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REPÚBLICA ARGENTINA

Free boundary problems in Industry: Diffusion of a solvent into a polymer.

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Abstract

We studied a one-dimensional free boundary problem arising in the polymer industry, which solution has an interesting asymptotic behavior when a convective boundary condition is imposed. We prove the existence and uniqueness of the solution. Moreover, we show the asymptotic behavior of the free boundary and of the concentration of the solvent in the domain, for large t. Exact estimates and numerical results are obtained.

Keywords: Free boundary problems; Diffusion; Convective case; Asymptotic behavior.

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1 Introduction.

In this paper we consider a free boundary problem arising from a model for sorption of solvents into glassy polymers.
This model was proposed in by Astarita and Sarti ([1]). They assumed that the sorption process can be described using a free boundary model to simulate a sharp morphological discontinuity observed in the material between a penetrated zone, with a relatively high solvent content, and an glassy region where the solvent concentration is negligibly small (and actually taken to be zero in the model).
The solvent is supposed to diffuse in the penetrated zone according to Fick's law. Moreover the penetrating zone moves into the glassy zone driven by chemical and mechanical effects that are taken into account by an empirical law relating the speed of penetration to the concentration of solvent near the front. This law must account for two main facts observed in the penetration experiences: (i) there exists a threshold value for the solvent concentration under which no penetration occurs; (ii) above such value the speed of the front increases with the concentration near the front itself. A typical form is $v = \alpha|u-q|^m$ where v is the front speed, u is the value of the concentration at the front, $q > 0$ is the threshold value and α and m are positive constants ([1]).
An additional condition on the free boundary is obtained imposing mass conservation, i.e., equating the mass density current to the product of solvent concentration and the velocity of the free boundary.
This model has been the object of a number of papers. The problem has been studied with the condition of constant concentration at the boundary by Fasano *et al* ([2]). Comparini & Ricci investigated the problem assuming that the polymer is in perfect contact with a well-stirred bath ([3]). Comparini *et al* were interested in the case of a slab of non-homogeneous polymer ([4]). Andreucci & Ricci studied the problem assuming a flux condition at the fixed boundary ([5]). Here we are interested in a convective case, where it is supposed that there is a flux of solvent through the left side of a slab proportional to the difference between the solvent concentration at $x = 0$ and a given function of the time which represents an external solvent concentration ($h > 0$ is the proportionality constant). Denoting by $c(x,t)$ the normalized concentration and by $x = s(t)$ the location of the front in the slab the mathematical problem can be stated as follows:

Problem PS

Find a triple (T, s, c) such that: $T > 0$, $s \in C^1[0,T]$, $c \in C^{2,1}(D_T) \cap C(\bar{D}_T)$, where $D_T = \{(x,t) : 0 < t < T, 0 < x < s(t)\}$, and satisfying

$$
\begin{aligned}
c_{xx} - c_t &= 0 \quad \text{in} \quad D_T, && (1.1)\\
c_x(0,t) &= h\left[c(0,t) - g(t)\right], \quad g(0) = 1, \quad 0 \le t \le T && (1.2)\\
\dot{s}(t) &= f(c(s(t),t)), \quad 0 \le t \le T && (1.3)\\
c_x(s(t),t) &= -\dot{s}(t)\left[c(s(t),t) + q\right], \quad 0 \le t \le T && (1.4)\\
s(0) &= 0. && (1.5)
\end{aligned}
$$

The function $g(t)$ is positive and the quantity $q + g(t)$ represents the external concentration. In order to assure a stable process we suppose that $g \in C^{1+\alpha}[0,T]$, $\forall T > 0$, $g'(t) \le 0$ and $G \equiv \int_0^\infty g(t)\,dt < \infty$. Throughout the paper the function f will be supposed to satisfy $f \in C^{1+\alpha}(\tau, 1]$, $\forall \tau > 0$, $f'(c) > 0$ for $c \in (0, 1]$ and $f(0) = 0$. We note that there exists $\Phi = f^{-1}$ which has the same properties as f.

2 An auxiliary problem.

Equating (1.2) to (1.4) for $t = 0$, we have that $c^* \doteq c(0, 0)$ is the unique solution of $f(c^*)(c^* + q) = -h(c^* - 1)$. The solution satisfies $0 < c^* < 1$.
Let $r \in C^1[0, T] \cap C^2(0, T)$ be such that

$$r(0) = 0, \tag{2.6}$$
$$\dot{r}(0) = f(c^*), \tag{2.7}$$
$$0 \leq \dot{r}(t) \leq f(c^*) \qquad \text{in} \qquad [0, T], \tag{2.8}$$
$$|\ddot{r}(t)| \leq K \qquad \text{in} \qquad (0, T), \tag{2.9}$$

and consider the problem (**PA**) of finding $c \in C^{2,1}(D) \cap C(\bar{D})$, c_x continuous up to $x = r(t)$, $t \in (0, T)$, such that

$$c_{xx} - c_t = 0 \qquad \text{in} \qquad D = \{(x, t) : 0 < t < T, 0 < x < r(t)\}, \tag{2.10}$$
$$c_x(0, t) = h\left[c(0, t) - g(t)\right], \qquad g(0) = 1, \qquad 0 \leq t \leq T, \tag{2.11}$$
$$c_x(r(t), t) = -\dot{r}(t)\left[\Phi(\dot{r}(t)) + q\right], \qquad 0 \leq t \leq T. \tag{2.12}$$

Theorem 2.1 *Problem* **PA** *has a unique solution.*

Proof. It follows from [6] and [7, Thm. 5.1., p. 561]. ▮

Proposition 2.2 *For small T, the solution of* **PA** *satisfies:*

$$c_0 \leq c(x, t) < 1 \qquad 0 < x \leq r(t), \qquad 0 < t \leq T, \tag{2.13}$$
$$h(c^* - 1) \leq c_x(x, t) < h\left(1 - g(t)\right) \qquad 0 < t \leq T, \qquad 0 < x < r(t). \tag{2.14}$$

where c_0 is positive and it only depends on T.

Proof. Using the Hopf's lemma we can assume that c attains its maximum value on $x = 0$ since $c_x \leq 0$ on $x = r(t)$. Let be

$$\max_{\bar{D}} c = c(0, t_0)$$

If $t_0 = 0$, then $\max_{\bar{D}} c = c^* < 1$. Otherwise we have $0 > c_x(0, t_0) = h(c(0, t_0) - g(t_0))$, which implies $\max_{\bar{D}} c < g(t_0) \leq 1$. Thus we obtain the right side of (2.13). Now suppose that

$$\min_{\bar{D}} c_x = c_x(0, t_0),$$

for some $t_0 > 0$, then

$$0 \geq c_{xt}(0, t_0) = h\left(c_t(0, t_0) - g'(t_0)\right),$$

and $c_{xx}(0,t_0) \leq g'(t_0) \leq 0$ which contradicts the Hopf's lemma. Thus we have $\min\limits_{\bar{D}} c_x = c_x(0,0) = h(c^* - 1)$. Finally,

$$\begin{aligned}
c(x,t) &= c(0,t) + \int_0^x c_x(\xi,t)\,d\xi = \frac{1}{h}c_x(0,t) + g(t) + \int_0^x c_x(\xi,t)\,d\xi \\
&\geq c^* - 1 + g(t) + h(c^* - 1)f(c^*)t \\
&\geq c^* - 1 + g(T) + h(c^* - 1)f(c^*)T > 0,
\end{aligned}$$

for small T. ∎

Proposition 2.3 *Under assumptions* $(2.6)-(2.9)$ $c \in C^{2,1}(\bar{D})$, $c_{xt} \in C(\bar{D} - (0,0))$ *and there exists a constant* B *depending on* T, *and on* K *such that*

$$|c_t(x,t)| \leq B, \qquad \forall (x,t) \in D. \tag{2.15}$$

Proof. We note that we can reduce T, if necessary in order to have $\dot{r}(t) \geq f(1) - KT > 0$ $\forall t \in [0,T]$. Note that $w = c_t$ is the solution of

$$\begin{aligned}
w_{xx} - w_t &= 0 \qquad \text{in } D, && (2.16)\\
w_x(0,t) &= h\,(w(0,t) - g'(t)) \qquad 0 < t < T, && (2.17)\\
w_x(r,t) + \dot{r}(t)w(r(t),t) &= F(t) \qquad 0 < t < T, && (2.18)
\end{aligned}$$

with $F(t) = \frac{d}{dt}c_x(r,t)$.
Now suppose that w attains its maximum value at (x_0,t_0). If $t_0 > 0$ and $x_0 = r(t_0)$ then

$$\begin{aligned}
0 < w_x(x_0,t_0) &= F(t_0) - \dot{r}(t_0)w(x_0,t_0) \\
w(x_0,t_0) &\leq \frac{\sup|F|}{f(c^*) - KT} \\
&\leq \frac{K}{f(c^*) - KT}\left(c^* + q + f(c^*) + \sup\Phi'\right) \doteq \beta_1
\end{aligned}$$

If $x_0 = 0$ and $t_0 > 0$ we have

$$\begin{aligned}
h\,(w(x_0,t_0) - g'(t_0)) &= w_x(x_0,t_0) < 0 \\
w(x_0,t_0) &< g'(t_0) \leq \sup|g'| \doteq \beta_2
\end{aligned}$$

Finally, if $x_0 = 0 = t_0$ there are t_1, t_2 and t_3 in $(0,t)$ such that

$$\begin{aligned}
\frac{c_x(r(t),t) - c_x(0,t)}{r(t)} &= \frac{-\dot{r}(t)(\Phi(\dot{r}(t)) + q) - h(c(0,t) - g(t))}{r(t)} \\
c_{xx}(r(t_1),t) &= \frac{-\ddot{r}(t_2)\left[q + \Phi(\dot{r}(t_2)) + \dot{r}(t_2)\Phi'(\dot{r}(t_2))\right] - h\left[c_t(0,t_2) - g'(t_2)\right]}{\dot{r}(t_3)} \\
\left|c_t(r(t_1),t) + \frac{h}{\dot{r}(t_3)}c_t(0,t_2)\right| &\leq \frac{K\left[q + \sup\Phi + f(c^*)\sup\Phi'\right] + h\sup|g'|}{\dot{r}(t_3)}
\end{aligned} \tag{2.19}$$

taking $t \to 0$:

$$|c_t(0,0)| \leq \frac{K[q + \sup\Phi + f(c^*)\sup\Phi'] + h\sup|g'|}{h + f(c^*)} \doteq \beta_3.$$

Similarly, we get $\min_{\bar{D}} w \geq -\max(\beta_1, \beta_2, \beta_3)$. ∎

Now we investigate how the solution of **PA** depends on $r(t)$. Let $r_1(t)$, $r_2(t)$ satisfy (2.6) – (2.9) and let $c_1(x,t)$, $c_2(x,t)$ be the corresponding solutions of (2.10) – (2.12). We have

Proposition 2.4 *Under the assumptions above, constants $T_0 > 0$ and $N > 0$ can be found such that for any $T \in (0, T_0)$*

$$|c_1(r_1(t),t) - c_2(r_2(t),t)| \leq N||r_1 - r_2||_{C^1[0,T]}, \qquad 0 < t < T. \tag{2.20}$$

Proof. Let us define $\lambda = \min(r_1, r_2)$ and $D^* = \{(x,t) : 0 < x < \lambda(t),\ 0 < t < T\}$. Let be $M > 0$ and

$$W^{\pm} = c_1 - c_2 \pm xMR, \qquad \text{in} \qquad D^*,$$

with $R = ||r_1 - r_2||_{C^1[0,T]}$. Those functions satisfy

$$W_x^{\pm}(0,t) = hW^{\pm}(0,t) \pm MR \tag{2.21}$$

Let be $t > 0$ and suppose that $\lambda(t) = r_1(t)$. Then

$$\begin{aligned}
|(c_1 - c_2)_x(\lambda, t)| &\leq |c_{1x}(r_1, t) - c_{2x}(r_2, t)| + |c_{2x}(r_2, t) - c_{2x}(r_1, t)| \\
&\leq |-\dot{r}_1(\Phi(\dot{r}_1) + q) + \dot{r}_2(\Phi(\dot{r}_2) + q)| + |c_{2xx}(\xi_{12}, t)||(r_1 - r_2)(t)| \\
&< MR
\end{aligned} \tag{2.22}$$

if $M > (c^* + q) + f(c^*)\max\Phi' + B$ is taken (note that M is the same if $\lambda(t) = r_2(t)$). Thus we get $W_x^+(\lambda, t) > 0$ and $W_x^-(\lambda, t) < 0\ \forall t$. So, there are $t^{\pm} \geq 0$ such that $\min W^+ = W^+(0, t^+)$ and $\max W^- = W^-(0, t^-)$. Using Hopf's lemma and (2.21) we have:

$$\begin{aligned}
W^+(0, t^+) &> -\frac{M}{h}R \\
W^-(0, t^-) &< \frac{M}{h}R
\end{aligned}$$

which implies

$$\begin{aligned}
(c_1 - c_2)(x,t) + MRx \geq \ & W^+(0, t^+) \ \geq -\frac{M}{h}R \\
(c_1 - c_2)(x,t) - MRx \leq \ & W^-(0, t^-) \ \leq \frac{M}{h}R
\end{aligned}$$

or

$$|(c_1 - c_2)(x,t)| \leq \left(Mf(c^*)T + \frac{M}{h}\right)R. \tag{2.23}$$

∎

3 Local existence and uniqueness.

Let $\gamma(t)$ be a positive nonincreasing function defined for $t > 0$ and possibly diverging for $t \to 0^+$. Denote by $X(K, T, \gamma)$ the set of functions $r(t)$ satisfying (2.6) – (2.9) and such that, for some $\alpha \in (0, 1]$

$$|\ddot{r}(t_1) - \ddot{r}(t_2)| \leq \gamma(\tau)(t_1 - t_2)^{\alpha/2}, \qquad 0 < \tau \leq t_2 \leq t_1 \leq T. \tag{3.24}$$

Note that the set X is convex and compact in $C^1[0,T]$.
For any $r \in X$ let c be the solution of (2.10) – (2.12). Then, define the transformation $\tilde{r} = \mathcal{C}r$ as follows

$$\tilde{r}(0) = 0, \qquad \dot{\tilde{r}}(t) = f(c(r(t),t)), \qquad 0 < t < T. \tag{3.25}$$

(Remember $0 < c_0 \leq c < 1$ by (2.13).)
Now we prove

Theorem 3.1 *There exist K, T and γ such that the transformation $\tilde{r} = \mathcal{C}r$ is a continuous mapping of $X(K,T,\gamma) \subset C^1[0,T]$ into itself.*

Proof. Since $(2.6) - (2.8)$ are satisfied by contruction, to prove that $\mathcal{C}$ maps X into itself, we only need to prove that $\tilde{r}$ satisfies (2.9) y (3.24) for suitable K, T, γ. We have

$$\ddot{\tilde{r}}(t) = \left[c_x(r(t),t)\dot{r}(t) + c_t(r(t),t)\right] f'(c(r(t),t)), \qquad 0 < t < T. \tag{3.26}$$

Using (2.13) and (2.14), we find (2.9) yields taking $K = (hf(c^*)T + B) \max\limits_{[c_0,1]} f'$. To estimate the Hölder norm of $\ddot{\tilde{r}}(t)$ we need to estimate the norm of $c_x(x,t)$ in the space $C^{1+\alpha}$. This is accomplished as follows. Define $z(x,t) = c_x(x,t) + \dot{r}(t)\,[q + \Phi(\dot{r}(t))]$, which solves

$$\begin{aligned} z_{xx} - z_t &= -\ddot{r}(t)\,[q + \Phi(\dot{r}(t)) + \Phi'(\dot{r}(t))\dot{r}(t)] \qquad \text{in D}, \\ hz_x(0,t) - z_t(0,t) &= hg'(t) - \ddot{r}(t)\,[q + \Phi(\dot{r}(t)) + \Phi'(\dot{r}(t))\dot{r}(t)]\,, \qquad 0 < t < T, \\ z(r(t),t) &= 0, \qquad 0 < t < T. \end{aligned}$$

For any $\tau \in (0,T)$ transform the domain $0 < x < r(t)$, $\tau/2 < t < T$ into the rectangle $(0,1) \times (\tau/2,T)$ by the transformation $y = x/r(t)$ and apply the standard Schauder estimates (e.g. [7, Thm. 5.1., p. 561]) to the transformed function $\hat{z}(y,t)$, in the rectangle $(1/2,1) \times (\tau/2,T)$. We find

$$||z||_{C^\alpha} \leq \bar{\gamma}(\tau), \qquad (1/2,1) \times (\tau,T), \tag{3.27}$$

where $\bar{\gamma}$ depends on K, on f, on T, and on τ (and α). Thus defining $\gamma(t)$ as suggested by (3.27), $\tilde{r}$ will satisfy (3.24). The final step in proving Theorem 3.1 is to prove that the transformation $\mathcal{C}$ is continuous. But this is an immediate consequence of (2.20) and (3.25) because

$$||\tilde{r}_1 - \tilde{r}_2||_{C^1[0,T]} \leq (T+1)\max_{[c_0,1]} f' N ||r_1 - r_2||_{C^1[0,T]}.$$

∎

Hence a $T_0 > 0$ can be found such that the following theorem holds

Theorem 3.2 *Problem* **PS** *admits a solution for $T \leq T_0$. Moreover, $c \in C^{2,1}(\bar{D}_T)$, $s \in C^2[0,T]$.*

Proof. This is a straightforward consequence of Theorem 3.1 and of Schauder's fixed point theorem. The regularity properties of c and s follow from Proposition 2.3 and the definition of X. ∎

A monotone dependence lemma will be useful in proving the uniqueness theorem. Let c_i, s_i, $i = 1, 2$, solve the problems

$$c_{ixx} - c_{it} = 0, \qquad 0 < x < s_i(t), \qquad t_i < t < T, \tag{3.28}$$

with initial conditions $s_i(t_i) = 0$ and satisfying boundary conditions (1.2) – (1.4) in the time intervals (t_i, T). We have

Lemma 3.1 *If $t_1 < t_2$, then*

$$s_1(t) > s_2(t), \qquad t_2 < t < T. \tag{3.29}$$

Proof. Note that the transformation

$$u(x,t) = -\int_x^{s(t)} [c(y,t) + q] \, dy, \tag{3.30}$$

carries (1.1) – (1.5) into the following problem:

$$u_{xx} - u_t = 0, \qquad \text{in} \qquad D_T, \tag{3.31}$$
$$u_t(0,t) = h\left[u_x(0,t) - q - g(t)\right], \qquad 0 < t < T, \tag{3.32}$$
$$u(s(t),t) = 0, \qquad 0 < t < T, \tag{3.33}$$
$$u_x(s(t),t) = \Phi(\dot{s}(t)) + q, \qquad 0 < t < T, \tag{3.34}$$
$$s(0) = 0. \tag{3.35}$$

Consider the function $u_i(x,t)$ obtained from $c_i(x,t)$ by means of (3.30). Assume that there exists a first time t_0 such that $s_1(t_0) = s_2(t_0) \equiv s_0$ and hence

$$\dot{s}_1(t_0) \le \dot{s}_2(t_0), \tag{3.36}$$

and so

$$(u_1 - u_2)(s_0, t_0) = 0, \tag{3.37}$$
$$(u_1 - u_2)_x(s_0, t_0) = \Phi(\dot{s}_1(t_0)) - \Phi(\dot{s}_2(t_0)) \le 0. \tag{3.38}$$

The Hopf's lemma and (3.32) assure that $u_1 - u_2$ cannot attain its maximum value at $x = 0$. But, for $t_2 \le t < t_0$ we have

$$(u_1 - u_2)(\lambda(t), t) = (u_1 - u_2)(s_2(t), t) = u_1(s_2(t), t) < 0,$$

thus (3.37) implies that $(u_1 - u_2)_x(s_0, t_0) > 0$ which contradicts (3.38).∎

Now we can prove uniqueness.

Theorem 3.3 *Problem* **PS** *cannot have two distinct solutions with the same T.*

Proof. As in [2].

4 Global existence.

Before proving global existence, let us perform an a priori analysis on the solutions of problem **PS**.

Proposition 4.1 *Assume s, c solve problem* **PS** *for a given $T < +\infty$. Then*

$$0 < \quad c(x,t) \quad < 1 \qquad 0 \le x \le s(t), \qquad t \ge 0, \tag{4.39}$$

$$h(c^* - 1) < \quad c_x(x,t) \quad < h(1 - g(t)) \qquad 0 \le x \le s(t), \qquad t > 0, \tag{4.40}$$

Proof. Using the Hopf's lemma we can assume that c attains its maximum value at $x = 0$ since $c_x = -f(c)(\Phi(\dot{s}) + q) \le 0$ on $x = s(t)$. Let be

$$c(0, t_0) = \max_{D_T} c.$$

If $t_0 = 0$, then $\max_{D_T} c = c^* < 1$. Otherwise we have $0 > c_x(0, t_0) = h(c(0, t_0) - g(t_0))$, which implies $\max_{D_T} c < g(t_0) \le 1$. Let be

$$c(x_1, t_1) = \min_{D_T} c.$$

If $x_1 = 0$ then there occurs either $\min_{D_T} c = c^* > 0$ or

$$\min_{D_T} c = g(t_1) + \frac{1}{h} c_x(0, t_1) \ge g(t_1) > 0.$$

Moreover, if $\min_{D_T} c = c(s(t_1), t_1) = 0$ (with $t_1 > 0$) then $c_x(s(t_1), t_1) = 0$, contradicting the boundary point principle. Thus, (2.6) holds and $c_x(0,t) < h(1 - g(t))$ for all t. Finally, let us suppose that

$$\min_{D_T} c_x = c_x(s(t_2), t_2) \qquad \text{with } t_2 \ge 0.$$

If $t_2 > 0$ then $0 \ge \frac{d}{dt} c_x(s(t),t)|_{t=t_2}$, i.e.

$$0 \le -[f'(c(s(t_2), t_2))(c(s(t_2), t_2) + q) + f(c(s(t_2, t_2)))][c_x(s(t_2), t_2)\dot{s}(t_2) + c_{xx}(s(t_2), t_2)] > 0,$$

which is a contradiction. Then $\min_{D_T} c_x = c_x(0,0) = h(c^* - 1)$. ∎

Proposition 4.2 *Under the assumptions above, the following estimate holds*

$$|c_t(x,t)| \le B_T, \qquad \forall (x,t) \in D_T, \tag{4.41}$$

with

$$B_T = \max\left\{ \max_{[0,T]} |g'|, f(1)^2(1 + q), |c_t(0,0)| \right\}. \tag{4.42}$$

Proof. Note from (1.2) that

$$c_t(0,t) = g'(t) + \frac{1}{h} c_{tx}(0,t), \qquad 0 < t \le T. \tag{4.43}$$

Moreover, from (1.3) and (1.4) we have $c_x = -f(c)(c + q)$ at $x = s(t)$ and deriving with respect to t we get

$$c_t f(c) + c_{tx} = -\left[f'(c)(c+q) + f(c)\right](c_x f(c) + c_t) \qquad \text{at} \qquad x = r(t) \tag{4.44}$$

$$c_t(s(t),t) = \left(\frac{\left[f'(c)(c+q) + f(c)\right] f^2(c)(c+q) - c_{tx}}{2f(c) + f'(c)(c+q)} \right)_{x=r(t)} \tag{4.45}$$

The proposition follows by using the Hopf's lemma. ∎

Theorem 4.3 *Problem* **PS** *admits a solution for arbitrary* $T > 0$.

Proof. Let us assume that

$$T^* = \sup\{T > 0 : \text{there exists a solution of } \mathbf{PS} \text{ for } T\} \tag{4.46}$$

is finite. Note from Thm. 3.3 and props. 4.1 and 4.2 that there exist the limits $s^* \equiv \lim_{t\to T^*} s(t)$, $c_0^* \equiv \lim_{t\to T^*} c(s(t),t))$, $\dot{s}^* \equiv \lim_{t\to T^*} \dot{s}(t)$ and $c_0^*(x) \equiv \lim_{t\to T^*} c(x,t)$ for $0 \le x < s^*$. Moreover, $c \in C^{2,1}(\bar{D}_{T^*} - D_{T^*/2})$ (see, e.g. [8]) and from (4.39) we have that $\dot{s}^* > 0$. Thus, for $\hat{T} > T^*$, consider the set of functions $r \in C^1[T^*, \hat{T}] \cap C^2(T^*, \hat{T})$ such that

$$r(T^*) = s^*, \tag{4.47}$$

$$\dot{r}(T^*) = \dot{s}^*, \tag{4.48}$$

$$0 \le \dot{r}(t) \le \dot{s}^* \qquad \text{in} \qquad [T^*, \hat{T}], \tag{4.49}$$

$$|\ddot{r}(t)| \le K \qquad \text{in} \qquad (T^*, \hat{T}). \tag{4.50}$$

There exists a unique solution for the problem of finding a function $c \in C^{2,1}(\bar{D}_{\hat{T}} - D_{T^*})$ satisfying (2.10) – (2.12) for $t \in [T^*, \hat{T}]$ and initial data $c(x,T^*) = c_0^*(x)$ (see, e.g. [8]). Similarly, as in section 3, there exists a function $s(t)$ which satisfies (4.47) – (4.50) and (1.3) for $T^* \le t \le \hat{T}$ for suitable $\hat{T} > T^*$, contradicting (4.46). ▮

5 Asymptotic behavior.

In this section we show some results about the behavior of the free boundary $s(t)$ when t goes to infinity.

Let $s(t)$, $c(x,t)$ solve problem **PS**. Using Green's identity we get:

$$0 = \oint_{\partial D_t} c(x,t)v(x,t)\,dx + (v(x,t)c_x(x,t) - c(x,t)v_x(x,t))\ dt \qquad t > 0, \tag{5.51}$$

which holds for every solution $v = v(x,t)$ of $v_{xx} + v_t = 0$ in D_t. Thus, taking $v(x,t) = 1$ we obtain

$$0 = \oint_{\partial D_t} c(x,t)\,dx + c_x(x,t)\,dt \qquad t > 0,$$

which gives

$$0 = \int_0^t c(s(\tau),\tau)\dot{s}(\tau)\,d\tau - \int_0^t \dot{s}(\tau)\,(c(s(\tau),\tau) + q)\ d\tau - \int_0^{s(t)} c(x,t)\,dx - \int_0^t c_x(0,\tau)\,d\tau$$

and then

$$qs(t) \;=\; -\int_0^{s(t)} c(x,t)\,dx - \int_0^t c_x(0,\tau)\,d\tau \tag{5.52}$$

$$\;=\; -\int_0^{s(t)} c(x,t)\,dx - h\int_0^t c(0,\tau)\,d\tau + h\int_0^t g(\tau)\,d\tau \tag{5.53}$$

so

$$s(t) \le \frac{h}{q}\int_0^t g(\tau)\,d\tau \le \frac{h}{q}G. \tag{5.54}$$

This upper bound is independent of f, and since $\dot{s}(t) = f(c(s(t),t)) > 0$ there exists

$$s_\infty \doteq \lim_{t\to\infty} s(t). \tag{5.55}$$

The following numerical result (see section 6) shows these facts for the case $q = 0.3$, $h = 10$, $g(t) = e^{-2t}$ and several functions f ($\frac{h}{q}G = 16.7$).

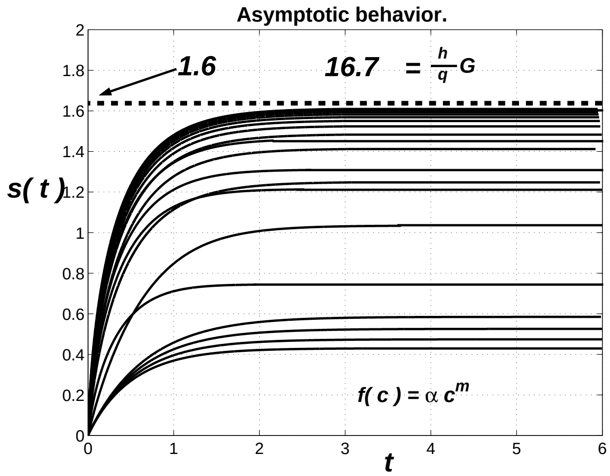

Figure 1: Plot of the free boundaries and their asymptotic behaviors for several function $f(c) = \alpha c^m$, $\alpha > 0$,$m > 0$.

The figure 1 shows that all the free boundaries are bounded by a constant closed to 1.6, so $\frac{h}{q}G$ appears to be a very large bound, and we can look for a better one. In order to do it, we will obtain two additional equations for s and c ((5.56) and (5.57) below). First, taking $v(x,t) = x$ in (5.51) we have

$$0 = \oint_{\partial D_t} c(x,t)x\,dx + (xc_x(x,t) - c(x,t))\,dt,$$

it gives

$$0 = \int_0^t c(s(\tau),\tau)s(\tau)\dot{s}(\tau)\,d\tau + \int_0^t [-(q + c(s(\tau),\tau))\dot{s}(\tau)s(\tau) - c(s(\tau),\tau)]\,d\tau - \\ - \int_0^{s(t)} c(x,t)x\,dx + \int_0^t c(0,\tau)\,d\tau,$$

$$\frac{q}{2}s^2(t) + \int_0^t c(s(\tau),\tau)\,d\tau = -\int_0^{s(t)} c(x,t)x\,dx + \int_0^t c(0,\tau)\,d\tau. \tag{5.56}$$

Similarly, taking $v(x,t) = t - \frac{x^2}{2}$ we get:

$$0 = \oint_{\partial D_t} c(x,t)\left(t - \frac{x^2}{2}\right)\,dx + \left[\left(t - \frac{x^2}{2}\right)c_x(x,t) + xc(x,t)\right]\,dt,$$

thus

$$\begin{aligned} 0 \;=\; & \int_t^0 \tau c_x(0,\tau)\,d\tau + \\ & + \int_0^t \left[c(s(\tau),\tau)\left(\tau - \frac{s^2(\tau)}{2}\right)\dot{s}(\tau) + \left(\tau - \frac{s^2(\tau)}{2}\right)c_x(s(\tau),\tau) + c(s(\tau),\tau)s(\tau)\right]\,d\tau + \\ & + \int_{s(t)}^0 c(x,t)\left(t - \frac{x^2}{2}\right)\,dx, \end{aligned}$$

and so

$$
\begin{aligned}
0 \;=\;& -\int_0^t \tau c_x(0,\tau)\,d\tau - \frac{q}{6}s^3(t) - q\int_0^t \tau\dot{s}(\tau)\,d\tau + \\
&+\int_0^t c(s(\tau),\tau)s(\tau)\,d\tau + \frac{1}{2}\int_0^{s(t)} x^2 c(x,t)\,dx - t\int_0^{s(t)} c(x,t)\,dx. \qquad (5.57)
\end{aligned}
$$

Lemma 5.1 *The following equation holds:*

$$
\lim_{t\to\infty}\int_0^{s(t)} c(x,t)\,dx = 0. \qquad (5.58)
$$

Proof. From (5.57) we have

$$
\begin{aligned}
\int_0^{s(t)} c(x,t)\,dx \;=\;& -\frac{1}{t}\int_0^t \tau c_x(0,\tau)\,d\tau - \frac{q}{6t}s^3(t) - \frac{q}{t}\int_0^t \tau\dot{s}(\tau)\,d\tau + \\
&+\frac{1}{t}\int_0^t c(s(\tau),\tau)s(\tau)\,d\tau + \frac{1}{2t}\int_0^{s(t)} x^2 c(x,t)\,dx \\
&\le -\frac{1}{t}\int_0^t \tau c_x(0,\tau)\,d\tau + \frac{1}{t}\int_0^t c(s(\tau),\tau)s(\tau)\,d\tau + \frac{s_\infty^3}{2t}.
\end{aligned}
$$

To prove the lemma it is enough that all these terms go to zero as $t\to\infty$. In order to do it, note that from (5.53),

$$
\int_0^t c(0,\tau)\,d\tau \le \int_0^t g(\tau)\,d\tau \le G,
$$

then, using (5.56)

$$
\int_0^t c(s(\tau),\tau)s(\tau)\,d\tau \le s_\infty \int_0^t c(s(\tau),\tau)\,d\tau \le s_\infty G,
$$

thus

$$
\lim_{t\to\infty}\frac{1}{t}\int_0^t c(s(\tau),\tau)s(\tau)\,d\tau = 0.
$$

On the other hand, from (5.52)

$$
-\int_0^t c_x(0,\tau)\,d\tau = \int_0^{s(t)} \left[q + c(x,t)\right]\,dx > 0 \qquad (5.59)
$$

and from (1.2) we have

$$
-\int_0^\infty c_x(0,\tau)\,d\tau = h\left(G - \int_0^\infty c(0,\tau)\,d\tau\right) < \infty. \qquad (5.60)
$$

By using integration by parts, (5.59), 5.60 and the L'Hôpital's rule we obtain

$$
\lim_{t\to\infty}\frac{1}{t}\int_0^t \tau c_x(0,\tau)\,d\tau = \lim_{t\to\infty}\left[\int_0^t c_x(0,\tau)\,d\tau - \frac{1}{t}\int_0^t\left(\int_0^\tau c_x(0,\tau')\,d\tau'\right)\,d\tau\right] = 0.
$$

∎

Lemma 5.2 *Assume that $f(c) = \alpha c$, $\alpha > 0$. Then the explicit formula holds:*

$$s_\infty = \sqrt{\left(\frac{1}{h} + \frac{1}{\alpha q}\right)^2 + \frac{2}{q}G} - \left(\frac{1}{h} + \frac{1}{\alpha q}\right). \tag{5.61}$$

Proof. Cancelling $\int_0^t c(0,\tau)\,d\tau$ from (5.53) and (5.56) we obtain

$$\frac{q}{2}s^2(t) + \frac{q}{h}s(t) = -\int_0^{s(t)} \left(\frac{1}{h} + x\right) c(x,t)\,dx + \int_0^t g(\tau)\,d\tau - \int_0^t c(s(\tau),\tau)\,d\tau, \tag{5.62}$$

and since $c(s(\tau),\tau) = \frac{1}{\alpha}\dot{s}(\tau)$, we get

$$\frac{q}{2}s^2(t) + \left(\frac{1}{\alpha} + \frac{q}{h}\right) s(t) = \int_0^t g(\tau)\,d\tau - \int_0^{s(t)} \left(\frac{1}{h} + x\right) c(x,t)\,dx,$$

observe that $\int_0^{s(t)} \left(\frac{1}{h} + x\right) c(x,t)\,dx \le \left(\frac{1}{h} + s_\infty\right) \int_0^{s(t)} c(x,t)\,dx$, and then by (5.58) we get

$$\frac{q}{2}s_\infty^2 + \left(\frac{1}{\alpha} + \frac{q}{h}\right) s_\infty = G.$$

∎

Theorem 5.1 *The following statement is true*

$$\sup_f s_\infty = \sqrt{\frac{1}{h^2} + \frac{2}{q}G} - \frac{1}{h}. \tag{5.63}$$

The supremum is taken on the set of the functions f belonging to $C^{1+\alpha}(\tau,1]$ $\forall \tau > 0$ satisfying $f'(c) > 0$ in $(0,1]$ and $f(0) = 0$.

Proof. Proceeding as in (5.62), we have

$$s^2(t) + \frac{2}{h}s(t) - \frac{2}{q}\int_0^t g(\tau)\,d\tau = -\frac{2}{q}\int_0^{s(t)} \left(\frac{1}{h} + x\right) c(x,t)\,dx - \int_0^t c(s(\tau),\tau)\,d\tau \le 0,$$

as $t \to \infty$ we get

$$s_\infty^2 + \frac{2}{h}s_\infty - \frac{2}{q}G \le 0$$

thus

$$s_\infty \le \sqrt{\frac{1}{h^2} + \frac{2}{q}G} - \frac{1}{h},$$

and (5.63) follows taking $\alpha \to \infty$ in (5.61). ∎

6 The numerical method.

In this section will be shown a numerical scheme based on the method introduced in [9] for one-dimensional parabolic free boundary problems with arbitrary implicit or explicit free boundary conditions.
In this method the continuous problem is time discretized and solved at successive time levels as a sequence of free boundary problems for ordinary differential equations. Specifically, at time level $t = t_n$ with $t_n - t_{n-1} = \Delta t$ the solution $\{C_n(x), S_n\}$ is computed as the exact solution of the discretized equations

$$\begin{aligned}
C_n'' - \frac{C_n - C_{n-1}}{\Delta t} &= 0 \qquad 0 < x < S_n, && (6.64)\\
C_n'(0) &= h\left(C_n(0) - g(t_n)\right), && (6.65)\\
\frac{S_n - S_{n-1}}{\Delta t} &= f(C_n(S_n)), \qquad S_0 = 0, && (6.66)\\
C_n'(S_n) &= -\frac{S_n - S_{n-1}}{\Delta t}(q + C_n(S_n)). && (6.67)
\end{aligned}$$

In (6.64) the function $C_{n-1}(x)$ is supposed to be defined over $[0, +\infty)$, and S_{n-1} supposed to be known as well. We write (6.64) as a first order system over $(0, S_n)$

$$\begin{aligned}
C_n' &= V_n, && (6.68)\\
V_n' &= \frac{1}{\Delta t}\left(C_n - C_{n-1}\right) && (6.69)
\end{aligned}$$

and exploit the observation that C_n and V_n are related through the Riccati transformation

$$C_n(x) = R(x)V_n(x) + W_n(x), \tag{6.70}$$

where

$$\begin{aligned}
R(x) &= \frac{\sqrt{\Delta t}}{\tanh\left(\frac{x+K}{\sqrt{\Delta t}}\right)}, \qquad K = \sqrt{\Delta t}\tanh^{-1}(h\sqrt{\Delta t}) && (6.71)\\
W_n' &= -\frac{R(x)}{\Delta t}\left(W_n - C_{n-1}(x)\right), \qquad W_n(0) = g(t_n). && (6.72)
\end{aligned}$$

The function W_n is solution of well defined initial value problem and may be considered available. The free boundary S_n is determined such that the triple C_n, V_n, S_n simultaneously satisfies (6.66), (6.67) and (6.70). Elimination of C_n and V_n from (6.67) and (6.70) shows that S_n must be a root of the scalar equation

$$\sigma_n(x) \doteq (x - S_{n-1})/\Delta t - f\left(\frac{W_n(x) - qR(x)(x - S_{n-1})/\Delta t}{1 + R(x)(x - S_{n-1})/\Delta t}\right) = 0. \tag{6.73}$$

Given S_n, we set

$$C_n(S_n) = \frac{W_n(S_n) - R(S_n)\dot{S}_n q}{1 + R(S_n)\dot{S}_n}, \tag{6.74}$$

so that

$$\dot{S}_n \doteq \frac{S_n - S_{n-1}}{\Delta t} = f(C_n(S_n)), \tag{6.75}$$

and

$$C_n'(S_n) = V_n(S_n) = -\dot{S}_n \frac{W_n(S_n) + q}{1 + R(S_n)\dot{S}_n}. \tag{6.76}$$

Thus, the triple $\{C_n(S_n), V_n(S_n), S_n\}$ is an exact solution of (6.66), (6.67) and (6.70). We remark that depending on Δt the functional $\sigma_n(x)$ may have a root smaller than S_{n-1}. Such a root would correspond to a negative concentration $C_n(S_n)$ and is not admissible. We shall therefore agree to choose for S_n the smallest root of $\sigma_n(x) = 0$ on (S_{n-1}, ∞). Such a root will be soon to exist.
Once S_n has been determined, one can find V_n by integrating backward over $[0, S_n)$ the equation

$$V_n' = \frac{1}{\Delta t}(R(x)V_n + W_n(x) - C_{n-1}(x)), \tag{6.77}$$

with $V_n(S_n)$ given by (6.76). The concentration $C_n(x)$ at time level t_n is obtained from (6.71). Finally, $C_n(x)$ is extended over $[S_n, \infty)$ as C^1 linear function. For the initial concentration we shall use

$$C_0(x) = -h(1 - c^*)x + c^*.$$

Lemma 6.1 *There exists a solution S_n of (6.73) on (S_{n-1}, ∞) and $S_n - S_{n-1} < f(1)\Delta t$. The function C_n satisfies $0 < C_n < 1$ on $[0, S_n]$ and $C_n' < 0$ on $[S_n, \infty)$.*

Proof. We note that $C_0(S_0) = c^* \in (0, 1)$ and $C_0' = -h(1 - c^*) < 0$. Let us proceed by induction and assume the result valid for $n - 1$. Integrating (6.72) we have

$$W_n(x) = \frac{1}{\sinh\left(\frac{x+K}{\sqrt{\Delta t}}\right)} \left[g(t_n) \sinh\left(\frac{K}{\sqrt{\Delta t}}\right) + \frac{1}{\sqrt{\Delta t}} \int_0^x \cosh\left(\frac{r + K}{\sqrt{\Delta t}}\right) C_{n-1}(r)\, dr \right],$$

since $C_{n-1} < 1$ by assumption, we get

$$\begin{aligned} W_n(x) &\leq \frac{1}{\sinh\left(\frac{x+K}{\sqrt{\Delta t}}\right)} \left[g(t_n) \sinh\left(\frac{K}{\sqrt{\Delta t}}\right) + \frac{1}{\sqrt{\Delta t}} \int_0^x \cosh\left(\frac{r + K}{\sqrt{\Delta t}}\right) dr \right], \\ &= \frac{1}{\sinh\left(\frac{x+K}{\sqrt{\Delta t}}\right)} \left[g(t_n) \sinh\left(\frac{K}{\sqrt{\Delta t}}\right) + \left(\sinh\left(\frac{x + K}{\sqrt{\Delta t}}\right) - \sinh\left(\frac{K}{\sqrt{\Delta t}}\right) \right) \right] \\ &\leq 1 \end{aligned}$$

moreover $W_n(S_{n-1}) > 0$. Hence the function

$$\frac{W_n(x) - qR(x)(x - S_{n-1})/\Delta t}{1 + R(x)(x - S_{n-1})/\Delta t}$$

is less than one and positive on some interval (S_{n-1}, x_0), vanishing on x_0 . Then,

$$\sigma_n(x_0) = \frac{x_0 - S_{n-1}}{\Delta t} - f(0) > 0,$$

what is more

$$\sigma_n(S_{n-1}) = -f(W_n(S_{n-1})) < 0,$$

thus there must be a point $S_n \in (S_{n-1}, x_0)$ where $\sigma_n(S_n) = 0$, $0 < C_n(S_n) < 1$ and $C_n'(S_n) < 0$. Integrating (6.70) we obtain:

$$\begin{aligned} 0 < C_n(x) &= \cosh\left(\frac{x+K}{\sqrt{\Delta t}}\right)\left[\frac{C_n(S_n)}{\cosh\left(\frac{S_n+K}{\sqrt{\Delta t}}\right)} - \frac{1}{\sqrt{\Delta t}}\int_{S_n}^{x} \frac{\sinh\left(\frac{r+K}{\sqrt{\Delta t}}\right)}{\cosh^2\left(\frac{r+K}{\sqrt{\Delta t}}\right)} W_n(r)\,dr\right] \\ &\leq \cosh\left(\frac{x+K}{\sqrt{\Delta t}}\right)\left[\frac{C_n(S_n)}{\cosh\left(\frac{S_n+K}{\sqrt{\Delta t}}\right)} - \frac{1}{\sqrt{\Delta t}}\int_{S_n}^{x} \frac{\sinh\left(\frac{r+K}{\sqrt{\Delta t}}\right)}{\cosh^2\left(\frac{r+K}{\sqrt{\Delta t}}\right)}\,dr\right] \\ &= C_n(S_n)\frac{\cosh\left(\frac{x+K}{\sqrt{\Delta t}}\right)}{\cosh\left(\frac{S_n+K}{\sqrt{\Delta t}}\right)} + 1 - \frac{\cosh\left(\frac{x+K}{\sqrt{\Delta t}}\right)}{\cosh\left(\frac{S_n+K}{\sqrt{\Delta t}}\right)} < 1 \qquad \forall x \in [0, S_n]. \end{aligned}$$

Finally, from (6.74) and (6.75) we conclude that $S_n - S_{n-1} = f(C_n(S_n))\Delta t < f(1)\Delta t$. ∎

7 Conclusions.

In this paper the main result is the asymptotic behavior of the free boundary. We remark that the upper bound (5.63) should be very useful for real applications, where the function f is a priori unknown and a estimate of s_∞ is needed, this is a remarkable fact because we can control $s(t)$ for large t whatever be the physical process that the movement of the free boundary obeys.

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