Behavior of the solution of a Stefan problem by changing thermal coefficients of the substance

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Abstract

We consider a one-dimensional one-phase Stefan problem for a semi-infinite substance. We suppose that there is a transient heat flux at the fixed face and the thermal coefficients are constant.

The goal of this paper is to determine the behavior of the free boundary and the temperature by changing the thermal coefficients. We use the maximum principle in order to obtain properties of monotony with respect to the latent heat of fusion, the specific heat and the mass density. We compute approximate solutions through the quasi-stationary, the Goodman’s heat-balance integral and the Biot’s variational methods and a numerical solution through a finite difference scheme. We show that the solution is not monotone with respect to the thermal conductivity.

The results obtained are important in technological applications.

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Keywords: Phase change material; One phase Stefan problem; Melting time; Heat balance integral method; Biot’s variational method; Quasi stationary method; Finite difference method

1. Introduction

Phase change materials (PCMs) are substances whose phase-change temperature makes it available to moderate the oscillations of temperature and to store energy of another substance put in contact with them. The heat storage by PCMs is almost isothermal, so it is preferable to the storage by sensible heat in applications which involve small changes of temperature. When a temperature jump occurs, the PCM absorbs the excess of energy changing its phase and then it gives the energy back in a later time [1].

Among the variety of uses of the PCMs we can mention the climate of buildings, the storage of energy in satellites and clothes and the transport of biological substances. In this last application we must consider that...
the breathing of substances generates a caloric energy. So, the temperature of the package rises and consequently the early degradation of the transported product can occur. For this reason, it is important to know the evolution of the temperature in the border of the PCM in contact with the biological substance and also the thickness of the layer of PCM able to absorb the excess of energy, in order to keep the temperature in the interior of the package in an optimal range. It is also important to determine how does that temperature vary with respect to the different thermal properties of the PCM \[2,3\].

When we consider a packaging of a PCM that recovers an organic substance to be transported, it is essential to find the thickness of this pack to insure the optimal temperature of conservation in the organic substance during total time of transport \[4–9\]. Because the sizes of the pack (wide, length and height) are sufficiently greater than its thickness, we can assume that the heat transfer occurs in only one direction. Moreover, we can suppose that the initial temperature is constant and equal to the phase change temperature since the PCM and the substance are pre-cooling. So we think in a one-phase one-dimensional Stefan problem.

The goal of the present work is to establish if there is or not any monotone dependence of the solution for a one-dimensional Stefan problem with respect to the variation of some thermal coefficients of a substance (for example a PCM).

We consider the following one-dimensional one-phase Stefan problem (melting case):

\[
\text{Problem } P: \text{Find the function } s(t) \text{ (free boundary or solid–liquid interphase) defined for } t > 0, \text{ and the temperature } [10–12]:
\]

\[
T(x, t) = \begin{cases} 
T(x, t) & \text{if } 0 \leq x < s(t), \quad t > 0, \\
T_f & \text{if } x \geq s(t), \quad t > 0.
\end{cases}
\]

so that they satisfy

\[
\begin{align*}
T_t &= \alpha T_{xx}, \quad 0 < x < s(t), \quad t > 0; \\
kT_x(0, t) &= -K(t), \quad t > 0; \\
T(s(t), t) &= T_f, \quad t > 0; \\
kT_s(s(t), t) &= -\rho\ell s'(t) \quad t > 0; \\
s(0) &= 0,
\end{align*}
\]

where \(K = K(t) > 0\) is a given smooth function which represents the heat flux on the fixed border \(x = 0\); \(k, \rho, c\) and \(\ell\) are the thermal conductivity, the mass density, the specific heat and the latent heat of fusion per unity of mass respectively; \(\alpha = \frac{k}{\rho c}\) is the thermal diffusivity and \(T_f\) is the phase-change temperature.

Numerical solution of the phase-change problem, in general, requires solution of the heat conduction equation with an adequate treatment of the phase front.

For the numerical treatment of this free boundary problem we can mention \[13–20\].

In Section 2 we show properties of monotony for the solution of Stefan problem \(P\) with respect to the physical parameters \(\ell, c\) and \(\rho\) by using the maximum principle. In Section 3 we obtain approximate solutions of
2. Study of monotony of the solution with respect to the physical parameters

In this section we use the maximum principle and the result of the following Lemma, when it is required, in order to establish some properties of monotony for the solution of problem \( P \). We consider the compatibility conditions \( T_0(b) = T_f \) and \( T_0'(0) = -\frac{K(0)}{k} \).

**Lemma 1.** Let be the Stefan problem

\[
T_t = \kappa T_{xx}, \quad 0 < x < s(t), \quad t > 0; \tag{3.1}
\]
\[
kT_s(0, t) = -K(t), \quad t > 0; \tag{3.2}
\]
\[
T(s(t), t) = T_f, \quad t > 0; \tag{3.3}
\]
\[
kT_s(s(t), t) = -\rho \ell s'(t), \quad t > 0; \tag{3.4}
\]
\[
T(x, 0) = T_0(x) > T_f, \quad 0 < x < b; \tag{3.5}
\]
\[
s(0) = b \geq 0. \tag{3.6}
\]

We have that:

(i) If \( T'_0(x) \leq 0 \) in \( 0 \leq x \leq b \), then \( T_s(x, t) \leq 0 \) in \( 0 \leq x \leq s(t) \), \( t \geq 0 \).

(ii) If \( T'_0(x) \geq 0 \) in \( 0 \leq x \leq b \) and \( K'(t) \geq 0 \) \( \forall t > 0 \), we obtain \( T_{xx}(x, t) \geq 0 \) in \( 0 \leq x \leq b \), for all \( t \geq 0 \).

**Proof.** The maximum principle applied to problem given by Eqs. (3.1)–(3.6) implies that \( T(x, t) \geq T_f \), \( 0 < x < s(t) \), \( t > 0 \) and therefore \( s'(t) > 0 \) for \( t > 0 \).

(i) We define the auxiliary function \( w(t) = T_s(x, t) \), which verify the associated problem:

\[
w_t = \kappa w_{xx}, \quad 0 < x < s(t), \quad t > 0; \tag{4.1}
\]
\[
w(0, t) = \frac{-K(t)}{k} < 0, \quad t > 0; \tag{4.2}
\]
\[
w(s(t), t) = -\frac{\rho \ell}{k} s'(t) < 0, \quad t > 0; \tag{4.3}
\]
\[
w(x, 0) = T'_0(x) \leq 0, \quad 0 < x < b; \tag{4.4}
\]
\[
s(0) = b. \tag{4.5}
\]

Then, from the maximum principle and \( K(t) > 0 \) and \( T'_0(x) \leq 0 \) the thesis holds.

(ii) We consider the auxiliary function \( v(x, t) = T_{xx}(x, t) \), which satisfies the associated problem:

\[
v_t = \kappa v_{xx}, \quad 0 < x < s(t), \quad t > 0; \tag{5.1}
\]
\[
v(0, t) = \frac{-K(t)}{\kappa k} \leq 0, \quad t > 0; \tag{5.2}
\]
\[
v(s(t), t) = \frac{\rho \ell}{k} s^2(t) > 0, \quad t > 0; \tag{5.3}
\]
\[
v(x, 0) = T''_0(x) \geq 0, \quad 0 < x < b; \tag{5.4}
\]
\[
s(0) = b. \tag{5.5}
\]

Then, from the maximum principle and \( K'(t) \geq 0 \) and \( T''_0(x) \geq 0 \) we get the thesis. □
Proposition 2. Problem $P$ depends monotonically on the thermal coefficients $\ell$, $c$ and $\rho$, that is,

(a) If $\ell_1 < \ell_2$ and $\{T_i(x,t), s_i(t)\}$ is the solution of the problem $P$ for the data $\ell_i(i = 1, 2)$ and $s_1(0) \geq s_2(0)$, then we have:

$$s_1(t) \geq s_2(t), \quad t > 0;$$

$$T_1(x,t) \geq T_2(x,t), \quad 0 \leq x \leq s_2(t), \quad t > 0.$$  \hspace{1cm} (6.1)

(b) If $c_1 < c_2$ and $\{T_i(x,t), s_i(t)\}$ is the solution of the problem $P$ for the data $c_i(i = 1, 2)$, and $s_1(0) \geq s_2(0)$, then we have:

$$s_1(t) \geq s_2(t), \quad t > 0;$$

$$T_1(x,t) \geq T_2(x,t), \quad 0 \leq x \leq s_2(t), \quad t > 0.$$  \hspace{1cm} (6.2)

(c) If $\rho_1 < \rho_2$ and $\{T_i(x,t), s_i(t)\}$ is the solution of the problem $P$ for the data $\rho_i(i = 1, 2)$, and $s_1(0) \geq s_2(0)$, then we have:

$$s_1(t) \geq s_2(t), \quad t > 0;$$

$$T_1(x,t) \geq T_2(x,t), \quad 0 \leq x \leq s_2(t), \quad t > 0.$$  \hspace{1cm} (6.3)

Proof. The three results are similar but the proofs are different because we must change the coefficients in the heat equation or in the Stefan condition or in both conditions at the same time.

(a) We consider two cases, $s_1(0) > s_2(0)$ and $s_1(0) \geq s_2(0)$.

Case I: Let us suppose $b_1 = s_1(0) > s_2(0) = b_2$ and we consider for $\ell_i(i = 1, 2)$ the corresponding problem $(i = 1, 2)$:

$$T_i = \alpha T_{xx}, \quad 0 < x < s_i(t), \quad t > 0;$$

$$kT_i(0,t) = -K(t), \quad t > 0;$$

$$T_i(s_i(t),t) = T_f, \quad t > 0;$$

$$kT_i(s_i(t),t) = -\rho_i s_i(t), \quad t > 0;$$

$$T_i(x,0) = T_0(x) \geq T_f, \quad 0 < x < b_i;$$

$$s_i(0) = b_i.$$  \hspace{1cm} (9.6)

Let $t_0$ be the first moment such that $s_1(t_0) = s_2(t_0)$ and $s_2(t) < s_1(t)$ for all $0 < t < t_0$, then it will occur

$$s_1'(t_0) \leq s_2'(t_0).$$  \hspace{1cm} (10)

If we define the function $W(x,t) = T_1(x,t) - T_2(x,t)$, $\forall(x,t) \in D^*$ with $D^* = \{(x,t)/0 < x < s_2(t), \quad 0 < t < t_0\}$ then we have:

$$W_t - \alpha W_{xx} = 0, \quad \forall(x,t) \in D^*;$$

$$W_x(0,t) = 0, \quad 0 < t < t_0;$$

$$W(x,0) = 0, \quad 0 \leq x \leq b_2;$$

$$W(s_2(t),t) = T_1(s_2(t),t) - T_f > 0, \quad 0 < t < t_0;$$

$$s_2(0) = b_2.$$  \hspace{1cm} (11.5)

since by the maximum principle $T_1(x,t) > T_f$ in its domain of definition. By the same principle we conclude that $W \geq 0$ in $Cl(D^*)$. At $x = s_1(t_0) = s_2(t_0)$, we have that $W(s_2(t_0),t_0) = 0$, therefore $W$ attains a minimum at $(s_2(t_0),t_0)$. By the strong maximum principle, we have that $W_x(s_2(t_0),t_0) < 0$. But from the Stefan condition Eq. (9.4) and $\ell_1 < \ell_2$ we obtain that

$$W_x(s_2(t_0),t_0) = T_1_x(s_1(t_0),t_0) - T_2_x(s_2(t_0),t_0) = -\frac{\rho_1}{k} s_1'(t_0) + \frac{\rho_2}{k} s_2'(t_0) \geq \frac{\rho_2}{k} [s_2'(t_0) - s_1'(t_0)] \geq 0,$$  \hspace{1cm} (12)
which leads to a contradiction and therefore
\[ s_1(t) > s_2(t), \quad \forall t \geq 0 \quad \text{and} \quad T_1(x, t) \geq T_2(x, t), \quad \forall 0 \leq x \leq s_2(t), \quad t > 0. \]

**Case II:** We consider now the case \( b_1 = s_1(0) \geq s_2(0) = b_2. \) Let \( \delta > 0, \) then \( b_2 \leq b_1 < b_1 + \delta. \) We consider a problem like Eqs. (9.1)-(9.5) with thermal coefficients \((k, \rho, c, \ell_i), s_i(0) = b_1 + \delta\) and we call \((s_\delta, T_\delta)\) the solution of this new problem. We take \( T_0(x) = T_f \) for \( b_1 \leq x \leq b_1 + \delta. \) It results \( s_1(t) < s_\delta(t), \quad \forall t \geq 0 \) and \( T_1(x, t) \leq T_\delta(x, t), \quad \forall 0 \leq x \leq s_1(t) \) and \( t > 0 \) by the maximum principle. From the **Case I** we have that \( s_2(t) < s_\delta(t), \quad \forall t \geq 0 \) and \( T_2(x, t) \leq T_\delta(x, t), \quad \forall 0 \leq x \leq s_2(t) \) and \( t > 0. \) The integral relation between the free boundary \( s_i \) and the temperature \( T_i \) with \( i = 1, \delta \) is given by [21]:

\[
s_i(t) \left( \frac{\ell_i}{c} - T_f \right) = s_i(0) \left( \frac{\ell_i}{c} - T_f \right) + \int_0^{s_i(t)} T_0(x) dx + \frac{1}{\rho c} \int_0^t K(\tau) d\tau - \int_0^{s_i(t)} T_i(x, t) dx.
\]

Subtracting the expressions for \( i = 1 \) and \( i = \delta \) we get

\[
\left[ s_\delta(t) - s_1(t) \right] \left( \frac{\ell_1}{c} - T_f \right) = \delta \frac{\ell_1}{c} - \int_0^{s_\delta(t)} T_\delta(x, t) dx + \int_0^{s_1(t)} T_1(x, t) dx
\]

\[
= \delta \frac{\ell_1}{c} + \int_0^{s_\delta(t)} \left[ T_1(x, t) - T_\delta(x, t) \right] dx - \int_0^{s_1(t)} T_\delta(x, t) dx \leq \delta \frac{\ell_1}{c} - T_f [s_\delta(t) - s_1(t)],
\]

taking into account that \( T_\delta(x, t) - T_1(x, t) \geq 0 \) and \( T_\delta(x, t) \geq T_f. \) Then, \( s_\delta(t) - s_1(t) \leq \delta, \) that is, to say:

\[
s_2(t) < s_\delta(t) \leq s_1(t) + \delta, \quad \forall \delta > 0 \tag{13}
\]

and consequently, letting \( \delta \to 0, \) we obtain that \( s_2 \leq s_1 \) in the common domain of existence.

(b) We consider again two possible cases, \( s_1(0) > s_2(0) \) and \( s_1(0) \geq s_2(0). \)

**Case I:** Let us suppose \( b_1 = s_1(0) > s_2(0) = b_2 \) and we consider for \( c_i (i = 1, 2) \) the corresponding problem:

\[
T_i = \alpha_i T_{xx}, \quad 0 < x < s_1(t), \quad t > 0; \tag{14.1}
\]

\[
-kT_i(0, t) = -K(t), \quad t > 0; \tag{14.2}
\]

\[
T_i(s_1(t), t) = T_f, \quad t > 0; \tag{14.3}
\]

\[
kT_i(s_1(t), t) = -\rho \ell s'_1(t), \quad t > 0; \tag{14.4}
\]

\[
T_i(x, 0) = T_0(x) > T_f, \quad 0 < x < b_1; \tag{14.5}
\]

\[
s_1(0) = b_1, \tag{14.6}
\]

with \( x_1 = \frac{k}{\rho c_1} \) and \( x_2 = \frac{k}{\rho c_2}. \) Let \( t_0 \) be the first moment such that \( s_1(t_0) = s_2(t_0) \) and \( s_2(t) < s_1(t) \) for all \( 0 < t < t_0, \) then it will occur

\[
s'_1(t_0) \leq s'_2(t_0). \tag{15}
\]

If we define the function \( W(x, t) = T_1(x, t) - T_2(x, t), \forall (x, t) \in D^* \) with

\[
D^* = \{(x, t)/0 < x < s_2(t), 0 < t < t_0\},
\]

then we have:

\[
W_1 - \frac{k}{\rho c_1} W_{xx} = \frac{k}{\rho} \left( \frac{1}{c_1} - \frac{1}{c_2} \right) T_{1u} \geq 0, \quad \forall (x, t) \in D^*, \tag{16.1}
\]

\[
W_1(0, t) = 0, \quad 0 < t < t_0; \tag{16.2}
\]

\[
W_1(x, 0) = 0, \quad 0 < x < b_2; \tag{16.3}
\]

\[
W_1(s_2(t), t) = T_1(s_2(t), t) - T_f > 0, \quad 0 < t < t_0; \tag{16.4}
\]

\[
s_2(0) = b_2 \tag{16.5}
\]

as a consequence of **Lemma 1** and \( T_1(x, t) \geq T_f \) by the maximum principle. Then, we conclude that \( W \geq 0 \) in \( Cl(D^*). \) At \( x = s_1(t_0) = s_2(t_0), \) we have that \( W(s_2(t_0), t_0) = 0, \) therefore \( W \) attains a minimum at \( (s_2(t_0), t_0). \) By the strong maximum principle, we have that \( W_x(s_2(t_0), t_0) < 0. \) But from the Stefan condition Eq. (14.4) we obtain that

\[
W_x(s_2(t_0), t_0) = T_1, (s_1(t_0), t_0) - T_2, (s_2(t_0), t_0) = -\frac{\rho \ell}{k} s'_1(t_0) + \frac{\rho \ell}{k} s'_2(t_0) = \frac{\rho \ell}{k} \left[ s'_2(t_0) - s'_1(t_0) \right] \geq 0 \tag{17}
\]
which leads to a contradiction and therefore
\[ s_1(t) > s_2(t), \quad \forall t \geq 0 \quad \text{and} \quad T_1(x, t) \geq T_2(x, t), \quad \forall 0 \leq x \leq s_2(t), \quad t > 0. \]

**Case II:** We consider now the case \( b_1 = s_1(0) \geq s_2(0) = b_2 \). Let \( \delta > 0 \), then \( b_2 \leq b_1 < b_1 + \delta \). We propose a problem like the problem given by Eqs. (14.1)–(14.5) with thermal coefficients \( (k, \rho_1, c_1, \ell) \), \( s_1(0) = b_1 + \delta \) and we call \((s_0, T_0)\) the solution of this new problem by considering \( T_0(x) = T_f \) for \( b_1 \leq x \leq b_1 + \delta, \ t > 0 \). It results \( s_1(t) < s_0(t), T_1(x, t) \leq T_0(x, t), \forall 0 \leq x \leq s_1(t) \) and \( t > 0 \) by the maximum principle. From the **Case I** we have that \( s_2(t) < s_0(t), \forall t \geq 0 \) and \( T_2(x, t) \leq T_0(x, t), \forall 0 \leq x \leq s_2(t) \) and \( t > 0 \). The integral relation between the free boundary \( s \) and the temperature \( T \) with \( r = 1 \), \( \delta \) is given now by \([21]\):
\[
s(t) \left( \frac{\ell}{c_1} - T_f \right) = s(0) \left( \frac{\ell}{c_1} - T_f \right) + \int_0^{s(t)} T_0(x)dx + \frac{1}{\rho c_1} \int_0^t \mathcal{K}(\tau)d\tau - \int_0^{s(t)} T(x, t)dx.
\]
Then, we obtain:
\[
[s_0(t) - s(t)] \left( \frac{\ell}{c_1} - T_f \right) = \delta \frac{\ell}{c_1} - \int_0^{s(t)} [T_1(x, t) - T_0(x, t)]dx - \int_0^{s(t)} T_0(x, t)dx \leq \delta \frac{\ell}{c_1} - T_f [s_0(t) - s(t)].
\]
Taking into account that \( T_0(x, t) - T_1(x, t) \geq 0 \), and \( T_0(x, t) \geq T_f \), then we have \( s_0(t) - s(t) \leq \delta \) that is to say:
\[
s_2(t) < s_2(t) \leq s_1(t) + \delta, \quad \forall \delta > 0.
\]
Consequently, letting \( \delta \to 0 \), we obtain that \( s_2(t) \leq s_1(t) \) in the common domain of existence.

(c) We consider again two possible cases, \( s_1(0) > s_2(0) \) and \( s_1(0) \geq s_2(0) \).

**Case I:** Let us suppose \( b_1 = s_1(0) > s_2(0) = b_2 \) and we consider for \( \rho_i (i = 1, 2) \) the corresponding problem:
\[
T_i = x_i T_{ix}, \quad 0 < x < s_1(t), \quad t > 0;
\]
\[
k T_i(0, t) = -K(t); \quad t > 0;
\]
\[
T_i(s_1(t), t) = T_f, \quad t > 0;
\]
\[
k T_i(s_1(t), t) = -\rho_i s_i^\prime(t), \quad t > 0;
\]
\[
T_f(0, t) = T_0 > T_f, \quad 0 \leq x \leq b_i;
\]
\[
s_1(0) = b_1,
\]
with \( s_1 = \frac{1}{\rho_1 c} \) and \( s_2 = \frac{1}{\rho_2 c} \). Let \( t_0 \) be the first moment such that \( s_1(t_0) = s_2(t_0) \) and \( s_2(t) < s_1(t) \) for all \( 0 < t < t_0 \), then it will occur
\[
s_1^\prime(t_0) \leq s_2^\prime(t_0).
\]
If we define the function \( W(x, t) = T_1(x, t) - T_2(x, t), \forall (x, t) \in D_t^t \) with \( D_t^t = \{(x, t)/0 < x < s_2(t), 0 < t < t_0\} \) then we have:
\[
W - \frac{k}{\rho_1 c} W = k \left( \frac{1}{\rho_1} - \frac{1}{\rho_2} \right) T_2, \quad \forall (x, t) \in D_t^t; \quad \forall (x, t) \in D_t^t;
\]
\[
W(0, t) = 0, \quad 0 < t < t_0;
\]
\[
W(x, 0) = 0, \quad 0 \leq x \leq b_2;
\]
\[
W(s_2(t), t) = T_1(s_2(t), t) - T_f > 0, \quad 0 < t < t_0;
\]
\[
s_2(0) = b_2
\]
as a consequence of the **Lemma 1** and the maximum principle. Then we conclude that \( W \geq 0 \) in \( Cl(D_t^t) \). At \( x = s_1(t_0) = s_2(t_0) \), we have that \( W(s_2(t_0), t_0) = 0 \), therefore \( W \) attains a minimum at \( (s_2(t_0), t_0) \). By the strong maximum principle, we have that \( W_x(s_2(t_0), t_0) < 0 \). But from the Stefan condition Eq. (19.4) we obtain that:
\[
W_x(s_2(t_0), t_0) = -\frac{\rho_1 \ell}{k} s_1^\prime(t_0) + \frac{\rho_2 \ell}{k} s_2^\prime(t_0) = \frac{\ell}{k} \left[ \rho_2 s_2^\prime(t_0) - \rho_1 s_1^\prime(t_0) \right] > 0
\]
(22)
which leads to a contradiction and therefore

\[ s_1(t) > s_2(t), \quad \forall t \geq 0 \quad \text{and} \quad T_1(x,t) \geq T_2(x,t), \quad \forall 0 \leq x \leq s_2(t), \quad t > 0. \]

**Case II:** We consider now the case \( b_1 = s_1(0) \geq s_2(0) = b_2 \). Let \( \delta > 0 \), then \( b_2 \leq b_1 < b_1 + \delta \). We propose a problem like the problem given by Eqs. (19.1)–(19.5) with thermal coefficients \((k, \rho_1, c, \ell)\), \( s_0(0) = b_1 + \delta \) and we call \((s_0, T_0)\) the solution of this new problem by considering \( T_0(x) = T_f \) for \( b_1 \leq x \leq b_1 + \delta \). It results \( s_1(t) < s_0(t), \forall t \geq 0 \) and \( T_1(x,t) \leq T_0(x,t), \forall 0 \leq x \leq s_1(t) \) and \( t > 0 \) by the maximum principle. From the Case I we have that \( s_2(t) < s_0(t), \forall t \geq 0 \) and \( T_2(x,t) \leq T_0(x,t), \forall 0 \leq x \leq s_2(t) \) and \( t > 0 \). The integral relation between the free boundary and the temperature for problems whose solutions are \((s_i, T_i)\), with \( i = 1, \delta \) is now given by [21]:

\[ s_i(t)\left(\frac{\ell}{c} - T_f\right) = s_i(0)\left(\frac{\ell}{c} - T_f\right) + \int_0^{s_i(0)} T_0(x)dx + \frac{1}{\rho_1 c} \int_0^t K(\tau) d\tau - \int_0^{s_i(t)} T_i(x,t)dx. \]

Then we obtain:

\[ [s_\delta(t) - s_1(t)]\left(\frac{\ell}{c} - T_f\right) = \delta \left[ \frac{\ell}{c} - \int_0^{s_1(t)} [T_1(x,t) - T_\delta(x,t)]dx - \int_{s_1(t)}^{s_\delta(t)} T_\delta(x,t)dx \right] \leq \delta \left(\frac{\ell}{c} - T_f\right)[s_\delta(t) - s_1(t)] \]

because \( T_\delta(x,t) - T_1(x,t) \geq 0 \), and \( T_\delta(x,t) \geq T_f \). Then we have \( s_\delta(t) - s_1(t) \leq \delta \) that is to say:

\[ s_2(t) < s_\delta(t) \leq s_1(t) + \delta, \quad \forall \delta > 0. \]

Consequently, letting \( \delta \to 0 \), we obtain that \( s_2(t) \leq s_1(t) \) in the common domain of existence. \( \Box \)

**Remark.** We can not obtain any conclusion through the maximum principle about variations in the thermal conductivity \( k \). This case can be studied by numerical approximations and it will be done in Section 4.

### 3. Approximate solutions of the problem \( P \)

With the aim to obtain the behavior of the solution of problem \( P \) when there exists a variation in the thermal conductivity, we compute the solution to this problem through approximate methods and a numerical method. First we check all these methods with a test problem and then, we use the best of them in order to obtain the desired conclusion.

From now, we consider that the solution of the problem \( P \) can be obtained like:

\[ T(x,t) = u(x,t) + T_f, \]

where \( u(x,t) \) satisfies the same problem (2) with \( T_f = 0 \), i.e.,

\[
\begin{align*}
    u_t &= u_{xx}, \quad 0 < x < s(t), \quad t > 0; \\
    ku_x(0,t) &= -K(t), \quad t > 0; \\
    u(s(t),t) &= 0, \quad t > 0; \\
    ku_x(s(t),t) &= -\rho \ell s'(t), \quad t > 0; \\
    s(0) &= 0.
\end{align*}
\]

**3.1. Heat balance integral method**

The Goodman’s heat balance integral method [22], in analogous form to the integral moment method used in the theory of the boundary layers in fluids mechanics, is based on the physical concept of “thermal depth of penetration”. That is to say, the effect of the excitation in the fixed border \( x = 0 \) does not propagate immediately to all the domain, but in a limited interval \([0, \delta(t)]\). Outside this interval the temperature is the initial temperature. For one-phase problems, this thermal layer agrees with the free boundary \( s(t) \).
By using the heat balance integral method we must solve the following problem:

\[
\frac{d}{dt} \int_0^s u(x, t) dx = \frac{1}{\rho c} [K(t) - \rho \ell \phi'(t)], \quad t > 0; \tag{26.1}
\]

\[
u_s^2(s(t), t) = \frac{\ell}{c} u_{ss}(s(t), t), \quad t > 0; \tag{26.2}
\]

\[u(s(t), t) = 0, \quad t > 0; \tag{26.3}
\]

\[k u_s(0, t) = -K(t), \quad t > 0; \tag{26.4}
\]

\[s(0) = 0. \tag{26.5}
\]

For the non-unique solution of problem (26.1)–(26.5) we can propose a solution. In [23] an exponential type solution is used. We choose the quadratic approximant used by Goodman [22] for \(u(x, t)\) given by

\[u(x, t) = A(t) \left( 1 - \frac{x}{s(t)} \right) + B(t) \left( 1 - \frac{x}{s(t)} \right)^2, \tag{27}
\]

where \(A(t), B(t)\) and \(s(t)\) are unknown functions.

**Proposition 3.** The solution of problem \(P\), through the heat balance integral method, is given by:

\[T(x, t) = T_f + \frac{\ell}{c} \left[ \phi(t) + \frac{1}{2} \phi^2(t) - \frac{cK(t)}{k\ell} x + \frac{1}{2} \left( \frac{xK(t)c}{k\ell(1 + \phi(t))} \right)^2 \right], \tag{28.1}
\]

\[s(t) = \frac{k\ell}{cK(t)} \phi(t)[1 + \phi(t)], \tag{28.2}
\]

where the function \(\phi = \phi(t)\) is the unique solution of the following Cauchy’s problem:

\[\phi'(t) = \frac{A_1(t)}{1 + 3\phi(t) + 2\phi^2(t) + \frac{2}{3} \phi^3(t)} [A_2(t) + A_3(t) \phi(t)(\phi(t) + 1)], \quad t > 0; \tag{29.1}
\]

\[\phi(0) = 0, \tag{29.2}
\]

with:

\[A_1(t) = \frac{c^2}{K(t)\ell^2}, \quad A_2(t) = \frac{K(t)^3}{k\rho c} \]

and

\[A_3(t) = \left( 6 + 3\phi(t) + \phi^2(t) \right) \frac{K'(t)\ell^2}{6c^2}. \]

**Proof.** If we replace Eq. (26) in Eqs. (25.2) and (25.4), we obtain:

\[B(t) = \frac{c}{2r} A_2(t), \quad s(t) = \frac{k}{K(t)} \left[ A(t) + \frac{c}{r} A_2(t) \right]. \tag{30}
\]

We define the function \(\phi(t) = \frac{\phi}{A(t)}\). From the condition Eq. (26.1) we obtain Eq. (28) where \(\phi\) is given as the solution of Eqs. (29.1),(29.2). This problem is well defined because the expression

\[1 + 3\phi(t) + 2\phi^2(t) + \frac{2}{3} \phi^3(t)\]

is a positive and strictly increasing function if \(\phi(t)\) is non-negative. Moreover Eqs. (29.1),(29.2) has a unique solution because, if we call \(f(\phi, t) = \frac{A_1(t)}{1 + 3\phi(t) + 2\phi^2(t) + \frac{2}{3} \phi^3(t)} [A_2(t) + A_3(t) \phi(t)(\phi(t) + 1)]\), we obtain that \(f\) and \(\frac{\partial f}{\partial \phi}\) are both continuous functions when \(K\) and \(K'\) are continuous functions of \(t \geq 0\). Then the proposition holds. \(\square\)
3.2. Biot’s variational method

The Biot’s variational method [24,25] is based on irreversible thermodynamic arguments and it is characterized by:

(i) A vectorial field called “heat displacement” which depends on the space coordinates, on the time and on a set of generalized coordinates suitably chosen for the problem.

(ii) The concepts of thermal potential, dissipation function and generalized thermal force.

Let \( H = H(x,t,s) \) the heat displacement and \( s = s(t) \) a generalized coordinate. We must solve the following variational equation:

\[
\frac{\partial V}{\partial s} + \frac{\partial D}{\partial s} = Q_s,
\]

where the functions \( V \) the thermal potential, \( D \) the dissipation function and \( Q_s \), the generalized thermal force, are defined by the following expressions:

\[
V = \frac{1}{2} \int_0^{s(t)} \rho c u^2 dx; \tag{32}
\]

\[
D = \frac{1}{2} \int_0^{s(t)} \frac{1}{k} \left( \frac{\partial H}{\partial t} \right)^2 dx; \tag{33}
\]

\[
Q_s = -u \frac{\partial H}{\partial s} \bigg|_{x=0}. \tag{34}
\]

The functions \( H, u \) and \( s \) satisfy the set of conditions Eqs. (25.2) and (25.3) and

\[
\frac{\partial H}{\partial x} = -\rho c u, \quad 0 < x < s(t), \quad t > 0, \tag{35.1}
\]

\[
\left. \frac{dH}{dt} \right|_{x=s(t)} = \rho \ell \dot{s}'(t), \quad t > 0, \tag{35.2}
\]

**Proposition 4.** If we consider for \( u \) a polynomial expression with respect to the space variable then the solution of the problem \( P \) through the Biot’s variational method Eqs. (31)–(35) is given by:

\[
T(x,t) = T_f + u(x,t) = T_f + \frac{K(t)s(t)}{2k} \left( 1 - \frac{x}{s(t)} \right)^2 \tag{36}
\]

where \( s(t) \) is the solution of the following Cauchy problem:

\[
s'(t) = \frac{K(t)\rho \ell + B_1(t)s(t) - B_2(t)s^2(t) - B_3(t)s^3(t)}{2(\rho \ell)^2 + B_4(t)s(t) + B_5(t)s^2(t)}, \tag{37.1}
\]

\[
s(0) = 0, \tag{37.2}
\]

with

\[
B_1(t) = \frac{11K^2(t)}{60x}; \quad B_2(t) = \frac{\rho \ell K'(t)}{12x}; \quad B_3(t) = \frac{5K(t)K'(t)}{252x^2}; \quad B_4(t) = \frac{\rho \ell K(t)}{2x}; \quad B_5(t) = \frac{11K^2(t)}{210x^2}.
\]

**Proof.** We propose a quadratic form for \( u \) in the space variable \( x \) of the type

\[
u(x,t) = A(t) \left( 1 - \frac{x}{s(t)} \right)^2.
\]

From Eq. (25.2) we obtain \( A(t) = \frac{K(t)s(t)}{2k}. \)
Taking into account Eq. (35.1), from Eq. (38) we have \( \frac{\partial H}{\partial x} = \frac{K(t)s(t)}{2x}(1 - \frac{x}{s(t)})^2 \) and therefore

\[
H(x,t,s) = \frac{K(t)s^2}{6x}
\left(1 - \frac{x}{s(t)}\right)^3 + G(t,s).
\]  

(39)

As in \( x = s \) we have that \( \dot{H} = \rho\ell\dot{s}' \), we choose \( G(t,s) = \rho\ell s \). After some computations we obtain:

\[
V_s = \frac{3K^2(t)s^2}{40k\alpha},
\]

(40)

\[
Q_s = \frac{K(t)s}{3k} + \rho\ell,
\]

(41)

\[
\frac{\partial D}{\partial s'} = \left(\frac{(\rho\ell)^3 s}{k} + \frac{\rho\ell K(t)s^2}{24k\alpha} + \frac{11K^2(t)s^3}{420/\alpha^2k}\right) s' + s\frac{\rho\ell K'(t)}{24k\alpha} + s\frac{\rho\ell K'(t)}{504/\alpha^2k}.
\]

(42)

Replacing Eqs. (40)–(42) in the variational Eq. (31) we get the Cauchy problem given by Eqs. (37.1) and (37.2). This problem is well-defined because the expression \( 2(\rho\ell)^2 + B_4(t)s(t) + B_5(t)s^2(t) \) is a quadratic function without real zeros. Furthermore, there exist a unique solution to the problem Eqs. (37.1) and (37.2). In effect, if we call

\[
f(s,t) = \frac{K(t)\rho\ell + B_1(t)s(t) - B_2(t)s^2(t) - B_3(t)s^3(t)}{2(\rho\ell)^2 + B_4(t)s(t) + B_5(t)s^2(t)},
\]

and considering that \( K \) and \( K' \) are continuous functions on \( t > 0 \), we have that \( f \) and \( \frac{\partial f}{\partial s} \) are both continuous functions when \( t > 0 \).

**Remark.** If \( K'(t) \leq 0 \), the second member in Eq. (37.1) is a positive function, then \( s(t) \) is a strictly increasing function.

### 3.3. Quasi-stationary method

The quasi-stationary method [1,10,11,26] is used to model physical processes that develop very slowly \( (u_t \sim 0) \). In these processes the latent heat of fusion \( \ell \) tends to infinity and consequently the Stefan number \( \text{Ste} = \frac{c_T}{\ell} \) tends to zero. Using this approximate method we obtain, for problem Eq. (2), the associated problem [22]:

\[
u_{xx} = 0, \quad 0 < x < s(t), \quad t > 0;
\]

(43.1)

\[
k u_x(0,t) = -K(t), \quad t > 0;
\]

(43.2)

\[
u(s(t),t) = 0, \quad t > 0;
\]

(43.3)

\[
k u_x(s(t),t) = -\rho\ell\dot{s}'(t), \quad t > 0;
\]

(43.4)

\[
u(0) = 0.
\]

(43.5)

**Proposition 5.** The solution of the problem \( P \) through the quasi-stationary method given by Eqs. (43.1)–(43.5), is:

\[
T(x,t) = T_f + \frac{K(t)}{k}[s(t) - x], \quad s(t) = \frac{1}{\rho\ell} \int_0^t K(\tau)d\tau.
\]

(44)

**Proof.** We propose a solution \( u(x,t) \) of the problem Eqs. (43.1)–(43.5) in the form

\[
u(x,t) = a(t)x + b(t),
\]

(45)

where \( a(t) \) and \( b(t) \) are unknown functions. From Eq. (43.3) we get \( b(t) = -a(t)s(t) \) and from Eq. (43.2) we have \( a(t) = -\frac{1}{s(t)}K(t) \). The Stefan condition Eq. (43.4), with these \( a(t) \) and \( b(t) \), gives the expressions Eq. (44) for \( s(t) \) and \( T(x,t) \).
3.4. Implicit finite difference method

 Provided that \( \{T(x, t), s(t)\} \), solution of the problem \( P \), is a pair of sufficiently regular functions, we can use a finite difference scheme to approximate this problem [13,17,27].

 Without loss of generality, we suppose \( 0 \leq x \leq E \) (\( E \) fixed, \( E \geq 0 \)) and we define a variable grid with constant space step and equal to \( \Delta x = \frac{E}{N} \) (\( N \) is the number of space intervals). Then we take \( x_i = (i-1)\Delta x, \quad i = 1, \ldots, N + 1 \). The heat equation in the problem \( P \) is transformed into:

\[
\frac{dT_i}{dt} = 2T_i - T_{i+1} - T_{i-1} \quad \frac{\Delta t}{\Delta x^2}
\]

with \( T_i = T(x_i, t) \forall t > 0 \).

 We call \( t_f \) the time such that \( s(t_f) = E \) and let us divide the interval \([0, t_f]\) in \( N \) subintervals of variable size \( \Delta t_j \) with \( j = 1, \ldots, N \). These time steps are such that the moving boundary coincides with a grid line in space at each time level, that is, to say:

\[
s(t_{j+1}) = j\Delta x, \quad \text{with} \quad t_{j+1} = t_j + \Delta t_j,
\]

that is, equivalent to \( (s(t_{j+1}), t_{j+1}) \) be a node of the mesh.

 In order to determine the step \( \Delta t_j \), we consider an equivalent integral form of the Stefan condition in \( P \) [21]:

\[
s(t) \left( \frac{\ell}{c} - T_f \right) = \frac{1}{pc} \int_0^t K(\tau) d\tau - \int_0^s(t) T(x, t) dx,
\]

which connects the free boundary position and the temperature. Replacing Eq. (47) in Eq. (48) with \( t = t_{j+1} \), we obtain

\[
j\Delta x \left( \frac{\ell}{c} - T_f \right) = \frac{1}{pc} \int_0^{t_{j+1}} K(\tau) d\tau - \int_0^{j\Delta x} T(x, t_{j+1}) dx.
\]

 We make the approximations

\[
\int_0^{j\Delta x} T(x, t_{j+1}) dx \simeq \sum_{i=2}^{j+1} \Delta x T_{i,j+1}
\]

\[
\int_0^{t_{j+1}} K(\tau) d\tau \simeq \sum_{m=1}^{j} \Delta t_m K_{m+1}
\]

with \( T_{i,j+1} = T(x_i, t_{j+1}), K_{m+1} = K(\tau_{m+1}) \) and, for each \( j = 1, \ldots, N \), we suppose that \( \Delta t_1, \Delta t_2, \ldots, \Delta t_{j-1} \) and \( T(x_i, t_j), i = 1, \ldots, j \) are known. Then, we obtain the following iterative scheme in order to calculate approximately \( \Delta t_j \):

\[
\Delta(t_{j+1}) t_j = \frac{\rho c}{K_{j+1}} \left[ j \left( \frac{\ell}{c} - T_f \right) \Delta x + \Delta x \sum_{i=2}^{j+1} T_{i,j+1}^{(j)} - \frac{1}{pc} \sum_{m=1}^{j-1} \Delta t_m K_{m+1} \right], \quad q \geq 0,
\]

where \( T_{i,j+1}^{(q)} = T^{(q)}(x_i, t_{j+1}) \) and \( \Delta(t_{j+1}) t_j > 0 \) is chosen arbitrarily. Considering \( T_{i,j+1}^{(q)} = T_f, q \geq 0 \), the solution proceeds iteratively by using Eq. (50) to correct the assumed time step.

 In order to find the components \( T_{i,j+1}^{(q+1)}, i = 1, \ldots, j \), we make a finite-difference representation of both, the first member of the equation Eq. (46) and the flux condition in the fixed border \( x = 0 \) in the problem \( P \). Then we solve the associated linear system:

\[
\frac{T_{i,j+1}^{(q+1)} - T_{i,j}}{\Delta(t_{j+1}) t_j} = \alpha \frac{T_{i+1,j+1}^{(q+1)} - 2T_{i,j+1}^{(q+1)} + T_{i-1,j+1}^{(q+1)}}{\Delta x^2}, \quad i = 2, \ldots, j;
\]

\[
T_{1,j+1}^{(q+1)} = \frac{T_{j+1}^{(q+1)}}{2j+1} + \frac{K(t_{j+1}) \Delta x}{k},
\]

(51)
whose matrix expression is $Av = b$, with $v = (T_{i,j+1}^{(q+1)})_{i=2,...,j}$,

$$A = \begin{pmatrix} 1 + 2r & -r & 0 & 0 & \ldots & 0 & 0 \\ -r & 1 + 2r & -r & 0 & \ldots & 0 & 0 \\ 0 & \ldots & \ldots & -r & 1 + 2r & -r \\ 0 & \ldots & 0 & -r & 1 + 2r \end{pmatrix}, \quad b = \begin{pmatrix} T_{2,j} + rA^{T} \Delta x^{-1} \\ T_{3,j} \\ \vdots \\ T_{j-1,j} \\ (1 + r)T_{j} \end{pmatrix},$$

with $r = \frac{\Delta t}{\Delta x}$. The matrix $A \in \mathbb{R}^{(j-1) \times (j-1)}$ is a non-singular tridiagonal matrix, and then the system Eq. (51) has unique solution.

The iteration Eq. (50) is repeated until we get the desired tolerance. With the value of the time step $\Delta t_{j} = \Delta^{q+1} t_{j}$, for some appropriate $q^{*}$, we take the temperature vector $T_{i,j+1} = T_{i,j+1}^{\text{ES}}$ for $i = 1, \ldots, j + 1$ and $j = 1, \ldots, N$.

**Remark.** It is important to note that we must solve at each time a linear system of equations but there is not restrictions about convergence, because it is an implicit scheme [17,20].

### 3.5. Test problem

In this section, in order to validate the approximate methods described above, we make a program in Scilab for each one of these methods and we obtain a comparative graphic of the numerical solutions with respect to the exact solution of the following test problem:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \alpha u_{xx}, & 0 < x < s(t), & 0 < t < t_f; \\
ku_x(0,t) &= -K(t), & 0 < t < t_f; \\
ku_x(s(t),t) &= 0, & 0 < t < t_f; \\
ku_x(s(t),t) &= -\rho \xi s(t), & 0 < t < t_f; \\
s(0) &= 0;
\end{align*}
\]

where $K(t) = \frac{k}{\text{erf}(\frac{x}{\sqrt{4at}})}$ is the flux function on the fixed border $x = 0$ and we consider $c = \rho = \ell = k = 1$. For this problem, the exact solution has the form [10,21,28]:

\[
\begin{align*}
u(x,t) &= 1 - \frac{\text{erf}\left(\frac{x}{\sqrt{4at}}\right)}{\text{erf}(\xi)}, & s(t) = 2\xi \sqrt{at}
\end{align*}
\]

![Fig. 1. $s(t)$ versus $t$.](image-url)
and $\xi$ is the unique solution of the equation

$$\xi e^{\xi^2} \text{erf}(\xi) = \frac{c}{\ell \sqrt{\pi}}.$$ 

In the following graphics (see Figs. 1–3) we represent the exact solution (ES), the analytical approximate solutions obtained through the heat balance integral method (HBIM), the Biot’s variational method (BM) and the quasi-stationary method (QM) and the numerical solution given by the finite difference method (FDM).

We see in Table 1 the corresponding relative errors for the different methods. We consider the Euclidean norm to compute the errors. We conclude that the finite difference scheme is the best, because for this method

![Fig. 2. $T(0,t)$ versus $t$.](image2)

![Fig. 3. $T(x,t_f)$ versus $x$.](image3)

<table>
<thead>
<tr>
<th></th>
<th>HBIM</th>
<th>BM</th>
<th>QM</th>
<th>FDM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s(t)$</td>
<td>5.79</td>
<td>1.076</td>
<td>0.458</td>
<td>0.568</td>
</tr>
<tr>
<td>$T(0,t)$</td>
<td>0.464</td>
<td>0.852</td>
<td>0.441</td>
<td>0.188</td>
</tr>
<tr>
<td>$T(x,t_f)$</td>
<td>0.392</td>
<td>0.625</td>
<td>0.469</td>
<td>0.340</td>
</tr>
</tbody>
</table>
the error for the temperature’s distribution at the final time is minimum, while the error for the free boundary is acceptable.

4. Numerical results

As we have seen in the previous section, we obtain more adjusted results using the finite difference method, so we will use this method in order to analyze the behavior of the solution of the problem \( P \) with respect to variations in the value of the thermal conductivity.

With that purpose, we will consider in the problem \( P \) a constant heat flux on the fixed border \( x = 0 \) and the values of the thermal coefficients which correspond to the paraffin PCM (his commercial name is Rubitherm).

Let be the problem:

\[
\begin{align*}
T_t &= \alpha T_{xx}, \quad 0 < x < s(t), \quad t > 0; \\
kT_x(0, t) &= -K, \quad t > 0; \\
T(s(t), t) &= T_f, \quad t > 0; \\
kT_x(s(t), t) &= -\rho \ell s'(t), \quad t > 0; \\
s(0) &= 0;
\end{align*}
\]

(54)

\[ \text{Fig. 4. } s(t) \text{ versus } t. \]

\[ \text{Fig. 5. } T(0, t) \text{ versus } t. \]
where \( \alpha = \frac{k}{\rho c} \) is the thermal diffusivity, the thermal conductivity is \( k = 0.2 \text{ W m}^{-1} \text{C}^{-1} \), the mass density is \( \rho = 770 \text{ kg m}^{-3} \), the latent heat is \( \ell = 214000 \text{ J kg}^{-1} \), the specific heat is \( c = 2100 \text{ J kg}^{-1} \text{C}^{-1} \) and the phase change temperature is \( T_f = 2 \text{ C} \). In addition we suppose a fictitious constant heat flux \( K = 100 \text{ W m}^{-2} \). In the \textit{Fig. 4}, we see the evolution of the free boundary for different values for the thermal conductivity such as \( k/10, k/4, k/2, k, 2k, 4k \) and \( 10k \), where \( k \) is the real value for the thermal conductivity of the paraffin. This evolution agrees with the physical idea because at greater conductivity, we need less time to melt the material.

In \textit{Fig. 5} we can analyze the behavior of the temperature in the border in contact with the heat source. For each of the values of the conductivity we observe a decreasing monotone behavior. That is correct, because the system is less time in contact with the heat source.

In \textit{Fig. 6} we represent the temperature distributions at a fixed time \( t^* = 122h \). For three values of the thermal conductivity: \( k/10, k \) and \( 10k \); we choose this time because in that moment none substance is totally melted. We observe that the corresponding curves intersect and so there is not monotonicity.

The curves in \textit{Fig. 7} correspond at a fixed time \( t^* = 300 \text{ h} \), which is the time when the material with the higher conductivity is totally melted. Again we observe that there is not monotonicity.

5. Conclusions

We consider a one-phase one dimensional Stefan problem with a variable heat flux condition on the fixed face \( x = 0 \). We have proved the monotone decreasing behavior of the free boundary and temperature
distribution with respect to the latent heat, specific heat and mass density of a substance by using the maximum principle.

We apply three analytical methods (Heat balance integral method, Biot’s variational method and Quasistationary method) and a numerical method (Implicit finite difference method with variable grid in the time) with the aim to approximate the solution to the problem $P$. We developed the corresponding four programs in Scilab.

We obtain more adjusted results by using the finite difference method and we used it in order to analyze the behavior of the solution of the Stefan problem with respect to the thermal conductivity. We have showed that there is no monotonicity with respect to this thermal coefficient.

References