of a semi-infinite material with temperature-dependent thermal conductivity through a phase-change process with an overspecified condition on the fixed face (flux and convective boundary conditions) through a free boundary problem (Stefan problem with 5 cases). A new error function is introduced as part of the similarity-type solution, which depends on a parameter related to thermal conductivity. For the special case in which the parameter assumes values close to zero (positive or negative), we show that the new error function presents some characteristic features of the classical error function, such as monotony, concavity, and boundedness. We also study the sensitivity of the solution depending on different thermal parameters applied to aluminum and uranium.

Keywords Phase-change processes · Unknown thermal coefficient · Free boundary problem · Convective boundary conditions · Error function · Nonlinear second order ordinary differential equation

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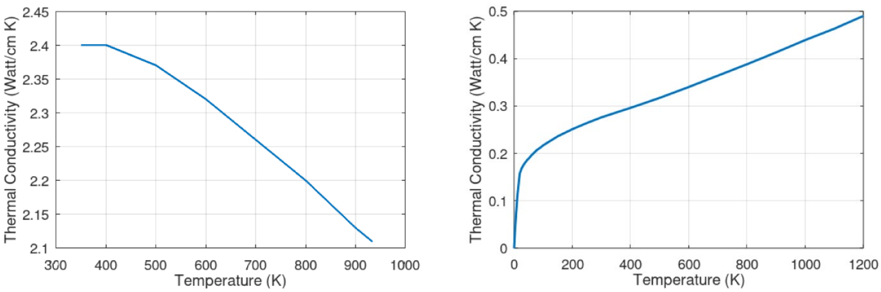
Introduction

Phase-change phenomena play a crucial role in a wide range of physical and engineering systems, including industrial processes such as glass manufacturing and continuous metal casting [4, 15], as well as environmental phenomena like permafrost evolution and snow avalanche dynamics [20]. The study of these processes is fundamental not only for advancing the theoretical understanding of heat transfer with moving boundaries, but also for improving real-world applications. For a detailed overview of the current applications and ongoing challenges in the field of free boundary problems, we refer the reader to [10, 27] and the references therein.

In this article, we study a phase-change process that models the solidification of a homogeneous material, with an external temperature imposed at a fixed boundary. A common simplification is to assume Dirichlet boundary conditions at this fixed boundary, based on the idealized assumption that the external temperature is instantaneously transferred to the material. Instead, we adopt a more realistic approach by considering a Robin or convective condition, in which heat transfer at the boundary is proportional to the difference between the external and internal temperatures (see, for example, [1, 6]). Another usual simplification in modeling phase-change processes is to treat thermophysical properties as constant. While this assumption may be acceptable for many cases involving moderate temperature variations [1], it does not reflect actual physical behavior. In Fig. 1, we show the thermal conductivity of Aluminum and Uranium [29], both of which are key materials in industrial and nuclear applications. Notably, near their melting points (933.2 K for Aluminum and 1405 K for Uranium), thermal conductivity can be reasonably approximated by a linear function. We therefore consider a more realistic model, assuming that thermal conductivity varies linearly with temperature.

In 1974, Cho and Sunderland studied a phase-change process for a one-dimensional semi-infinite material with temperature-dependent lineal thermal conductivity [11]. The phase-change process had a constant temperature imposed at the fixed boundary of the material. They presented an exact similarity solution, obtained through an auxiliary function that they have called Modified Error (ME) function and that was defined as the solution to a nonlinear ordinary differential problem of second order. In [7] the modeling of the imposed temperature at the fixed boundary was improved by considering a convective boundary condition, obtaining a solution of similarity type. The authors introduced an auxiliary function



(a) Aluminum (b) Uranium

Fig. 1 Thermal conductivity as a function of temperature for different materials, near their fusion temperatures: **a** aluminum and **b** uranium called Generalized Modified Error (GME) function, which was defined as the solution to a nonlinear ordinary differential problem of second order.

The thermal coefficients, e.g. the conductivity, latent heat, specific heat, and density of mass, characterize each material and are required to model any thermal process, and therefore they should be known a priori. A simple method for the determination of thermal coefficients is to add an extra boundary condition, obtaining an overspecified system. This allow us to find analytically, not only the solution of the temperature, but also a thermal coefficient. In [25] a phase-change process was studied, with a Dirichlet and flux condition at the fixed face $x = 0$, with temperature-dependent thermal conductivity. Unknown thermal coefficient where found in 4 cases of free boundary problems, and 5 cases of moving boundary problems. In [23] the same process was considered, but an extra parameter related to the ME function was also determined in 5 cases of free boundary problems, and 10 cases of moving boundary problems when an overspecified heat flux and temperature boundary conditions were imposed. Other papers related to determination of thermal coefficients are [13, 17, 18, 21].

In this article we consider a phase-change process, with a Robin (or convective) and Neumann (or heat flux) condition at the fixed face $x = 0$, with temperature-dependent thermal conductivity. These two boundary conditions allow us to obtain a similarity type solution through a new error function, which was defined as the solution to a nonlinear ordinary differential problem of second order similar to the previous error functions but with Dirichlet boundary conditions in a finite interval. We analyze 5 cases of free boundary problems (Stefan problem), giving the analytical expression for the simultaneously determination of different thermal coefficients, the temperature and the free boundary.

The unknown thermal coefficients to be identified at the same time will be selected from the following: density (ρ), latent heat (l), specific heat (c), thermal conductivity (k_0), and the slope of the thermal conductivity represented by the parameter β. In general, these types of problems are ill-posed, and for ill-posed problems a small perturbation in the input data may produce a big change in the output data. We will obtain the formulae for the unknown thermal coefficients and study the behavior of the solution parameters when a slightly modification is made in the data parameters, through a sensitivity analysis for the Aluminum and Uranium, both important materials for industrial and nuclear activities.

In Sect. 2, we give the mathematical formulation for the determination of one unknown thermal coefficient, and we prove the existence and uniqueness of the solution for small positive values of the parameter which characterizes the slope of the thermal conductivity as a function of the temperature.

In Sect. 3, for a one-phase Stefan problem, we determine the temperature $T(x, t)$, the free boundary interface $s(t) = 2\lambda\sqrt{\alpha_0 t}$ and the following parameters in 5 different cases for a free boundary problem:

$$\text{FB}: \ (1)\ \lambda,\ l \quad (2)\ \lambda,\ k_0 \quad (3)\ \lambda,\ \rho \quad (4)\ \lambda,\ c \quad (5)\ \lambda,\ \beta \tag{1}$$

Table 1 summarizes the formulae for the unknown thermal coefficients corresponding to the five cases for the free boundary problem (2). In Sect. 4, we study the sensitivity of the thermal coefficients when there are estimated.

Table 1 Formulae for the unknown thermal coefficients for the five cases with free boundary formulation taking into account that $\varphi = \varphi_\lambda(\eta)$ or $\varphi = \varphi_{\lambda,\beta}(\eta)$ is the solution to equation (6)

Case N°	Unknown coefficient	Solution
FB-1	λ, l	$\begin{cases} l = \frac{1}{2}c(1+\beta)(T_f - T_\infty)F_1(\lambda) \\ \varphi'_\lambda(0) = \dfrac{2h_0}{\sqrt{k_0\rho c}}\dfrac{\varepsilon_0}{(1+\varepsilon_0\beta)} \end{cases}$
FB-2	λ, k_0	$\begin{cases} k_0 = \dfrac{4\varepsilon_0^2 h_0^2}{\rho c\,(1+\varepsilon_0\beta)^2\,\varphi'(0)^2} \\ F_1(\lambda) = \dfrac{2\,l}{c(T_f - T_\infty)(1+\beta)} \end{cases}$
FB-3	λ, ρ	$\begin{cases} \rho = \dfrac{4\varepsilon_0^2 h_0^2}{k_0 c\,(1+\varepsilon_0\beta)^2\,\varphi'(0)^2} \\ F_1(\lambda) = \dfrac{2\,l}{c(T_f - T_\infty)(1+\beta)} \end{cases}$
FB-4	λ, c	$\begin{cases} c = \dfrac{4\varepsilon_0^2 h_0^2}{\rho k_0\,(1+\varepsilon_0\beta)^2\,\varphi'(0)^2} \\ F_1(\lambda) = \dfrac{l k_0 \rho (T_f - T_\infty)\varphi'(0)^2}{2q_0^2}\dfrac{(1+\varepsilon_0\beta)^2}{1+\beta} \end{cases}$
FB-5	λ, β	$\begin{cases} \beta = \dfrac{1}{\varepsilon_0}\left(\dfrac{2h_0\varepsilon_0}{\sqrt{\rho c k_0}}\dfrac{1}{\varphi'(0)} - 1\right) \\ F_1(\lambda) = \dfrac{2\,l}{c(T_f - T_\infty)}\dfrac{1}{1 + \frac{1}{\varepsilon_0}\left(\frac{2h_0\varepsilon_0}{\varphi'(0)\sqrt{\rho c k_0}} - 1\right)} \end{cases}$

Formulation for the Determination of Unknown Thermal Coefficients

We analyze a solidification problem in a semi-infinite medium, subject to a convective boundary condition and an additional heat flux condition imposed at the fixed boundary $x = 0$:

$$\begin{cases} \rho c T_t(x,t) = (k(T(x,t)T_x(x,t))_x & 0 < x < s(t), t > 0 & \text{(2a)} \\ s(0) = 0 & & \text{(2b)} \\ T(x,0) = T(+\infty,t) = T_f & x > 0, t > 0 & \text{(2c)} \\ T(s(t),t) = T_f & t > 0 & \text{(2d)} \\ k(T_f)T_x(s(t),t) = \rho l \dot{s}(t) & t > 0 & \text{(2e)} \\ k(T(0,t))T_x(0,t) = \frac{h_0}{\sqrt{t}}(T(0,t) - T_\infty) & t > 0 & \text{(2f)} \\ k(T(0,t))T_x(0,t) = \frac{q_0}{\sqrt{t}} & t > 0 & \text{(2g)} \end{cases}$$

where $T(x, t)$ is the temperature of the solid phase, $\rho > 0$ 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_∞ is the external temperature at the fixed face $x = 0$ ($T_\infty < T_f$), h_0 is the coefficient that characterizes the heat transfer coefficient at $x = 0$ given by (2f), and q_0 is the coefficient that characterizes the heat flux at $x = 0$ given by (2g) which must be obtained experimentally through a phase-change process. The parameters mentioned before are all constant. The model assumes a thermal conductivity that varies linearly with temperature, represented by:

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

where $k_0 > 0$, $\beta > -1$ are given constants [11]. This thermal conductivity model is similar to the one considered in [23], with the key difference that it involves the external temperature T_∞ rather than the Dirichlet boundary temperature imposed at $x = 0$ in [23].

We remark that the phase-change problem (2), without the condition (2g), corresponds to a classical Stefan problem [5, 6, 28]. The condition (2g) is treated as an overspecified boundary condition at the fixed face $x = 0$, as studied in [26]. This formulation reduces to the traditional Stefan framework when the thermal conductivity is assumed to be constant (i.e., $\beta = 0$), with an overspecified boundary condition at $x = 0$; the simultaneous determination of thermal coefficients under such assumptions was recently analyzed in [24].

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 $\eta = \frac{x}{2\sqrt{\alpha_0 t}}$, where $\alpha_0 = \frac{k_0}{\rho c}$ is the thermal diffusivity.

Proposition 1 *The Stefan problem (2) when the function $x = s(t)$ is unknown has the similarity solution (T, s) given by:*

$$\begin{cases} T(x,t) = (T_f - T_\infty)\varphi\left(\frac{x}{2\sqrt{\alpha_0 t}}\right) + T_\infty, & if 0 < x < s(t), t > 0 \quad (4a) \\ s(t) = 2\lambda\sqrt{\alpha_0 t}, & if t > 0 \quad (4b) \end{cases}$$

if and only if the parameter $\lambda > 0$ and the unknown thermal coefficients satisfy the following conditions:

$$\begin{cases} \varphi'(\lambda) = \lambda \frac{2l}{(1+\beta)c(T_f - T_\infty)} & (5a) \\ \varphi'(0) = \frac{2h_0}{\sqrt{k_0 \rho c}} \frac{\varepsilon_0}{(1+\varepsilon_0\beta)} & (5b) \end{cases}$$

where the parameter $\lambda > 0$ and the function φ satisfy the following ordinary differential problem:

$$\begin{cases} [(1 + \beta\varphi(\eta))\varphi'(\eta)]' + 2\eta\varphi'(\eta) = 0, & 0 < \eta < \lambda \\ \varphi(0) = \varepsilon_0 \\ \varphi(\lambda) = 1 \end{cases} \tag{6}$$

assuming that ε_0 satisfies the following condition:

$$\varepsilon_0 = \frac{q_0}{h_0(T_f - T_\infty)} < 1. \tag{7}$$

Taking into account that the solution φ of the problem (6) is dependent of the parameters $\beta > -1$ and $\lambda > 0$ we can consider $\varphi(\eta) = \varphi_{\beta,\lambda}(\eta)$ or $\varphi(\eta) = \varphi_\lambda(\eta)$ in cases where β, λ or λ are unknowns for free boundary problems. We remark that the solution of the ordinary differential problem (6) is similar to the GME function defined in [7], and we will call it

Similar Generalized Modified Error (SGME) function. The main difference between the GME function and the SGME function lies in the boundary conditions of their respective differential problems. In the case of the GME, a nonlinear boundary condition involving the derivative at $x = 0$ is imposed. In contrast, the SGME formulation adopts a Dirichlet-type condition at $x = 0$. This modification significantly simplifies the numerical resolution of the problem, making the computation of the SGME function more accessible.

Existence and Uniqueness of the SGME Function

All throughout this Section we will consider $\lambda > 0$, and $\beta > -1$. Following [7] we will denote with X to the set of all bounded analytic functions $h : [0, \lambda] \to \mathbb{R}$. It is well known that X is a Banach space with the supremum norm $||\cdot||_\infty$, which is defined by:

$$||h||_\infty = \sup\{|h(x)| \,:\, 0 \le x \le \lambda\} \quad (h \in X). \tag{8}$$

The subset of X given by all non-negative functions which are bounded by 1 will be referred to as K, that is:

$$K = \{h \in X \,:\, 0 \le h \text{ and } ||h||_\infty \le 1\}. \tag{9}$$

Note that K is a non-empty closed subset in $(X, ||\cdot||_\infty)$. In order to study the solution to problem (6) through a fixed point theory, we will start by considering the linear problem given by the following conditions:

$$\begin{cases} [\Psi_h(\eta)y'(\eta)]' + 2\eta y(\eta) = 0, & 0 < \eta < \lambda \\ y(0) = \varepsilon_0 < 1 \\ y(\lambda) = 1 \end{cases} \tag{10}$$

where $\Psi_h = \Psi_h(\eta)$ is defined by

$$\Psi_h(\eta) = 1 + \beta h(\eta), \qquad \eta > 0 \tag{11}$$

for $\beta > -1, h \in K \subset X$.

Theorem 1 *Let $h \in K$ and $\beta > -1$. The function y is a solution to problem (10) if and only if $y = y(\eta)$ is given by*

$$y(\eta) = \varepsilon_0 + (1 - \varepsilon_0)\frac{1}{E_h}\int_0^\eta \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_h(\xi)}d\xi\right)}{\Psi_h(x)}dx, \quad 0 < \eta < \lambda, \tag{12}$$

where the constant $E_h > 0$ is defined by:

$$E_h = \int_0^\lambda \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_h(\xi)}d\xi\right)}{\Psi_h(x)}dx. \tag{13}$$

Proof It follows from regular computation for a linear ordinary differential problems, similarly to the one in [7, 8]. □

Lets define $\gamma_1 = \min\{1, 1+\beta\}$ and $\gamma_2 = \max\{1, 1+\beta\}$, note that both are positive constants. We need now some estimations which will be useful in the following:

Lemma 1 *Let* $h, h_1, h_2 \in K$, $\beta > -1$ *and* $0 \leq \eta \leq \lambda$. *Then, we have the following inequalities:*

$$\gamma_1 \leq \Psi_h \leq \gamma_2; \tag{14}$$

$$\| \Psi_{h_1} - \Psi_{h_2} \|_\infty \leq |\beta| \, \| h_1 - h_2 \|_\infty; \tag{15}$$

$$\int_0^\eta x^2 \exp\left(\frac{-x^2}{1+\beta}\right) dx \leq \frac{\sqrt{\pi}}{4} (\gamma_2)^{\frac{3}{2}}; \tag{16}$$

$$\frac{\sqrt{\pi}}{2\gamma_2}\sqrt{\gamma_1}\ \mathrm{erf}\left(\frac{\eta}{\sqrt{\gamma_1}}\right) \leq \int_0^\eta \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_h(\xi)} d\xi\right)}{\Psi_h(x)} dx \leq \frac{\sqrt{\pi}}{2\gamma_1}\sqrt{\gamma_2}\ \mathrm{erf}\left(\frac{\eta}{\sqrt{\gamma_2}}\right); \tag{17}$$

$$\frac{\sqrt{\pi}}{2\gamma_2}\sqrt{\gamma_1}\ \mathrm{erf}\left(\frac{\lambda}{\sqrt{\gamma_1}}\right) \leq E_h \leq \frac{\sqrt{\pi}}{2\gamma_1}\sqrt{\gamma_2}\ \mathrm{erf}\left(\frac{\lambda}{\sqrt{\gamma_2}}\right) \tag{18}$$

$$\int_0^\eta \left| \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)} d\xi\right) - \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_1}(\xi)} d\xi\right) \right| dx \leq \frac{\sqrt{\pi}}{6} \frac{\sqrt{\gamma_2}}{\gamma_1^2} \eta^3 |\beta| \, \| h_1 - h_2 \|_\infty; \tag{19}$$

$$|E_{h_2} - E_{h_1}| \leq \frac{\sqrt{\pi}}{2} \frac{\sqrt{\gamma_2}}{\gamma_1^2} \left(1 + \frac{\lambda^3}{3\gamma_1}\right) |\beta| \, \| h_1 - h_2 \|_\infty . \tag{20}$$

Proof The first three inequalities are obtained by elementary computations.

To prove (17), we use (14) to get:

$$\begin{aligned}
\int_0^\eta \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_h(\xi)} d\xi\right)}{\Psi_h(x)} dx &\leq \frac{1}{\gamma_1} \int_0^\eta \exp\left(-2\int_0^x \frac{\xi}{\gamma_2} d\xi\right) dx \\
&= \frac{1}{\gamma_1} \int_0^\eta \exp\left(-\frac{x^2}{\gamma_2}\right) dx \\
&= \frac{\sqrt{\pi}}{2} \frac{\sqrt{\gamma_2}}{\gamma_1}\ \mathrm{erf}\left(\frac{\eta}{\sqrt{\gamma_2}}\right).
\end{aligned}$$

The upper bound in (18) is obtained by using (17) and the lower bound, by using (14).

For (19), the proof is similar to that given in [7–9] and by using the previous inequalities.

For (20), the above inequalities are used and it is demonstrated that:

$$
\begin{aligned}
|E_{h_2}-E_{h_1}| &\le \int_0^\lambda \left| \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)}d\xi\right)}{\Psi_{h_2}(x)} - \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_1}(\xi)}d\xi\right)}{\Psi_{h_1}(x)} \right| dx \\
&\le \int_0^\lambda \frac{|\Psi_{h_1}(x)-\Psi_{h_2}(x)|}{\Psi_{h_1}(x)\Psi_{h_2}(x)} \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)}d\xi\right) dx \\
&+ \int_0^\lambda \frac{1}{\Psi_{h_1}} \left| \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)}d\xi\right) - \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_1}(\xi)}d\xi\right) \right| dx
\end{aligned}
$$

$$
\begin{aligned}
&\le \frac{|\beta|}{\gamma_1^2} \parallel \Psi_{h_1}-\Psi_{h_2} \parallel_\infty \int_0^\lambda \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)}d\xi\right) dx \\
&+ \frac{1}{\gamma_1}\int_0^\lambda \left| \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)}d\xi\right) - \exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_1}(\xi)}d\xi\right) \right| dx \\
&\le \frac{\sqrt{\pi}}{2}\frac{\sqrt{\gamma_2}}{\gamma_1^2}|\beta| erf\left(\frac{\lambda}{\sqrt{\gamma_2}}\right) \parallel h_2-h_1 \parallel_\infty + \frac{\sqrt{\pi}}{6}\frac{\sqrt{\gamma_2}}{\gamma_1^3}\lambda^3|\beta| erf\left(\frac{\lambda}{\sqrt{\gamma_2}}\right) \parallel h_1-h_2 \parallel_\infty \\
&\le \frac{\sqrt{\pi}}{2}\frac{\sqrt{\gamma_2}}{\gamma_1^2}\left(1+\frac{\lambda^3}{3\gamma_1}\right)|\beta| \parallel h_1-h_2 \parallel_\infty
\end{aligned}
$$

□

Theorem 2 *Let $y \in K$ and $\beta > -1$ be. Then y is a solution to problem (10) if and only if y is a fixed point of the operator $\tau : K \longrightarrow X$ defined by*

$$
\tau h(\eta) = \tau(h)(\eta) = \varepsilon_0 + (1-\varepsilon_0)\frac{1}{E_h}\int_0^\eta \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_h(\xi)}d\xi\right)}{\Psi_h(x)}dx, \quad 0<\eta<\lambda, \tag{21}
$$

where E_h was defined in (13). Moreover, the operator has the following properties:
(a) $\tau(K) \subset K \subset X$;
(b) *For $h_1, h_2 \in K$, we have*

$$
||\tau h_1 - \tau h_2||_\infty \le G(\beta)||h_1-h_2||_\infty \tag{22}
$$

where the real function $G(\beta)$ is defined by

$$
G(\beta) = G_\lambda(\beta) = \frac{2\gamma_2^3}{\gamma_1^4}\frac{(1-\varepsilon_0)}{\left(erf\left(\frac{\lambda}{\sqrt{\gamma_1}}\right)\right)^2}\left(1+\frac{\lambda^3}{3\gamma_1}\right)|\beta|; \tag{23}
$$

(c) *There exists a unique solution $\beta_0 = \beta_0(\lambda) < 0$ to the equation:*

$$
G(x) = 1, \qquad x \in (-1, 0); \tag{24}
$$

(d) *There exists a unique solution $\beta_1 = \beta_1(\lambda) > 0$ to the equation:*

$$
G(x) = 1, \qquad x > 0; \tag{25}
$$

(e) *τ is a contraction operator if,*

$$\beta_0(\lambda) < \beta < \beta_1(\lambda), \quad \forall \lambda > 0. \tag{26}$$

Proof The first part of the theorem is an immediate consequence of Theorem 1. To prove item (a), note that $\tau(h)$ is an analytic function because h is analytic. Besides it is positive and increasing, and $\tau h(\lambda) = 1$:

$$\tau h(\lambda) = \varepsilon_0 + (1-\varepsilon_0)\frac{1}{E_h}\int_0^\lambda \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_h(\xi)}d\xi\right)}{\Psi_h(x)}dx = \varepsilon_0 + \frac{1-\varepsilon_0}{E_h}E_h = 1,$$

therefore $||\tau h||_\infty \leq 1$, and $\tau(K) \subset K$.

For (b) using the inequalities (17)–(20) from Lemma 1 it can be shown that:

$$\begin{aligned}
|\tau h_1(\eta) - \tau h_2(\eta)| &\leq (1-\varepsilon_0)\left|\frac{1}{E_{h_2}} - \frac{1}{E_{h_1}}\right| \int_0^\eta \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)}d\xi\right)}{\Psi_{h_2}(x)}dx \\
&+ (1-\varepsilon_0)\frac{1}{E_{h_1}}\left|\int_0^\eta \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_2}(\xi)}d\xi\right)}{\Psi_{h_2}(x)} - \frac{\exp\left(-2\int_0^x \frac{\xi}{\Psi_{h_1}(\xi)}d\xi\right)}{\Psi_{h_1}(x)}dx\right| \\
&\leq \frac{2\gamma_2^3}{\gamma_1^4}\frac{(1-\varepsilon_0)}{\left(erf\left(\frac{\lambda}{\sqrt{\gamma_1}}\right)\right)^2}\left(1 + \frac{\lambda^3}{3\gamma_1}\right)|\beta| \parallel h_1 - h_2 \parallel_\infty \\
&= G(\beta) \parallel h_1 - h_2 \parallel_\infty .
\end{aligned}$$

To prove item d), it is enough to show that G is an increasing function with $G(0^+) = 0$ and $G(+\infty) = +\infty$. To prove item c), it is enough to show that G is an decreasing function with $G(-1) = +\infty$ and $G(0^+) = 0$. Therefore by using the previous results we have that τ is a contraction operator when (26) holds. □

Auxiliary Functions

Let us consider the following real function, that we will use in the analytical expressions for the thermal coefficients of the free boundary problems:

$$F_1(x) = \frac{\varphi'(x)}{x}. \tag{27}$$

To understand the behaviour of this auxiliary function, we first need to establish some properties of the SGME function.

Proposition 2 *The solution function φ of the overspecified Stefan problem (5) and (6) verifies the following properties:*

$$(i) 0 \le \varphi(\eta) \le 1, \quad (ii) 0 < \varphi'(\eta), \qquad (iii) \varphi'(0) = \frac{2h_0\varepsilon_0}{\sqrt{\rho c k_0}(1+\beta\varepsilon_0)} > 0,$$
$$(iv) \varphi''(\eta) < 0, \qquad (v) \varphi''(0) = -\frac{4\beta q_0^2}{\rho c k_0(1+\beta\varepsilon_0)(T_f - T_\infty)^2} < 0. \tag{28}$$

Proof (i) Follows from definition of K, (ii) follows from contradiction similarly as in [7], and (iii) follows from (5b). (iv) From (6), we obtain that

$$\varphi''(\eta) = -\frac{\beta(\varphi'(\eta))^2 + 2\eta\varphi'(\eta)}{1+\beta\varphi(\eta)} < 0. \tag{29}$$

Therefore, by using (29) and (iii) we get the expression (v). □

Proposition 3 *The function F_1 is continuous and have the following properties:*

$$(a) F_1(0^+) = +\infty, \qquad (b) F_1(+\infty) = 0, \qquad (c) F_1(x) > 0 \qquad (d) F_1^{'}(x) < 0. \tag{30}$$

Proof The first and third properties are an immediate consequence of (27), (28ii), and (28iv). From (27), we have:

$$F_1^{'}(x) = \frac{\varphi''(x) - F_1(x)}{x} < 0. \tag{31}$$

and then (d) holds.

To prove the second property we use the second property we use that $\varphi = \varphi(\eta)$ is concave in $[0, \lambda]$, then $\varphi(z) \le \varphi(x) + \varphi'(x)(z - x)$ since $\varphi'' < 0$. Taking $x = \lambda, z = 0$ we have that

$$\varphi(0) \le \varphi(\lambda) + \varphi'(\lambda)(0 - \lambda) = \varphi(\lambda) - \lambda\varphi'(\lambda),$$

thatis$\varphi'(\lambda) \le \dfrac{1-\varepsilon_0}{\lambda}$.Therefore, $\lim\limits_{x\to\lambda} \varphi'(x) = \varphi'(\lambda) \le \dfrac{1-\varepsilon_0}{\lambda}$,then $\lim\limits_{\lambda\to+\infty} \lim\limits_{x\to\lambda} \varphi'(x) = 0$.
From (27), we have that $0 \le \lim\limits_{x\to\lambda} F_1(x) = \dfrac{\varphi'(\lambda)}{\lambda} \le \dfrac{1-\varepsilon_0}{\lambda^2}$ and then we obtain

$$F_1(+\infty) = \lim_{\lambda\to+\infty} \lim_{x\to\lambda} F_1(x) = 0.$$

□

Determination of One Thermal Coefficient Through Free Boundary Problems

To estimate thermal parameters under various scenarios, we analyze five configurations where the unknowns are selected from physical properties such as latent heat, conductivity, or specific heat, detailed in (1). First we must show a preliminary result:

Proposition 4 *The Stefan problem (2) with an overspecified condition has the similarity solution (T, s) given by:*

$$\begin{cases} T(x,t) = (T_f - T_\infty)\varphi\left(\dfrac{x}{2\sqrt{\alpha_0 t}}\right) + T_\infty, & if\, 0 < x < s(t), t > 0 & (32a) \\ s(t) = 2\lambda\sqrt{\alpha_0 t}, & if\, t > 0 & (32b) \end{cases}$$

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

$$\begin{cases} \varphi'(\lambda) = \lambda\frac{2l}{(1+\beta)c(T_f - T_\infty)}, & (33a) \\ \varphi'(0) = \frac{2h_0}{\sqrt{k_0\rho c}}\frac{\varepsilon_0}{(1+\varepsilon_0\beta)}, & (33b) \end{cases}$$

where $\alpha_0 = \dfrac{k_o}{\rho c}$ is the thermal diffusivity and φ is the solution of problem (6).

We would like to remark that in most cases stated in (1), since the SGME function depends on λ, and both typically appear in the analytical expressions, an iterative process is required to determine the values that satisfy the equations. In Sect. 4, we employ the Levenberg–Marquardt algorithm, an iterative optimization method designed to solve nonlinear least squares problems. Starting from initial guesses—such as for λ and l—we solve system (6) for the SGME function in each iteration, and the algorithm updates the values of λ and l accordingly. This type of procedure has also been used in other works on the simultaneous determination of thermal coefficients [23, 25].

Case 1: Inferring Both $\{\lambda, l\}$

Proposition 5 *The temperature and the free boundary for problem (2) with unknown thermal coefficients $\{\lambda, l\}$ are given by (32), and l is given by the expression,*

$$l = \frac{c(1+\beta)(T_f - T_\infty)}{2}F_1(\lambda), \tag{34}$$

and λ is solution of the equation,

$$\varphi'(0) = \varphi'_\lambda(0) = \frac{2h_0}{\sqrt{k_0\rho c}}\frac{\varepsilon_0}{(1+\varepsilon_0\beta)}, \qquad \lambda > 0. \tag{35}$$

Proof From the condition (33a) we obtain (34), and from the condition (33b) we obtain the equation (35) which is solved by an iterative process. □

Case 2: Inferring Both $\{\lambda, k_0\}$

Proposition 6 *The temperature and the free boundary for problem (2) with unknown thermal coefficients $\{\lambda, k_0\}$ are given by (32), and k_0 is given by the expression,*

$$k_0 = \frac{4\varepsilon_0^2 h_0^2}{\rho c \left(1+\varepsilon_0\beta\right)^2 \varphi'(0)^2}, \tag{36}$$

and λ *is solution of the equation,*

$$\frac{\varphi'_\lambda(\lambda)}{\lambda} = F_1(\lambda) = \frac{2l}{c(T_f - T_\infty)(1+\beta)}, \qquad \lambda > 0. \tag{37}$$

Proof The first expression (36) is obtained from (33b), and the second one is obtained from (33a) through an iterative process. □

Case 3: Inferring Both $\{\lambda, \rho\}$

Proposition 7 *The temperature and the free boundary for problem (2) with unknown thermal coefficients* $\{\lambda, \rho\}$ *are given by (32), and* ρ *is given by the expression,*

$$\rho = \frac{4\varepsilon_0^2 h_0^2}{k_0 c \left(1+\varepsilon_0\beta\right)^2 \varphi'(0)^2}, \tag{38}$$

and λ *is solution of the equation,*

$$\frac{\varphi'_\lambda(\lambda)}{\lambda} = F_1(\lambda) = \frac{2l}{c(T_f - T_\infty)(1+\beta)}, \qquad \lambda > 0. \tag{39}$$

Proof It is similar to the Proof of Proposition 6 where (39) is an iterative process. □

Case 4: Inferring Both $\{\lambda, c\}$

Proposition 8 *The temperature and the free boundary for problem (2) with unknown thermal coefficients* $\{\lambda, c\}$ *are given by (32), and* c *is given by the expression,*

$$c = \frac{4\varepsilon_0^2 h_0^2}{\rho k_0 \left(1+\varepsilon_0\beta\right)^2 \varphi'(0)^2}, \tag{40}$$

and λ *is solution of the equation,*

$$\frac{\varphi'_\lambda(\lambda)}{\lambda} = F_1(\lambda) = \frac{l k_0 \rho (T_f - T_\infty)\varphi'(0)^2}{2q_0^2} \frac{\left(1+\varepsilon_0\beta\right)^2}{1+\beta}, \qquad \lambda > 0. \tag{41}$$

Proof It is similar to the Proof of Proposition 5 where (41) is an iterative process. □

Case 5: Inferring Both $\{\lambda, \beta\}$

Proposition 9 *The temperature and the free boundary for problem (2) with unknown thermal coefficients* $\{\lambda, \beta\}$ *are given by (32), and* β *is given by the expression,*

$$\beta = \frac{1}{\varepsilon_0}\left(\frac{2h_0\varepsilon_0}{\sqrt{\rho c k_0}}\frac{1}{\varphi'(0)} - 1\right), \tag{42}$$

and λ *is solution of the equation,*

$$\frac{\varphi'_\lambda(\lambda)}{\lambda} = F_1(\lambda) = \frac{2l}{c(T_f - T_\infty)}\frac{1}{1 + \frac{1}{\varepsilon_0}\left(\frac{2h_0\varepsilon_0}{\varphi'(0)\sqrt{\rho c k_0}} - 1\right)}, \qquad \lambda > 0. \tag{43}$$

Proof It is similar to the Proof of Proposition 5 where (43) is an iterative process. □

Sensitivity Analysis

In [3] Blackwell and Dowding analyzed the importance of the sensitivity of thermal parameters when they are estimated. They state that even though there are numerous investigations for the determination of thermal coefficients, the sensitivity is rarely analyzed [2]. The study of the sensitivity of the parameters in the determination process helps to understand the dependency on the experimental variables. In general, these types of problems are ill-posed [3, 14], and for ill-posed problems a small perturbation in the input data may produce a big change in the output data.

The sensitivity of a coefficient A with respect to another parameter B is defined as the partial derivative of A with respect to B, denoted by $\partial A/\partial B$. In the context of free boundary problems, the coefficient A corresponds to one of the thermal coefficients being determined simultaneously, while B is one of the thermal coefficients treated as known data.

To evaluate how the known parameters influence the unknown coefficients and to enable comparison between sensitivities, we introduce the dimensionless normalized sensitivity [22]:

$$S(A, B) := \frac{B}{A}\frac{\partial A}{\partial B}. \tag{44}$$

Because this quantity is dimensionless, it allows for the comparison of sensitivities across parameters with different units or magnitudes. This analysis quantifies how small perturbations in the known data influence the estimated parameters, by evaluating the percentage variation in the output per 1% change in each input [12, 16]. We approximate $S(A, B)$ using:

$$S(A, B)^+ \approx \frac{B}{A(B)}\frac{A(B^+) - A(B)}{B^+ - B} \quad \text{(right normalized sensitivity)},$$

$$S(A, B)^- \approx \frac{B}{A(B)}\frac{A(B^-) - A(B)}{B^- - B} \quad \text{(left normalized sensitivity)},$$

where $B^+ = B + \epsilon|B|$, $B^- = B - \epsilon|B|$ with $\epsilon > 0$, and $A(B), A(B^+), A(B^-)$ represent the values of the parameter A determined when the input data is B, B^+, or B^-, respectively.

Table 2 Thermal coefficients for aluminum and uranium

Parameter	Units	Aluminum	Uranium
k_0	$J/s\,m°C$	221.081	480.56
β	adim	−0.04411299	0.11601464
ρ	kg/m^3	2702	19050
c	$J/kg°C$	12769.74	16089.8724
l	J/kg	395652.6	83736
h_0	$kg/°Cs^{5/2}$	100000	100000
T_∞	$°C$	500	900
T_f	$°C$	660.37	1132.3
λ	adim	0.919889	1.400829
q_0	$kg/s^{5/2}$	5992871.96	16416411.83

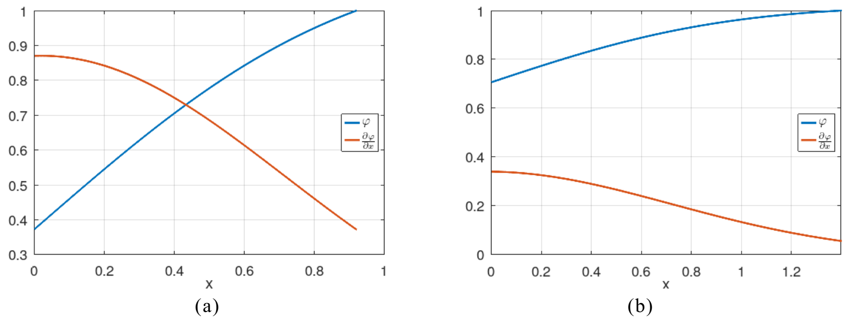


Fig. 2 SGME function and its derivative for **a** aluminum and **b** uranium

In this framework, the right normalized sensitivity quantifies the variation in A when B increases by 1%, while the left normalized sensitivity measures the variation in A when B decreases by 1%.

We used the free software SCILAB[1] for the numerical analysis. For each case, first we had to determine the solution to the corresponding system of equations. The command bvodeS was used to solve the differential problem (6), which allowed us to evaluate the SGME function at the necessary points. To find the solution to the system, we minimize the sum of the squares of the equations of the nonlinear system, using the Levenberg-Marquardt algorithm. Secondly, using the approximately solution to the system, we evaluated the unknown thermal coefficients.

We analyzed two different materials, Aluminum, who's thermal conductivity has a negative slope, and Uranium, with a positive slope. The thermal data was obtained from [29], and is summarized in Table 2.

Note that some parameters in Table 2 are obtained directly from [19, 29] $(k_0, \beta, \rho, c, l, T_f)$, others are assumed (h_0, T_∞), and others are determined (λ, q_0) solving the problem (2) without taking into account the last condition (2g). We also show the SGME function and its derivative for Aluminum and Uranium, in Fig. 2, for the domain $(0, \lambda)$.

[1] https://www.scilab.org.

Table 3 Left and right sensitivities for the five cases of free boundary problems for aluminum

Caso No	1		2		3		4		5	
Coef. Det	λ	l	λ	k_0	λ	ρ	λ	c	λ	β
l	–	–	−0.305	−0.329	−0.305	−0.329	−0.452	−0.488	−0.505	**11.470**
	–	–	−0.301	−0.326	−0.301	−0.326	−0.449	−0.486	−0.498	**11.359**
k_0	0.921	−3.087	–	–	−0.0001	−1.011	−0.452	−1.503	−0.611	**35.231**
	0.930	−3.022	–	–	0.0001	−0.989	−0.449	−1.471	−0.607	**34.503**
ρ	0.921	−3.087	−0.0001	−1.011	–	–	−0.452	−1.503	−0.611	**35.231**
	0.930	−3.022	0.0001	−0.989	–	–	−0.449	−1.471	−0.607	**34.503**
c	0.921	−2.056	0.304	−0.678	0.304	−0.678	–	–	−0.104	**23.616**
	0.930	−2.052	0.302	−0.668	0.302	−0.668	–	–	−0.106	**23.284**
β	−0.044	0.086	−0.018	0.028	−0.018	0.028	−0.005	0.042	–	–
	−0.044	0.089	−0.017	0.029	−0.017	0.029	−0.004	0.043	–	–

The highest sensitivity values are highlighted in bold

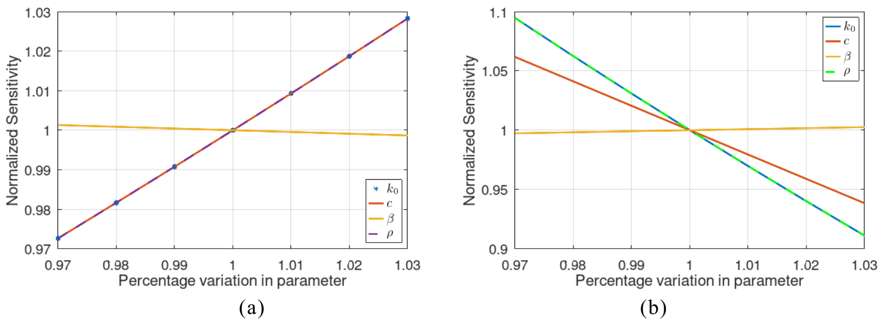


Fig. 3 Parametric change of **a** λ and **b** l versus the relative change of $\{k_0, \rho, c, \beta\}$ in Case 1 of the free boundary problem

Sensitivity Analysis for Aluminum Through Free Boundary Problems

Table 3 shows the left and right sensitivities for the free boundary problems. Case 5 is the most sensible one, where the parameter β have the highest sensitivities for almost every parameter. For this case, Fig. 4 shows the relationship between the parameter solutions λ and β and the given parameters $\{k_0, \rho, c, l\}$. Note that for the parameter λ the sensitivities are less than 0.61%, having in the vertical axis a scale between 0.95 and 1.05. Instead, for β, that have sensitivities up to 35.22%, the scale of the axis if between −0.5 and 2.5, resulting in higher slopes (sensitivities). The next case with the highest sensitivities is Case 1, shown in Fig. 3, where the parameter l has a sensitivity around 3% for k_0, ρ and c. The remaining cases have sensitivities less than 2%.

Sensitivity Analysis for Uranium Through Free Boundary Problems

Table 4 shows the left and right sensitivities for the free boundary problems. Again Case 5 is the most sensible one, shown in Fig. 6, where the parameter β have the highest sensitivities for almost every parameter. The next one is Case 1, where l have the highest sensitivity,

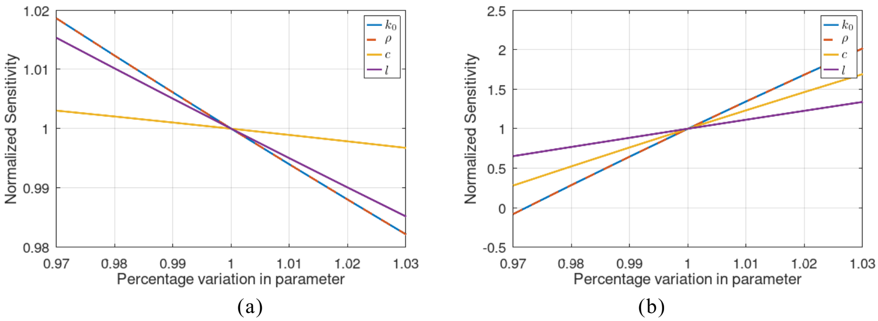


Fig. 4 Parametric change of **a** λ and **b** β versus the relative change of $\{l, k_0, \rho, c, \}$ in Case 5 of the free boundary problem

Table 4 Left and right sensitivities for the five cases of free boundary problems for uranium

Caso No	1		2		3		4		5	
Coef. Det	λ	l	λ	k_0	λ	ρ	λ	c	λ	β
l	–	–	−0.209	−0.113	−0.209	−0.113	−0.235	−0.127	−0.272	−1.304
	–	–	−0.207	−0.112	−0.207	−0.112	−0.233	−0.127	−0.269	−1.301
k_0	1.792	−8.956	–	–	−0.00001	−1.010	−0.235	−1.138	−0.556	**−11.649**
	1.903	−8.755	–	–	0.00001	−0.990	−0.233	−1.116	−0.548	**−11.418**
ρ	1.792	−8.956	−0.00001	−1.010	–	–	−0.235	−1.138	−0.556	**−11.649**
	1.903	−8.755	0.00001	−0.990	–	–	−0.233	−1.116	−0.548	**−11.418**
c	1.792	−7.866	0.209	−0.895	0.209	−0.895	–	–	−0.282	**−10.321**
	1.903	−7.843	0.207	−0.879	0.207	−0.879	–	–	−0.280	**−10.140**
β	0.207	−0.768	0.047	−0.086	0.047	−0.086	0.027	−0.097	–	–
	0.208	−0.767	0.047	−0.086	0.047	−0.086	0.027	−0.097	–	–

The highest sensitivity values are highlighted in bold

around 8%. The rest of the cases have sensitivities less than 1%. In Fig. 5, we show the normalized sensitivities for Case 2, which is one of the least sensitive cases. Although the plots for Cases 5 and 2 appear similar, there is a significant difference in the scale of the y-axis for the second parameter. In Case 5, the sensitivity for β reaches up to 1.4, whereas in Case 2, the sensitivity for k_0 only reaches 1.04. This means that the sensitivity is 40% in Case 5, compared to just 4% in Case 2.

Conclusions

We have considered a phase-change process with two conditions at the fixed boundary $x = 0$, a Robin and a Neumann type conditions. This overspecified condition allowed us to obtain formulae for the determination of one unknown thermal coefficient, in the five cases for free boundary problems.

A new error function is introduced as a solution of a non-linear ordinary differential problem, and we show that it presents some characteristic features of the classical error function,

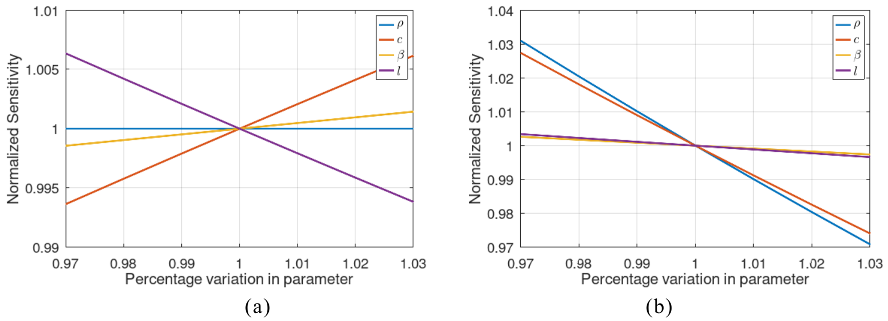


Fig. 5 Parametric change of **a** λ and **b** k_0 versus the relative change of $\{l, \rho, c, \beta\}$ in Case 2 of the free boundary problem

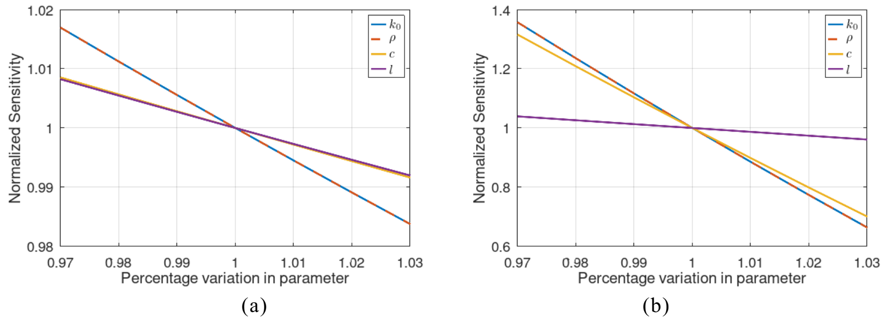


Fig. 6 Parametric change of **a** λ and **b** β versus the relative change of $\{l, k_0, \rho, c\}$ in Case 5 of the free boundary problem

such as monotony, concavity, and boundedness. The existance of this function was proven through the Fixed Point Theorem, for values close to zero.

The sensitivities for Aluminum and Uranium are very similar, resulting Case 5 the most sensible one. In general, the sensitivities for Aluminum are higher than Uranium, except for Case 1.

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Declarations

Conflict of interest The authors declare no Conflict of interest.

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