Int. J. Appl. Math. Comput. Sci., 2001, Vol.11, No.4, 921–955

APPROXIMATION OF A SOLIDIFICATION PROBLEM

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A two-dimensional Stefan problem is usually introduced as a model of solidification, melting or sublimation phenomena. The two-phase Stefan problem has been studied as a direct problem, where the free boundary separating the two regions is eliminated using a variational inequality (Baiocchi, 1977; Baiocchi *et al.*, 1973; Rodrigues, 1980; Saguez, 1980; Srunk and Friedman, 1994), the enthalpy function (Ciavaldini, 1972; Lions, 1969; Nochetto *et al.*, 1991; Saguez, 1980), or a control problem (El Bagdouri, 1987; Peneau, 1995; Saguez, 1980). In the present work, we provide a new formulation leading to a shape optimization problem. For a semidiscretization in time, we consider an Euler scheme. Under some restrictions related to stability conditions, we prove an L^2-rate of convergence of order 1 for the temperature. In the last part, we study the existence of an optimal shape, compute the shape gradient, and suggest a numerical algorithm to approximate the free boundary. The numerical results obtained show that this method is more efficient compared with the others.

Keywords: Stefan problem, free boundary, shape optimization, Euler method, finite-element method

1. Problem Statement

We consider the open bounded domain $\Omega \subset \mathbb{R}^2$ defined by

$$\Omega = \left\{ x = (x_1, x_2) \in \mathbb{R}^2 \mid 0 < x_1 < 1,\ 0 < x_2 < 1 \right\} \tag{1}$$

The boundary of Ω is written as $\partial\Omega$. Time is denoted by $t \in]0, T[\,,\ 0 < T < \infty$. The field of temperature is $\theta : \Omega \times]0, T[\longrightarrow \mathbb{R}^2$, so $\theta(x, t)$ is the temperature at point $x \in \Omega$ at time $t \in]0, T[$. Let us denote by θ_c the fusion/solidification temperature. At time $t \in]0, T[$, the open bounded domain $\Omega \subset \mathbb{R}$ is partitioned as follows:

$$\Omega = \Omega_L(t) \cup \Omega_S(t) \cup S(t), \tag{2}$$

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where

$$\Omega_L(t) = \{x \in \Omega \mid \theta(x,t) > \theta_c\}, \tag{3}$$

$$\Omega_S(t) = \{x \in \Omega \mid \theta(x,t) < \theta_c\}, \tag{4}$$

$$S(t) = \{x \in \Omega \mid \theta(x,t) = \theta_c\}. \tag{5}$$

The interface $S(t)$ separating the solid and liquid phases is a free boundary and is an unknown of the problem. The domain Ω is shown in Fig. 1.

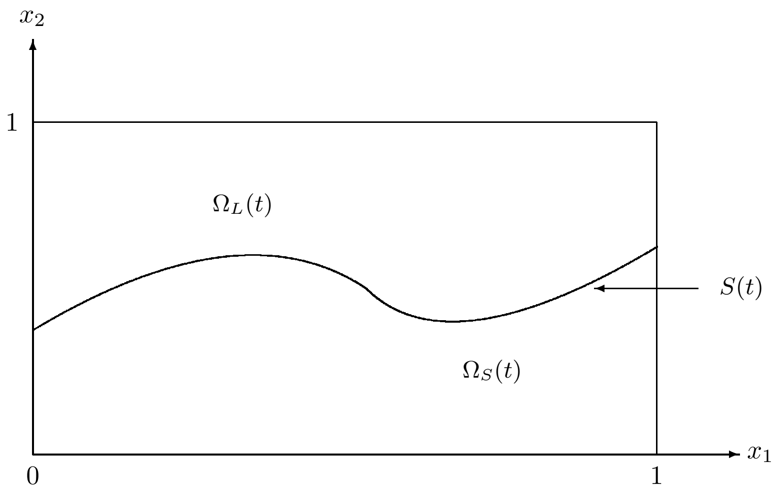


Fig. 1. The geometry of the domain.

We introduce the following notation:

$$Q = \Omega \times]0,T[, \tag{6}$$

$$Q_L = \bigcup_{t\in]0,T[} \big(\Omega_L(t) \times \{t\}\big), \tag{7}$$

$$Q_S = \bigcup_{t\in]0,T[} \big(\Omega_S(t) \times \{t\}\big), \tag{8}$$

$$\Sigma = \bigcup_{t\in]0,T[} \big(S(t) \times \{t\}\big). \tag{9}$$

Let functions $\theta_0 \in H^1(\Omega)$ and $\theta_{\partial\Omega} \in L^2(\partial\Omega)$ be given such that the following compatibility condition is satisfied:

$$\theta_0(x) = \theta_{\partial\Omega}(x), \quad \text{a.e. } x \in \partial\Omega.$$

Thus the unknowns (θ, Q_L) are the solutions of the following evolution free-boundary problem:

$$(P_1)\quad \begin{cases} \text{Find } \theta \text{ and } Q_L \text{ such that} \\ \dfrac{\partial \theta}{\partial t} - \operatorname{div}\left(C(\theta)\nabla\theta\right) = 0 & \text{in } Q_L \cup Q_S, \\ C(\theta) = \begin{cases} c_s & \text{if} \quad \theta < \theta_c, \\ c_l & \text{if} \quad \theta > \theta_c, \end{cases} \\ \theta(x,0) = \theta_0(x), & x \in \Omega, \\ \theta(x,t) = \theta_{\partial\Omega}(x), & x \in \partial\Omega, \quad t \in]0,T[, \\ \theta(x,t) < \theta_c, & (x,t) \in Q_S, \\ \theta(x,t) > \theta_c, & (x,t) \in Q_L, \\ \theta(x,t) = \theta_c, & (x,t) \in \Sigma, \\ \left[C(\theta)\nabla\theta \cdot \vec{n}\right]_{S(t)} = \lambda V \cdot \vec{n}, & x \in S(t), \quad t \in]0,T[. \end{cases}$$

Here λ is the latent heat of the material (a strictly positive coefficient), V signifies the velocity of the free boundary, c_s means the diffusivity of the solid part, c_l stands for the diffusivity of the liquid part (c_s and c_l are strictly positive coefficients), and n is the unitary normal to $S(t)$ pointing towards $\Omega_L(t)$.

The major difficulty in a direct problem lies in the fact that the moving boundary is utilized explicitly in the equation for the thermal state of the system. This difficulty is circumvented in Section 2, using the characteristic function of the liquid region. Such a formulation transforms the initial problem into a partial differential equation valid on the whole cavity occupied by the material. In Section 3 we recall the regularization method proposed in (Humeau and Souza del Cursi, 1993). In Section 4 we discretize the regularization problem and study the convergence of the proposed scheme. Section 5 estabilishes an approximation of the free boundary for the obtained stationary problem using a shape optimization method. The existence of the free boundary, details of the shape gradient computation, and numerical results are provided.

2. Problem Reformulation

Let us introduce the following spaces:

$$H = L^2(\Omega), \quad V = H^1(\Omega), \quad V_0 = H_0^1(\Omega), \tag{10}$$

with their usual scalar products

$$\mathcal{H} = L^2(0,T;H), \quad \mathcal{B} = L^2(0,T;V), \quad \mathcal{B}_0 = L^2(0,T;V_0), \tag{11}$$

respectively. Let $(\cdot,\cdot)$ denote the scalar product on H corresponding to the norm $\|\cdot\|$.

Consider the real-valued function

$$\chi_{Q_L}(x,t) = \begin{cases} 1 & \text{if } (x,t) \in Q_L, \\ 0 & \text{otherwise.} \end{cases} \tag{12}$$

The problem equivalent to (P_1) can be written as follows:

$$(P_2)\quad \begin{cases} \text{Find } \theta \in \mathcal{B} \text{ and } Q_L \subset Q \text{ such that} \\ \dfrac{\partial \theta}{\partial t} - \nabla \cdot (C(\theta)\nabla\theta) = -\lambda \dfrac{\partial}{\partial t}\chi_{Q_L} & \text{in } Q, \\ \theta(x,t) = \theta_{\partial\Omega}(x), & x \in \partial\Omega,\ t \in]0,T[, \\ \theta(x,0) = \theta_0(x), & x \in \Omega, \\ \theta(x,t) > \theta_c, & (x,t) \in Q_L, \\ \theta(x,t) < \theta_c, & (x,t) \in Q_S, \\ \theta(x,t) = \theta_c, & (x,t) \in \Sigma. \end{cases}$$

3. Problem Regularization

In order to overcome some numerical difficulties due to the discontinuity of the function $C(\theta)$, we consider the regularization method proposed in (Humeau and Souza del Cursi, 1993). Introduce $\phi : \mathbb{R} \longrightarrow \mathbb{R}$ given by

$$\phi(\beta) = 3\beta - 2\beta^2. \tag{13}$$

Let $\varepsilon > 0$ be a fixed parameter. We set

$$C_\varepsilon(\beta) = \begin{cases} C(\beta) & \text{if } \beta \notin (\theta_c - \varepsilon, \theta_c + \varepsilon), \\ c_s \phi\left(\dfrac{\varepsilon - \beta + \theta_C}{2\varepsilon}\right) + c_l \phi\left(\dfrac{\beta + \varepsilon - \theta_C}{2\varepsilon}\right) & \text{otherwise.} \end{cases}$$

Hence C_ε can be considered as a Lipschitz continuous approximation of C.

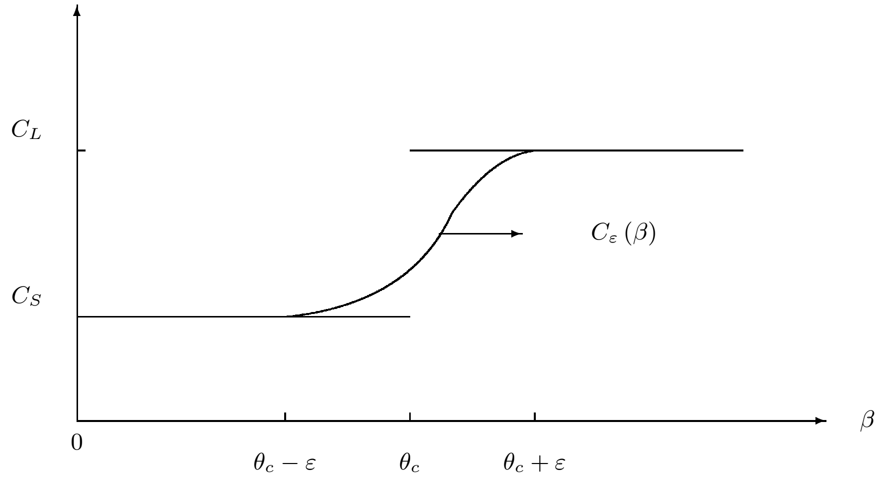


Fig. 2. Regularization of C.

The regularized problem associated with (P_2) can be formulated as follows:

$$(P_3)\quad \begin{cases} \text{Find } \theta_\varepsilon \in \mathcal{B} \text{ and } Q_L \subset Q \text{ such that} \\ \dfrac{\partial \theta_\varepsilon}{\partial t} - \nabla \cdot (C_\varepsilon(\theta_\varepsilon) \nabla \theta) = -\lambda \dfrac{\partial}{\partial t} \chi_{Q_L} & \text{in } Q, \\ \theta_\varepsilon(x,t) = \theta_{\partial\Omega}(x), & x \in \partial\Omega, t \in]0,T[, \\ \theta_\varepsilon(x,0) = \theta_0(x), & x \in \Omega, \\ \theta_\varepsilon(x,t) > \theta_c, & (x,t) \in Q_L, \\ \theta_\varepsilon(x,t) < \theta_c, & (x,t) \in Q_S, \\ \theta_\varepsilon(x,t) = \theta_c, & (x,t) \in \Sigma. \end{cases}$$

For notational convenience, in what follows the index ε will be omitted, so θ_ε and C_ε will be denoted respectively by θ and C. Consider a function $g \in H^1(\Omega)$ such that

$$g(x) = \begin{cases} \theta_0(x) & \text{if } x \in \Omega, \\ \theta_{\partial\Omega}(x) & \text{if } x \in \partial\Omega. \end{cases} \tag{14}$$

Introduce the change of variables

$$u(x,t) = \theta(x,t) - g(x) \quad \text{in } Q. \tag{15}$$

Then Problem (P_3) can be written as follows:

$$(P_4)\quad \begin{cases} \text{Find } u \in \mathcal{B}_0 \text{ and } Q_L \subset Q \text{ such that} \\ \dfrac{\partial u}{\partial t} - \nabla \cdot \left(C\,(u+g)\,\nabla\,(u+g)\right) = -\lambda \dfrac{\partial}{\partial t}\chi_{Q_L} & \text{in } Q, \\ u\,(x,0) = 0, & x \in \Omega, \\ u+g > \theta_c, & (x,t) \in Q_L, \\ u+g < \theta_c, & (x,t) \in Q_S, \\ u+g = \theta_c, & (x,t) \in \Sigma. \end{cases}$$

Consider now the problem

$$(P_5)\quad \begin{cases} \text{Find } u \in \mathcal{B}_0 \text{ such that} \\ \dfrac{\partial u}{\partial t} - \nabla \cdot \big(C\,(u+g)\,\nabla\,(u+g)\big) = -\lambda \dfrac{\partial}{\partial t}\chi_{Q_L} & \text{in } Q, \\ u\,(x,0) = 0, & x \in \Omega. \end{cases}$$

Let $\mathcal{V}$ be a closed subspace of $\mathcal{B}_0$ defined by

$$\mathcal{V} = \left\{ v \in \mathcal{B}_0 \;\middle|\; \frac{\partial v}{\partial t} \in \mathcal{H} \text{ and } v\,(x,0) = v\,(x,T) = 0,\ x \in \Omega \right\} \tag{16}$$

and equipped with the scalar product

$$(u,v)_{\mathcal{V}} = (u,v)_{\mathcal{B}_0} + \left(\frac{\partial u}{\partial t}, \frac{\partial v}{\partial t}\right)_{\mathcal{H}}. \tag{17}$$

The variational formulation associated with (P_5) is as follows:

$$(PV_5)\quad \begin{cases} \text{Find } u \in \mathcal{B}_0 \text{ such that} \\ \left(\dfrac{\partial}{\partial t}u, v\right) + \big(C\,(u+g)\,\nabla\,(u+g), \nabla v\big) = -\lambda \left(\dfrac{\partial}{\partial t}\chi_{Q_L}, v\right), \quad \forall v \in \mathcal{V}, \\ u\,(x,0) = 0,\ x \in \Omega. \end{cases}$$

The existence and uniqueness of the solution to (P_5) are established in (Haggouch, 1997; Humeau and Souza del Cursi, 1993), using the elliptic regularization method, cf. (Lions, 1969).

In the next section, we shall discretize Problem (P_5) in time and then study the convergence of the proposed scheme.

4. Time Discretization

Consider a strictly positive integer $N > 0$ which implies the discretization step $\tau = T/N$, and denote by t_n the grid points of $[0,T] : t_n = n\tau,\quad 0 \le n \le N$. We define

$$\Omega_L^n = \left\{ x \in \Omega \mid \theta\,(x,t_n) > \theta_c \right\}$$

and

$$\chi_{\Omega_L^n}(x) = \chi_{\Omega_L}(x, t_n) = \begin{cases} 1 & \text{if } \theta(x, t_n) > \theta_c, \\ 0 & \text{otherwise.} \end{cases}$$

Let

$$u_n(x) \simeq u(x, t_n), \quad u_{0n}(x) = u_0(x, t_n) = \theta_0(x, t_n) - g(x). \tag{18}$$

Then the discretization of Problem (P_5) can be written down as follows:

$$(P_n) \begin{cases} \text{Find } (u_{n+1})_{0 \le n \le N-1} \subset V_0^N \text{ such that} \\ \dfrac{u_{n+1} - u_n}{\tau} + \nabla \cdot \big(C(u_n + g)\nabla(u_{n+1} + g)\big) = -\lambda \dfrac{\chi_{\Omega_L^{n+1}} - \chi_{\Omega_L^n}}{\tau} \text{ in } \Omega. \end{cases}$$

Note that we have a linear problem that changes with each value of n. That means that solution to (P_n) requires N steps.

The variational problem associated with (P_n) is as follows:

$$(PV_n) \begin{cases} \text{Find } (u_{n+1})_{0 \le n \le N-1} \subset V_0^N \text{ such that} \\ \left(\dfrac{u_{n+1} - u_n}{\tau}, v\right) + \big(C(u_n + g)\nabla(u_{n+1} + g), \nabla v\big) \\ \qquad = -\lambda \left(\dfrac{\chi_{\Omega_L^{n+1}} - \chi_{\Omega_L^n}}{\tau}, v\right), \quad \forall v \in V_0. \end{cases}$$

Proposition 1. *The function u_n being a solution to (PV_n) satisfies the following discrete* a-priori *estimates:*

$$\max_{0 \le n \le N} \|u_n\| \le C_1,$$

$$\sum_{n=0}^{N-1} \|u_{n+1} - u_n\|^2 \le C_2,$$

$$\tau \sum_{n=1}^{N} \|\nabla u_n\|^2 \le C_3,$$

where C_1, C_2 and C_3 are constants independent of τ.

Proof. Setting $k_1 = \min(c_s, c_l)$ and $k_2 = \max(c_s, c_l)$, we have

$$k_1 \le C(\sigma) \le k_2. \tag{19}$$

Choosing $v = u_{n+1}$ in (PV_n) and applying the following elementary equality:

$$2p(p - q) = p^2 - q^2 + (p - q)^2, \quad \forall (p, q) \in \mathbb{R}^2, \tag{20}$$

we see that

$$\|u_{n+1}\|^2 - \|u_n\|^2 + \|u_{n+1} - u_n\|^2 + 2\tau k_1 \|\nabla u_{n+1}\|^2 + 2\tau k_1 \big(\nabla(g), \nabla u_{n+1}\big) + 2\lambda \left(\chi_{\Omega_L^{n+1}} - \chi_{\Omega_L^n}, u_{n+1}\right) \le 0. \tag{21}$$

Moreover, applying the Young inequality to the last terms of (21) yields

$$\begin{aligned} 2\tau k_1\big(\nabla(g), \nabla u_{n+1}\big) &\leq 2\tau k_1 \|\nabla g\| \ \|\nabla u_{n+1}\| \\ &\leq \frac{k_1^2 \|\nabla g\|^2}{\varepsilon} + \varepsilon\tau^2 \|\nabla u_{n+1}\|^2, \quad \forall\, \varepsilon > 0 \end{aligned} \tag{22}$$

and

$$\begin{aligned} 2\lambda\left(\chi_{\Omega_L^{n+1}} - \chi_{\Omega_L^n}, u_{n+1}\right) &\leq 2\lambda \left\|\chi_{\Omega_L^{n+1}} - \chi_{\Omega_L^n}\right\| \ \|u_{n+1}\| \\ &\leq 4\lambda\sqrt{\operatorname{mes}\Omega}\ \|u_{n+1}\| \\ &\leq \frac{4\lambda^2 \operatorname{mes}\Omega}{\beta} + \beta\|u_{n+1}\|^2, \quad \forall\, \beta > 0. \end{aligned} \tag{23}$$

Therefore, choosing arbitrary β and ε such that $(1-\beta) > 0$ and $(2k_1 - \varepsilon\tau) > 0$, we get

$$\begin{aligned} (1-\beta)\|u_{n+1}\|^2 - \|u_n\|^2 + \|u_{n+1} - u_n\|^2 + \tau\,(2k_1 - \varepsilon\tau)\|\nabla u_{n+1}\|^2 \\ \leq \frac{k_1^2 \|\nabla g\|^2}{\varepsilon} + \frac{4\lambda^2 \operatorname{mes}\Omega}{\beta} \leq c. \end{aligned}$$

Summing this inequality over $n,\ 0 \leq n \leq p-1,\ 1 \leq p \leq N$, and using the fact that $u_0 = 0$, we get

$$(1-\beta)\|u_p\|^2 + \sum_{n=0}^{p-1} \|u_{n+1} - u_n\|^2 + (2k_1 - \varepsilon\tau)\sum_{n=1}^{p} \tau\|\nabla u_n\|^2 \leq \beta \sum_{n=1}^{p-1} \|u_n\|^2 + pc.$$

By the discrete Gronwall inequality (Raviart and Girault, 1981), we obtain

$$(1-\beta)\|u_p\|^2 + \sum_{n=0}^{p-1} \|u_{n+1} - u_n\|^2 + (2k_1 - \varepsilon\tau)\sum_{n=1}^{p} \tau\|\nabla u_n\|^2 \leq pce^{\beta\, p}.$$

Hence there exist constants C_1, C_2 and C_3 independent of τ such that

$$\max_{0\leq n\leq N} \|u_n\| \leq C_1, \quad \sum_{n=0}^{N-1} \|u_{n+1} - u_n\|^2 \leq C_2, \quad \sum_{n=1}^{N} \tau\|\nabla u_n\|^2 \leq C_3,$$

which completes the proof. ■

Using these estimations and non-linear analysis, we can show the following theorems (Humeau and Souza del Cursi, 1993):

Theorem 1. *Problem* (P_n) *has a unique solution* u_n *in* V_0.

Consider

$$t_{i+\frac{1}{2}} = t_i + \frac{\tau}{2}, \quad t_{i-\frac{1}{2}} = t_i - \frac{\tau}{2}, \quad I_i = \left[t_{i-\frac{1}{2}}, t_{i+\frac{1}{2}}\right] \cap]0, T[,$$

$$\mathcal{I}_i = \begin{cases} 1 & \text{if } t \in I_i, \\ 0 & \text{otherwise} \end{cases}$$

and

$$u^N(x,t) = \sum_{n=0}^{N} u_n(x)\, \mathcal{I}_n(t).$$

Theorem 2. *The sequence* $\left\{u^N\right\}_{N>0}$ *converges weakly in* $\mathcal{B}_0$ *to a solution* u *to Problem* (P_5) *as* $N \to \infty$.

5. Error Analysis

In this paragraph, we use a regularization of χ_{Ω_L} to obtain a continuous function χ_{Ω_L} such that $\partial \chi_{\Omega_L}/\partial t$ and $\partial^2 \chi_{\Omega_L}/\partial t^2$ are regular. We consider, for example, the following regularization: For $\varepsilon > 0$, define

$$\chi^{\varepsilon}_{\Omega_L}\big(u(x,t)\big) = \begin{cases} \chi_{\Omega_L}\big(u(x,t)\big) & \text{if } u(x,t) \notin (0,\varepsilon), \\ \psi\left(\dfrac{u(x,t)}{\varepsilon}\right) & \text{otherwise,} \end{cases} \tag{24}$$

where ψ is a function of $C^1(Q)$. For notational simplicity, in place of $\chi^{\varepsilon}_{\Omega_L}$ we will write χ_{Ω_L}.

In the following, we suppose that

$$\frac{\partial u}{\partial t} \in L^2(0,T;V_0), \quad \frac{\partial^2 u}{\partial t^2} \in L^2\left(0,T;V'\right), \quad \frac{\partial^2 \chi_{\Omega_L}}{\partial t^2} \in L^2\left(0,T;V'\right). \tag{25}$$

Then we can deduce that

$$\begin{aligned} & u \in C^0(0,T;V_0), && \frac{\partial u}{\partial t} \in C^0(0,T;H), \\ & \chi_{\Omega_L} \in C^0(0,T;V_0), && \frac{\partial \chi_{\Omega_L}}{\partial t} \in C^0(0,T;H). \end{aligned} \tag{26}$$

First of all, we show that the consistency error is of order one and that the proposed scheme is stable.

5.1. Estimate of the Consistency Error

Let $\chi_{\Omega_L}(t)$ and $u(t)$ be two functions defined on Ω by

$$\chi_{\Omega_L}(t) : x \longrightarrow \chi_{\Omega_L}\big(u(x,t)\big)$$

and

$$u(t) : x \longrightarrow u(x,t)\,.$$

We define the consistency error $\varepsilon_n \in V^{'}$ by

$$\begin{aligned}\langle \varepsilon_n, v\rangle \;=\; & \frac{1}{\tau}\big(u(t_{n+1}) - u(t_n), v\big) + \big(C\big(u(t_n)+g\big)\nabla\big(u(t_{n+1})+g\big), \nabla v\big)\\ & + \frac{\lambda}{\tau}\big(\chi_{\Omega_L}(t_{n+1}) - \chi_{\Omega_L}(t_n), v\big),\end{aligned} \tag{27}$$

where $V^{'}$ is the dual space of V, and $\langle\cdot,\cdot\rangle$ denotes the duality product between V and $V^{'}$.

Lemma 1. (Lions, 1969) *When* $n = 2$, *all the elements* φ *of* V_0 *satisfy*

$$\|\varphi\|_{L^4(\Omega)} \le 2^{\frac{1}{4}}\,\|\varphi\|^{\frac{1}{2}}\,\|\nabla\varphi\|^{\frac{1}{2}}\,.$$

Suppose that a constant $M > 0$ exists such that for all $t \in [0,T]$ we have

(H) $$\big\|\nabla\big(u(t)+g\big)\big\|_{L^4(\Omega)} < M.$$

Consider

$$\begin{aligned}&\frac{\partial}{\partial t}\big(u(t_{n+1}), v\big) + \big(C\big(u(t_{n+1})+g\big)\nabla\big(u(t_{n+1})+g\big), \nabla v\big)\\ &\qquad + \lambda\frac{\partial}{\partial t}\big(\chi_{\Omega_L}(t_{n+1}), v\big) = 0.\end{aligned} \tag{28}$$

Calculating the difference of (27) and (28), we get

$$\begin{aligned}\langle \varepsilon_n, v\rangle \;=\; & \left(\frac{u(t_{n+1}) - u(t_n)}{\tau} - \frac{\partial u}{\partial t}(t_{n+1}), v\right)\\ & + \lambda\left(\frac{\chi_{\Omega_L}(t_{n+1}) - \chi_{\Omega_L}(t_n)}{\tau} - \frac{\partial}{\partial t}\chi_{\Omega_L}(t_{n+1}), v\right)\\ & - \big(C\big(u(t_{n+1})+g\big) - C\big(u(t_n)+g\big)\nabla\big(u(t_{n+1})+g\big), \nabla v\big)\,.\end{aligned}$$

By Taylor's formula with integral remainder, defined by

$$\begin{aligned}\frac{1}{\tau}\big(f(t_{n+1}) - f(t_n), v\big) \;=\; & \left(\frac{\partial}{\partial t} f(t_{n+1}), v\right)\\ & + \frac{1}{\tau}\int_{t_n}^{t_{n+1}} (t - t_{n+1}) \left\langle \frac{\partial^2}{\partial t^2} f(t), v\right\rangle \mathrm{dt}\end{aligned} \tag{29}$$

for $f = u$ and $f = \chi_{\Omega_L}$, we obtain

$$\begin{aligned}\langle \varepsilon_n, v\rangle \;=\; & \frac{1}{\tau}\int_{t_n}^{t_{n+1}} (t - t_{n+1}) \left\langle \frac{\partial^2 u}{\partial t^2}(t), v\right\rangle \mathrm{d}t \\ & + \frac{\lambda}{\tau}\int_{t_n}^{t_{n+1}} (t - t_{n+1}) \left\langle \frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t), v\right\rangle \mathrm{d}t \\ & - \big(\big(C\big(u(t_{n+1}) + g\big) - C\big(u(t_n) + g\big)\big)\nabla\big(u(t_{n+1}) + g\big), \nabla v\big). \qquad (30)\end{aligned}$$

But

$$\begin{aligned}& \big|\big(\big(C\big(u(t_{n+1}) \;+\; g\big) - C\big(u(t_n) + g\big)\big)\nabla\big(u(t_{n+1}) + g\big), \nabla v\big)\big| \\ & \quad \le \big\|\big(C\big(u(t_{n+1}) + g\big) - C\big(u(t_n) + g\big)\big)\nabla\big(u(t_{n+1}) + g\big)\big\| \; \|\nabla v\| \\ & \quad \le \max_{\sigma\in\mathbb{R}}\big|C'(\sigma)\big| \, \big\|\big(u(t_{n+1}) - u(t_n)\big)\nabla\big(u(t_{n+1}) + g\big)\big\| \; \|\nabla v\| \\ & \quad \le \max_{\sigma\in\mathbb{R}}\big|C'(\sigma)\big| \, \big\|\big(u(t_{n+1}) - u(t_n)\big)\big\|_{L^4(\Omega)} \big\|\nabla\big(u(t_{n+1}) + g\big)\big\|_{L^4(\Omega)} \; \|\nabla v\| \,.\end{aligned}$$

From Lemma 1 and the hypothesis (H), we deduce that

$$\begin{aligned}& \big|\big(\big(C\big(u(t_{n+1}) \;+\; g\big) - C\big(u(t_n) + g\big)\big)\nabla\big(u(t_{n+1}) + g\big), \nabla v\big)\big| \\ & \qquad\qquad \le\; c_1 \big\|\big(u(t_{n+1}) - u(t_n)\big)\big\|^{\frac{1}{2}} \; \big\|\nabla\big(u(t_{n+1}) - u(t_n)\big)\big\|^{\frac{1}{2}} \; \|\nabla v\| \,,\end{aligned}$$

where

$$c_1 = 2^{\frac{1}{4}} \, M \, \max_{\sigma\in\mathbb{R}}\big|C'(\sigma)\big| \tag{31}$$

Since the embedding $H^1(\Omega) \to L^2(\Omega)$ is compact and $u(t_n) \in H_0^1(\Omega)$, we obtain

$$\begin{aligned}& \big|\big(\big(C\big(u(t_{n+1}) + g\big) - C\big(u(t_n) \;+\; g\big)\big)\nabla\big(u(t_{n+1}) + g\big), \nabla v\big)\big| \\ & \qquad\qquad\qquad \le\; c_2 \, \big\|\nabla\big(u(t_{n+1}) - u(t_n)\big)\big\| \; \|\nabla v\| \,. \qquad (32)\end{aligned}$$

Let

$$u(t_{n+1}) - u(t_n) = \int_{t_n}^{t_{n+1}} \frac{\partial u(t)}{\partial t}\,\mathrm{d}t. \tag{33}$$

Then we have

$$\begin{aligned}
\left\|\int_{t_n}^{t_{n+1}} \frac{\partial u(t)}{\partial t}\,\mathrm{d}t\right\|_{V_0}^2 &= \int_\Omega \left[\nabla \int_{t_n}^{t_{n+1}} \frac{\partial u(t)}{\partial t}\,\mathrm{d}t\right]^2 \mathrm{d}x = \int_\Omega \left[\int_{t_n}^{t_{n+1}} \nabla \frac{\partial u(t)}{\partial t}\,\mathrm{d}t\right]^2 \mathrm{d}x \\
&\leq \int_\Omega \left[\tau \int_{t_n}^{t_{n+1}} \left|\nabla \frac{\partial u(t)}{\partial t}\right|^2 \mathrm{d}t\right] \mathrm{d}x \\
&\leq \tau \int_{t_n}^{t_{n+1}} \left[\int_\Omega \left|\nabla \frac{\partial u(t)}{\partial t}\right|^2 \mathrm{d}x\right] \mathrm{d}t \\
&\leq \tau \int_{t_n}^{t_{n+1}} \left\|\frac{\partial u(t)}{\partial t}\right\|_{V_0}^2 \mathrm{d}t. \qquad (34)
\end{aligned}$$

By the definition of the norm $\|\cdot\|_{V'}$:

$$\|\varepsilon_n\|_{V'} = \sup_{v\in V} \frac{\langle \varepsilon_n, v\rangle}{\|v\|_V}, \qquad (35)$$

from (30) we get

$$\begin{aligned}
\|\varepsilon_n\|_{V'} \leq\; &\frac{1}{\tau}\int_{t_n}^{t_{n+1}} (t-t_{n+1}) \left\|\frac{\partial^2 u}{\partial t^2}\right\|_{V'} \mathrm{d}t \\
&+ \frac{\lambda}{\tau}\int_{t_n}^{t_{n+1}} (t-t_{n+1}) \left\|\frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t)\right\|_{V'} \mathrm{d}t \\
&+ c_2\left(\tau \int_{t_n}^{t_{n+1}} \left\|\frac{\partial u(t)}{\partial t}\right\|_{V_0}^2 \mathrm{d}t\right)^{\frac{1}{2}}. \qquad (36)
\end{aligned}$$

But

$$\begin{aligned}
&\frac{1}{\tau}\int_{t_n}^{t_{n+1}} (t-t_{n+1}) \left\|\frac{\partial^2 u(t)}{\partial t^2}\right\|_{V'} \mathrm{d}t \\
&\qquad \leq \frac{1}{\tau}\left(\int_{t_n}^{t_{n+1}} (t-t_{n+1})^2\right)^{\frac{1}{2}} \left(\int_{t_n}^{t_{n+1}} \left\|\frac{\partial^2 u(t)}{\partial t^2}\right\|_{V'}^2 \mathrm{d}t\right)^{\frac{1}{2}} \\
&\qquad \leq \left(\tau \int_{t_n}^{t_{n+1}} \left\|\frac{\partial^2 u(t)}{\partial t^2}\right\|_{V'}^2 \mathrm{d}t\right)^{\frac{1}{2}} \qquad (37)
\end{aligned}$$

and

$$\frac{1}{\tau}\int_{t_n}^{t_{n+1}}(t-t_{n+1})\left\|\frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t)\right\|_{V'}\mathrm{d}t$$
$$\leq \frac{1}{\tau}\left(\int_{t_n}^{t_{n+1}}(t-t_{n+1})^2\right)^{\frac{1}{2}}\left(\int_{t_n}^{t_{n+1}}\left\|\frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t)\right\|_{V'}^2\mathrm{d}t\right)^{\frac{1}{2}}$$
$$\leq \left(\tau\int_{t_n}^{t_{n+1}}\left\|\frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t)\right\|_{V'}^2\mathrm{d}t\right)^{\frac{1}{2}}. \tag{38}$$

Substituting (37) and (38) into (36), we get

$$\|\varepsilon_n\|_{V'} \leq \left(\tau\int_{t_n}^{t_{n+1}}\left\|\frac{\partial^2 u(t)}{\partial t^2}\right\|_{V'}^2\mathrm{d}t\right)^{\frac{1}{2}} + \lambda\left(\tau\int_{t_n}^{t_{n+1}}\left\|\frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t)\right\|_{V'}^2\mathrm{d}t\right)^{\frac{1}{2}}$$
$$+ c_2\left(\tau\int_{t_n}^{t_{n+1}}\left\|\frac{\partial u(t)}{\partial t}\right\|_{V_0}^2\mathrm{d}t\right)^{\frac{1}{2}}. \tag{39}$$

Then

$$\|\varepsilon_n\|_{V'}^2 \leq c\tau\left[\int_{t_n}^{t_{n+1}}\left\{\left\|\frac{\partial^2 u(t)}{\partial t^2}\right\|_{V'}^2 + \left\|\frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t)\right\|_{V'}^2 + \left\|\frac{\partial u(t)}{\partial t}\right\|_{V_0}^2\right\}\mathrm{d}t\right]. \tag{40}$$

Summing this inequality over $n,\ 0\leq n\leq p-1,\ 1\leq p\leq N$, we obtain

$$\tau\sum_{n=0}^{p-1}\|\varepsilon_n\|_{V'}^2 \leq c\tau^2\left[\left\|\frac{\partial^2 u(t)}{\partial t^2}\right\|_{L^2(0,T;V')}^2 + \left\|\frac{\partial^2}{\partial t^2}\chi_{\Omega_L}(t)\right\|_{L^2(0,T;V')}^2\right.$$
$$\left.+\left\|\frac{\partial u(t)}{\partial t}\right\|_{L^2(0,T;V_0)}^2\mathrm{d}t\right]. \tag{41}$$

Using (25), we get the following result:

Proposition 2. *Suppose that u satisfies the regularity conditions (25) and that there exists a constant $M>0$ such that for all $t\in[0,T]$ we have $\|\nabla(u(t)+g)\|_{L^4(\Omega)} < M$. Then the consistency error is of order 1, i.e.*

$$\left(\tau\sum_{n=0}^{p-1}\|\varepsilon_n\|_{V'}^2\right)^{\frac{1}{2}} \leq c\tau, \qquad 1\leq p\leq N, \tag{42}$$

where $c>0$ is a constant independent of τ.

5.2. Stability of the Scheme

For all $n \in \{0, \ldots, N-1\}$, we have

$$\frac{1}{\tau}\left(u_{n+1}-u_n, v\right)+\big(C\left(u_n+g\right) \nabla\left(u_{n+1}+g\right), \nabla v\big)$$
$$+\ \frac{\lambda}{\tau}\Big(\chi_{\Omega_L^{n+1}}-\chi_{\Omega_L^n}, v\Big)=0. \tag{43}$$

Set

$$e^n=u\left(t_n\right)-u_n. \tag{44}$$

Proposition 3. *If* $u_0=u\left(t_0\right)$*, the following stability criterion holds for* $1 \leq p \leq N$*:*

$$\left\|e^p\right\|^2+\sum_{n=0}^{p-1}\left\|e^{n+1}-e^n\right\|^2+\tau k_1 \sum_{n=1}^p\left\|\nabla e^n\right\|^2 \leq\left(\frac{2 \tau}{k_1} \sum_{n=0}^{p-1}\left\|\varepsilon_n^*\right\|_{V'}^2\right) \exp (c T),$$

where $c>0$ *is a constant independent of* τ *and* $k_1=\min(c_s, c_l)$*.*

Proof. Subtracting (27) from (43) yields

$$\begin{aligned}\big(e^{n+1}-e^n, v\big)\ &+\ \tau k_1\left(\nabla e^{n+1}, \nabla v\right)\\ &+\ \tau\Big(\big(C\big(u\left(t_n\right)+g\big)-C\left(u_n+g\right)\big) \nabla\big(u\left(t_{n+1}\right)+g\big), \nabla v\Big)\\ &\leq\ \tau\left\langle\varepsilon_n, v\right\rangle, \quad \forall v \in V_0, \quad 0 \leq n \leq N-1.\end{aligned} \tag{45}$$

Taking $v=e_{n+1}$ in (45) and applying the inequality

$$\big|C(\alpha)-C(\beta)\big| \leq \max_{\sigma \in \mathbb{R}}\big|C^{'}(\sigma)\big|\ |\alpha-\beta|, \tag{46}$$

we see that

$$\begin{aligned}&\left\|e^{n+1}\right\|^2-\left\|e^n\right\|^2+\left\|e^{n+1}-e^n\right\|^2+2 \tau k_1\left\|\nabla e^{n+1}\right\|^2\\ &\qquad \leq 2 \tau\left\langle\varepsilon_n, e^{n+1}\right\rangle+2 \tau \max_{\sigma \in \mathbb{R}}\big|C^{'}(\sigma)\big|\left(e^n \nabla\big(u\left(t_{n+1}\right)+g\big), \nabla e^{n+1}\right).\end{aligned} \tag{47}$$

The right-hand side is estimated as follows:

$$\begin{aligned}2\left|\left\langle\varepsilon_n, e^{n+1}\right\rangle\right|\ &\leq\ 2\left\|\varepsilon_n\right\|_{V'}\ \left\|e^{n+1}\right\|_V\\ &\leq\ \frac{2}{k_1}\left\|\varepsilon_n\right\|_{V'}^2+\frac{k_1}{2}\left\|\nabla e^{n+1}\right\|^2.\end{aligned} \tag{48}$$

Using Lemma 1 and the assumption (H), we get

$$\begin{aligned}
2\left(e^n\nabla\big(u\left(t_{n+1}\right)+g\big),\nabla e^{n+1}\right) &\leq 2\left\|e^n\right\|_{L^4(\Omega)}\left\|\nabla\big(u\left(t_{n+1}\right)+g\big)\right\|_{L^4(\Omega)}\left\|\nabla e^{n+1}\right\| \\
&\leq 2\,M\,2^{\frac{1}{4}}\left\|e^n\right\|^{\frac{1}{2}}\left\|\nabla e^n\right\|^{\frac{1}{2}}\left\|\nabla e^{n+1}\right\| \\
&\leq c_1\left[\frac{1}{\varepsilon}\big(\left\|e^n\right\|\left\|\nabla e^n\right\|\big)+\varepsilon\left\|\nabla e^{n+1}\right\|^2\right] \\
&\leq c_1\left[\frac{1}{\varepsilon}\left(\frac{1}{2\delta}\left\|e^n\right\|^2+\frac{\delta}{2}\left\|\nabla e^n\right\|^2\right)+\varepsilon\left\|\nabla e^{n+1}\right\|^2\right], \quad (49)
\end{aligned}$$

where $\varepsilon > 0$ and $\delta > 0$ are arbitrary. Hence we have the estimate

$$\begin{aligned}
&2\tau\max_{\sigma\in\mathbb{R}}\left|C^{'}\left(\sigma\right)\right|\left(e^n\nabla\left(u\left(t_{n+1}\right)+g\right),\nabla e^{n+1}\right) \\
&\qquad\leq\frac{k_1}{4}\tau\left(\left\|\nabla e^n\right\|^2+\left\|\nabla e^{n+1}\right\|^2\right)+\tau c_2\left\|e^n\right\|^2. \qquad (50)
\end{aligned}$$

Substituting (48) and (50) into (47), we get

$$\begin{aligned}
&\left\|e^{n+1}\right\|^2-(1+\tau c_2)\left\|e^n\right\|^2+\left\|e^{n+1}-e^n\right\|^2+\frac{5k_1}{4}\tau\left\|\nabla e^{n+1}\right\|^2 \\
&\qquad\leq\frac{k_1}{4}\tau\left\|\nabla e^n\right\|^2+\frac{2\tau}{k_1}\left\|\varepsilon_n\right\|_{V'}^2. \qquad (51)
\end{aligned}$$

If we sum this last relation over $n,\ 0\leq n\leq p-1,\ 1\leq p\leq N$, and use the fact that $e_0=0$, then we obtain

$$\begin{aligned}
&\left\|e^p\right\|^2+\sum_{n=0}^{p-1}\left\|e^{n+1}-e^n\right\|^2+\tau k_1\sum_{n=1}^{p}\left\|\nabla e^n\right\|^2 \\
&\qquad\leq\tau c_2\sum_{n=1}^{p-1}\left\|e^n\right\|^2+\frac{2\tau}{k_1}\sum_{n=0}^{p-1}\left\|\varepsilon_n\right\|_{V'}^2.
\end{aligned}$$

The discrete Gronwall inequality gives

$$\begin{aligned}
\left\|e^p\right\|^2+\sum_{n=0}^{p-1}\left\|e^{n+1}-e^n\right\|^2+\tau k_1\sum_{n=1}^{p}\left\|\nabla e^n\right\|^2 &\leq\left(\frac{2\tau}{k_1}\sum_{n=0}^{p-1}\left\|\varepsilon_n\right\|_{V'}^2\right)\exp(c_2p\tau) \\
&\leq\left(\frac{2\tau}{k_1}\sum_{n=0}^{p-1}\left\|\varepsilon_n\right\|_{V'}^2\right)\exp(c_2T). \quad (52)
\end{aligned}$$

■

Combining Propositions 2 and 3, we derive immediately the following result:

Theorem 3. *Under the assumptions of Proposition 2, there exists a constant* $c > 0$ *independent of* τ *such that*

$$\max_{0 \leq n \leq N} \|u(t_n) - u_n\| + \left(\tau \sum_{n=0}^{p-1} \|u(t_n) - u_n\|_V^2 \right)^{\frac{1}{2}} \leq c\tau. \tag{53}$$

6. Formulation in the Framework of Shape Optimization

Under some regularity of the free boundary, we shall expose a new formulation of the semi-discrete problem associated with (P_3), using the shape optimization techniques. The existence results for an optimal domain and the shape gradient are presented. For the computation of the gradient, we suggest the material derivative (Zolésio, 1981) and the duality methods (Lions, 1968).

The partial differential equation in Problem (P_3) is approximated as

$$\frac{\theta_{n+1} - \theta_n}{\tau} - \nabla \cdot \big(C(\theta_n) \nabla \theta_{n+1} \big) = -\lambda \frac{\chi_{\Omega_L^{n+1}} - \chi_{\Omega_L^n}}{\tau}, \quad \forall n \in \{0, \dots, N-1\}. \tag{54}$$

We introduce functions a_n and b_n defined as follows:

$$\begin{aligned} a_n(x) &= \tau C\big(\theta_n(x)\big), & x \in \Omega, \\ b_n(x) &= \lambda \chi_{\Omega_L^n} + \theta_n(x), & x \in \Omega. \end{aligned}$$

Thus we get the following semi-discretized problem associated with (P_3):

$$(P_6) \quad \left\{ \begin{array}{l} \text{Find } (\theta_{n+1})_{0 \leq n \leq N-1} \subset V^N \text{ and } \big(\Omega_L^{n+1}\big)_{0 \leq n \leq N-1} \subset (\mathcal{O}_{\text{ad}})^N \text{ such that} \\ \theta_{n+1} > \theta_c \text{ in } \Omega_L^{n+1}, \\ \theta_{n+1} < \theta_c \text{ in } \Omega_S^{n+1}, \\ \theta_{n+1} = \theta_c \text{ on } S^{n+1}, \\ \text{and } \theta_{n+1} \text{ is the solution of the problem} \\ P\big(\Omega_L^{n+1}\big) \left\{ \begin{array}{l} \text{Find } \theta_{n+1} \in V \text{ such that} \\ \theta_{n+1} - \nabla \cdot (a_n \nabla \theta_{n+1}) = -\lambda \chi_{\Omega_L^{n+1}} + b_n \quad \text{in } \Omega, \\ \qquad \theta_{n+1} = \theta_{\partial\Omega} \quad \text{on } \partial\Omega, \end{array} \right. \end{array} \right.$$

where $\mathcal{O}_{\text{ad}}$ is the set of admissible domains that will be defined later.

For notational convenience, we eliminate the indices n, and the sequences θ_n, Ω_S^n, Ω_L^n, S^n, a_n and b_n are denoted by θ, Ω_S, Ω_L, S, a and b, respectively.

Introduce the cost functional

$$\begin{aligned}\mathcal{J}(\Omega_L) &\equiv \mathcal{J}\big(\Omega_L, \theta(\Omega_L)\big)\\ &= \frac{1}{2}\int_\Omega \chi_{\Omega_S}\Big[\big(\theta(\Omega_L)-\theta_c\big)^+\Big]^2 \mathrm{d}x + \frac{1}{2}\int_\Omega \chi_{\Omega_L}\Big[\big(\theta_c-\theta(\Omega_L)\big)^+\Big]^2 \mathrm{d}x. \qquad (55)\end{aligned}$$

The optimal shape design problem is formulated as follows:

$$(\mathcal{P}_{\mathrm{op}}) \quad \begin{cases} \min\limits_{\Omega_L\in\mathcal{O}_{\mathrm{ad}}} \mathcal{J}(\Omega_L) \quad \text{such that} \\ \theta(\Omega_L) \ \text{ is the solution of } P(\Omega_L). \end{cases}$$

By setting

$$\mathcal{F} = \Big\{\big(\Omega_L, \theta(\Omega_L)\big) \mid \Omega_L \in \mathcal{O}_{\mathrm{ad}} \text{ and } \theta(\Omega_L) \text{ is the solution to } P(\Omega_L)\Big\}, \quad (56)$$

the optimization problem can be written as

$$(\mathcal{P}_{\mathrm{op}}) \quad \big\{\text{minimize } \mathcal{J}(\Omega_L) \mid (\Omega_L, \theta(\Omega_L)) \in \mathcal{F}\big\}. \quad (57)$$

The new formulation we propose makes use of the regularity of the free boundary. The existence of the latter was proved in (Baiocchi *et al.*, 1973; Lions, 1969; Saguez, 1980). As in (Lions, 1969), we assume that the free boundary is of measure zero on Ω and, moreover, we suppose that it is defined by a curve described by the equation $x_2 = \alpha(x_1)$, where α is a regular function. Then there exists a solution in $\mathcal{F}$ such that $\mathcal{J}(\Omega_L) = 0$. We deduce easily the equivalence of Problems (P_6) and $(\mathcal{P}_{\mathrm{op}})$. In the next section, we shall study Problem $(\mathcal{P}_{\mathrm{op}})$.

6.1. Existence Result

The existence of an optimal solution to $(\mathcal{P}_{\mathrm{op}})$ requires the choice of an adequate topology on the admissible domain, permitting to obtain the compactness of $\mathcal{O}_{\mathrm{ad}}$ and the lower semicontinuity of $\mathcal{J}$.

The set of admissible functions which parameterize the free boundary S is defined as follows:

$$\begin{aligned}\mathcal{U}_{\mathrm{ad}} = \Big\{\alpha \in C\big([0,1]\big) \ \Big| \ &\big|\alpha(x_1) - \alpha(\overline{x_1})\big| \le k\,|x_1 - \overline{x_1}| \quad \forall\, x_1, \overline{x_1} \in [0,1],\\ &\alpha(0) = c_1,\ \alpha(1) = c_2 \text{ and } \alpha(x_1) < c_3,\ \ x_1 \in [0,1]\Big\}.\end{aligned}$$

The constants $k\ c_1$, c_2 and c_3 are chosen in such a way that $\mathcal{U}_{\mathrm{ad}}$ is not empty. $\mathcal{U}_{\mathrm{ad}}$ is equipped with the following norm:

$$\|\alpha\|_\infty = \max_{0\le x_1\le 1} \big|\alpha(x_1)\big|, \quad \alpha \in \mathcal{U}_{\mathrm{ad}}. \quad (58)$$

We define

$$\alpha_n \underset{n\to\infty}{\rightrightarrows} \alpha \ \text{ in } \ [0,1] \iff \|\alpha_n - \alpha\|_\infty \underset{n\to\infty}{\to} 0, \quad (59)$$

and the convergence in $\mathcal{U}_{\text{ad}}$ by

$$\text{‘}\alpha_n \underset{n\to\infty}{\to} \alpha\text{’ in } \mathcal{U}_{\text{ad}} \iff \alpha_n \underset{n\to\infty}{\rightrightarrows} \alpha \text{ in } [0,1]. \tag{60}$$

The different regions can be characterized by

$$\Omega_L(\alpha) = \big\{x \in \Omega \mid x_2 > \alpha(x_1)\big\}, \tag{61}$$

$$\Omega_S(\alpha) = \big\{x \in \Omega \mid x_2 < \alpha(x_1)\big\}, \tag{62}$$

$$S(\alpha) = \big\{x \in \Omega \mid x_2 = \alpha(x_1)\big\}, \tag{63}$$

and

$$\chi_{\Omega_L(\alpha)} = \begin{cases} 1 & \text{if } x_2 > \alpha(x_1), \\ 0 & \text{otherwise.} \end{cases}$$

We consider $\mathcal{O}_{\text{ad}}$ as the set of the admissible domains

$$\mathcal{O}_{\text{ad}} = \big\{\Omega(\alpha) \subset \Omega \mid \alpha \in \mathcal{U}_{\text{ad}}\big\}, \tag{64}$$

where

$$\Omega(\alpha) = \Omega_L(\alpha) \cup \Omega_S(\alpha) \cup S(\alpha).$$

We require $\mathcal{O}_{\text{ad}}$ to be equipped with the appropriate topology and convergence defined by

$$\text{‘}\Omega_n \underset{n\to\infty}{\to} \Omega\text{’} \iff \text{‘}\alpha_n \underset{n\to\infty}{\to} \alpha\text{’ in } \mathcal{U}_{\text{ad}}, \tag{65}$$

where $\Omega_n = \Omega(\alpha_n)$ and $\Omega = \Omega(\alpha)$.

Let $\alpha \in \mathcal{U}_{\text{ad}}$. For any $\Omega_L(\alpha)$ we consider the following boundary-value problem:

$$P(\alpha) \quad \begin{cases} \text{Find } \theta(\alpha) \in V \text{ such that} \\ \theta(\alpha) - \nabla\cdot\big(a\nabla\theta(\alpha)\big) = -\lambda\,\chi_{\Omega_L(\alpha)} + b & \text{in } \Omega, \\ \theta(\alpha) = \theta_{\partial\Omega} & \text{on } \partial\Omega. \end{cases}$$

The cost functional is given by

$$\begin{aligned} \mathcal{J}(\alpha) &\equiv \mathcal{J}\big(\alpha,\theta(\alpha)\big) \\ &= \frac{1}{2}\int_\Omega \chi_{\Omega_S(\alpha)} \Big[\big(\theta(\alpha) - \theta_c\big)^+\Big]^2 \mathrm{d}x + \frac{1}{2}\int_\Omega \chi_{\Omega_L(\alpha)} \Big[\big(\theta_c - \theta(\alpha)\big)^+\Big]^2 \mathrm{d}x. \end{aligned} \tag{66}$$

We set

$$\mathcal{F} = \Big\{\big(\alpha,\theta(\alpha)\big) \;\Big|\; \alpha \in \mathcal{U}_{\text{ad}} \text{ and } \theta(\alpha) \text{ is the solution to } P(\alpha)\Big\}, \tag{67}$$

endowed with the topology defined by the following convergence:

$$`\big(\Omega_L(\alpha_n), \theta(\alpha_n)\big) \underset{n\to\infty}{\to} \big(\Omega_L(\alpha), \theta(\alpha)\big)' \iff \begin{cases} \Omega_L(\alpha_n) \underset{n\to\infty}{\to} \Omega_L(\alpha) & \text{in } \mathcal{O}_{\mathrm{ad}}, \\ \theta(\alpha_n) \underset{n\to\infty}{\rightharpoonup} \theta(\alpha) \ \text{(weakly)} & \text{in } \mathcal{B}. \end{cases} \tag{68}$$

Thus the optimization problem is written as

$$\mathcal{P}_{\mathrm{op}}(\alpha) \ \ \big\{\text{minimize } \mathcal{J}(\alpha) \ \big| \ \big(\alpha, \theta(\alpha)\big) \in \mathcal{F}\ \big\}.$$

Using the approach presented in (Haslinger and Neittaanmäki, 1988), we have the following results, and the details of the proofs are given in (Haggouch, 1997).

Proposition 4. *Let* $\theta_n = \theta(\alpha_n)$ *be the solutions of* $P(\alpha_n)$, $\alpha_n \in \mathcal{U}_{\mathrm{ad}}$ *and* $\Omega_L^n = \Omega_L(\alpha_n)$. *Then there exist a subsequence of* $\{(\alpha_n, \theta_n)\}$ *(again denoted by* $\{(\alpha_n, \theta_n)\}$*) and elements* $\alpha \in \mathcal{U}_{\mathrm{ad}}$, $\theta \in V$ *such that*

$$`\Omega_L^n \underset{n\to\infty}{\to} \Omega_L(\alpha)' \ \text{ in } \mathcal{O}_{\mathrm{ad}} \ \text{ and } \theta_n \underset{n\to\infty}{\rightharpoonup} \theta \ \text{ (weakly) in } \mathcal{B}$$

Moreover, θ *solves* $P(\alpha)$.

Proposition 5. *The function* $\alpha \to \mathcal{J}(\alpha)$ *is continuous on* $\mathcal{U}_{\mathrm{ad}}$.

Using these propositions, we establish our next theorem.

Theorem 4. *There exists at least one solution to Problem* $\mathcal{P}_{\mathrm{op}}(\alpha)$, $\alpha \in \mathcal{U}_{\mathrm{ad}}$.

Proof. We define q by

$$q = \inf_{\alpha \in \mathcal{U}_{\mathrm{ad}}} \mathcal{J}(\alpha). \tag{69}$$

Let $\Omega_L^n = \Omega_L(\alpha_n)$, $\alpha_n \in \mathcal{U}_{\mathrm{ad}}$ be a minimizing sequence, i.e.

$$\lim_{n\to\infty} \mathcal{J}(\alpha_n) = q, \tag{70}$$

and $\theta(\alpha_n)$ be the solution to Problem $P(\alpha_n)$.

Proposition 2 implies that there exist a subsequence $\big\{\big(\alpha_{n_j}, \theta\big(\alpha_{n_j}\big)\big)\big\} \subset \{(\alpha_n, \theta(\alpha_n))\}$ and an element $\{(\alpha^*, \theta(\alpha^*))\} \in \mathcal{F}$ such that

$$\alpha_{n_j} \underset{j\to\infty}{\rightrightarrows} \alpha^* \ \text{ in } [0,1] \tag{71}$$

and

$$\theta\big(\alpha_{n_j}\big) \underset{j\to\infty}{\rightharpoonup} \theta(\alpha^*) \ \text{ (weakly) in } V. \tag{72}$$

By Proposition 3, we have

$$\lim_{j\to\infty} \mathcal{J}\left(\alpha_{n_j}\right) = \mathcal{J}\left(\alpha^*\right). \tag{73}$$

The uniqueness of the limit implies

$$\inf_{\alpha\in\mathcal{U}_{\rm ad}} \mathcal{J}\left(\alpha\right) = \mathcal{J}\left(\alpha^*\right). \tag{74}$$

■

6.2. Numerical Approximation of the Free Boundary

6.2.1. Existence of the Gradient

Consider a vector field $\mathcal{W}$, defined on $[0,\beta]\times U$ with values in $\mathbb{R}^2$, U being an open neighborhood of Ω and $\beta>0$. Let $\mathcal{W}\in C\left([0,\beta], \mathcal{D}^k\left(U,\mathbb{R}^2\right)\right)$, $k\geq 1$. We transform Ω into Ω_τ through the function $\mathcal{T}_\tau$ defined by

$$\mathcal{T}_\tau\left(X\right) = x\left(\tau, X\right), \tag{75}$$

where $x\left(\tau,X\right)$ is the unique solution to the differential equation

$$\mathcal{P}\quad\left\{\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\tau}x\left(\tau,X\right) &= \mathcal{W}\big(\tau, x\left(\tau,X\right)\big),\\ x\left(\tau,0\right) &= X.\end{aligned}\right.$$

We suppose that this transformation makes the domain Ω invariant and preserves the functional spaces, i.e.

$$\phi\in H^1(\Omega)\Longleftrightarrow \phi\circ T_\tau^{-1}\in H^1(\Omega). \tag{76}$$

Note that $\mathcal{T}_\tau$ transforms the open domains Ω_L and Ω_S onto the open domains Ω_L^τ and Ω_S^τ, and maps the associated boundaries $\partial\Omega_L$ and $\partial\Omega_S$ onto the boundaries $\partial\Omega_L^\tau$ and $\partial\Omega_S^\tau$, respectively.

Let $\tau\in[0,\beta]$ and θ_τ be the solution to the problem

$$P\left(\Omega_L^\tau\right)\quad\left\{\begin{aligned} &\text{Find }\ \theta_\tau\in V \text{ such that}\\ &\theta_\tau - \nabla\cdot\left(a\nabla\theta_\tau\right) = -\lambda\ \chi_{\Omega_L^\tau} + b \quad \text{in }\ \Omega,\\ &\qquad\qquad\qquad \theta_\tau = \theta_{\partial\Omega} \qquad\qquad \text{on }\ \partial\Omega.\end{aligned}\right.$$

The variational formulation associated with $P\left(\Omega_L^\tau\right)$ is given by

$$PV\left(\Omega_L^\tau\right)\quad\left\{\begin{aligned} &\text{Find }\ \theta_\tau\in V \text{ such that }\quad \forall\phi\in V_0,\\ &\int_\Omega \theta_\tau\,\phi\,\mathrm{d}x_\tau + \int_\Omega a\nabla\theta_\tau\cdot\nabla\phi\,\mathrm{d}x_\tau = -\lambda\int_\Omega \chi_{\Omega_L^\tau}\phi\,\mathrm{d}x_\tau + \int_\Omega b\,\phi\,\mathrm{d}x_\tau,\\ &\qquad\qquad\qquad\qquad \theta_\tau = \theta_{\partial\Omega}\quad \text{in }\ \partial\Omega.\end{aligned}\right.$$

Applying the change of variable $x_\tau = \mathcal{T}_\tau(X)(x)$ to the first equation of $PV(\Omega_L^\tau)$, we obtain

$$\int_\Omega \theta^\tau \phi \gamma(\tau) \, \mathrm{d}x + \int_\Omega A(\tau) a \nabla \theta^\tau \cdot \nabla \phi \, \mathrm{d}x$$
$$= -\lambda \int_{\Omega_L} \phi \big|_{\Omega_L^\tau} \circ \mathcal{T}_\tau \gamma(\tau) \, \mathrm{d}x + \int_\Omega b \phi \gamma(\tau) \, \mathrm{d}x, \qquad (77)$$

where $\theta^\tau = \theta_\tau \circ \mathcal{T}_\tau$, $\gamma(\tau) = \det(D\mathcal{T}_\tau)$ and $A(\tau) = \gamma(\tau) D\mathcal{T}_\tau^{-1}.^T \left(D\mathcal{T}_\tau^{-1}\right)$.

We define the material derivative of $\theta(\Omega_L)$ as the solution to $P(\Omega_L)$ in the direction of the vector field $\mathcal{W}$, i.e.

$$\dot{\theta}(\Omega, \mathcal{W}) = \lim_{\tau \to 0} \frac{1}{\tau} \big(\theta(\Omega_\tau) \circ \mathcal{T}_\tau - \theta(\Omega) \big), \qquad (78)$$

provided that this limit exists. Thus, deriving (77) with respect to τ at $\tau = 0$, we get the variational problem associated with the material derivative of θ as a solution to $P(\Omega_L)$:

$$(\dot{P}) \quad \begin{cases} \text{Find } \dot{\theta} \in V_0 \quad \text{such that} \quad \forall \phi \in V_0, \\ \displaystyle\int_\Omega \dot{\theta} \, \phi \, \mathrm{d}x + \int_\Omega a \nabla \dot{\theta} \cdot \nabla \phi \, \mathrm{d}x + \int_\Omega \theta \phi \, \mathrm{div}(\mathcal{W}) \, \mathrm{d}x + \int_\Omega A'(0) a \nabla \theta \cdot \nabla \phi \, \mathrm{d}x \\ \qquad = -\lambda \int_{\Omega_L} \mathrm{div}(\phi \mathcal{W}) \, \mathrm{d}x, \end{cases}$$

where $A'(0) = \mathrm{div}\, \mathcal{W}(0) I - \big(D\mathcal{W}(0) +^T D\mathcal{W}(0) \big)$.

Consider the shape derivative $\theta' = \dot{\theta} - \nabla \theta \cdot \mathcal{W}$ of the solution to $P(\Omega_L)$. We show that θ' exists in H and is determined as the solution to the following variational problem:

$$(P') \quad \begin{cases} \text{Find } \theta' \in H \text{ such that } \theta' = 0 \text{ on } \partial\Omega \text{ and} \\ \displaystyle\int_\Omega \theta' \phi \, \mathrm{d}x + \int_\Omega a \nabla \theta' \cdot \nabla \phi \, \mathrm{d}x = -\lambda \int_{\Omega_L} \mathrm{div}(\phi \mathcal{W}) \, \mathrm{d}x, \quad \forall \phi \in \mathcal{D}(\Omega). \end{cases}$$

($\theta' = 0$ on $\partial\Omega$ because $\mathcal{W} = 0$ on $\partial\Omega$). The Eulerian derivative of the functional $\mathcal{J}(\Omega_L)$ at Ω_L in the direction of a vector field $\mathcal{W}$ is defined as the limit

$$\mathrm{d}\mathcal{J}(\Omega_L, \mathcal{W}) = \lim_{\tau \to 0} \frac{1}{\tau} \big(\mathcal{J}(\Omega_\tau) - \mathcal{J}(\Omega) \big) \qquad (79)$$

provided that this limit exists.

Based on the foregoing results, one can deduce that the following theorem takes place:

Theorem 5. *For any vector field* $\mathcal{W} \in C\left([0,\beta], \mathcal{D}^k\left(U, \mathbb{R}^2\right)\right)$*, the Eulerian derivative of the functional* $\mathcal{J}(\Omega_L)$ *at* Ω_L *in the direction of a vector field* $\mathcal{W}$ *exists and is given by*

$$\begin{aligned} \mathrm{d}\mathcal{J}(\Omega_L, \mathcal{W}) \;=\; & \int_{\Omega_S} \left[(\theta-\theta_c)^+ \right] \theta' \, \mathrm{d}x + \int_{\Omega_S} \operatorname{div}\left(\frac{1}{2} \left[(\theta-\theta_c)^+ \right]^2 \mathcal{W}(0) \right) \mathrm{d}x \\ & - \int_{\Omega_L} \left[(\theta_c-\theta)^+ \right] \theta' \, \mathrm{d}x + \int_{\Omega_L} \operatorname{div}\left(\frac{1}{2} \left[(\theta_c-\theta)^+ \right]^2 \mathcal{W}(0) \right) \mathrm{d}x, \end{aligned}$$

where θ *and* θ' *are the solutions to* $P(\Omega_L)$ *and* (P')*, respectively.*

6.2.2. Calculation of the Gradient

Consider the Lagrangian functional defined by

$$\begin{aligned} \mathcal{L}(\Omega_L, \theta, \phi) \;=\; & \mathcal{J}(\Omega_L) + (\theta, \phi)_H + (a\nabla\theta, \nabla\phi)_H \\ & + \lambda \left(\chi_{\Omega_L(\alpha)}, \phi \right)_H - (b, \phi)_H, \quad \forall \phi \in V_0. \end{aligned} \tag{80}$$

To determine the adjoint state p, one can solve the following equation:

$$\lim_{\omega \to 0} \frac{\partial}{\partial \omega} \mathcal{L}(\Omega_L, \theta + \omega\phi, p) = 0, \quad \forall \phi \in V_0. \tag{81}$$

Then we obtain the adjoint problem

$$(P_a) \quad \begin{cases} \text{Find } p \in V_0 \text{ such that } \forall \phi \in V_0 \\ \displaystyle\int_\Omega p\phi \, \mathrm{d}x + \int_\Omega a\nabla p \cdot \nabla\phi \, \mathrm{d}x \\ \qquad\qquad = -\displaystyle\int_{\Omega_S} (\theta-\theta_c)^+ \phi \, \mathrm{d}x + \int_{\Omega_L} (\theta_c-\theta)^+ \phi \, \mathrm{d}x. \end{cases}$$

Taking $\phi = \theta'$ in (P_a) and $\phi = p$ in (P'), we get the final expression for the Eulerian derivative of the functional $\mathcal{J}(\Omega_L)$ at Ω_L in the direction of a vector field $\mathcal{W}$:

$$\begin{aligned} \mathrm{d}\mathcal{J}(\Omega_L, \mathcal{W}) \;=\; & \int_{\Omega_S} \operatorname{div}\left(\frac{1}{2} \left[(\theta-\theta_c)^+ \right]^2 \mathcal{W} \right) \mathrm{d}x \\ & + \int_{\Omega_L} \operatorname{div}\left[\left(\frac{1}{2} \left[(\theta_c-\theta)^+ \right]^2 + \lambda p \right) \mathcal{W} \right] \mathrm{d}x. \end{aligned}$$

The Hadamard formula (Zolésio, 1979) implies the existence of a scalar distribution G on S such that

$$\mathrm{d}\mathcal{J}(\Omega_L, \mathcal{W}) = \int_S G\, \mathcal{W} \cdot n \, \mathrm{d}\sigma. \tag{82}$$

Note that our aim is to minimize the functional $\mathcal{J}(\Omega_L)$ using some descent method. Accomplish this in practice, we must solve the following variational problem:

$$(P_u)\quad \begin{cases} \text{Find } \ u \in V_0 \ \text{ such that} \\ \displaystyle\int_\Omega \nabla u \cdot \nabla \phi \,\mathrm{d}x = \int_S G\, v \cdot n \,\mathrm{d}\sigma, \quad \forall v \in V_0. \end{cases}$$

Problem (P_u) permits us to compute a descent direction in order to approximate S.

We can avoid solving this accessory problem by using the duality method (Lions, 1968) to compute the gradient and deform the domain. We recall that

$$\Omega_L = \Omega_L(\alpha) = \big\{x \in \Omega \mid x_2 > \alpha(x_1)\big\}. \tag{83}$$

Set

$$\mathcal{J}(\alpha) = \frac{1}{2}\int_0^1 \int_0^{\alpha(x_1)} \Big[\big(\theta(\alpha) - \theta_c\big)^+\Big]^2 \mathrm{d}x + \frac{1}{2}\int_0^1 \int_{\alpha(x_1)}^1 \Big[\big(\theta_c - \theta(\alpha)\big)^+\Big]^2 \mathrm{d}x, \tag{84}$$

where $\theta(\alpha)$ is the solution to the variational problem

$$PV(\Omega_L)\quad \begin{cases} \text{Find } \ \theta \in V \ \text{ such that } \ \forall \phi \in V_0, \\ \displaystyle\int_\Omega \theta\phi \,\mathrm{d}x + \int_\Omega a\nabla\theta \cdot \nabla\phi \,\mathrm{d}x \ = \ -\lambda \int_0^1 \int_{\alpha(x_1)}^1 \phi \,\mathrm{d}x + \int_\Omega b\phi \,\mathrm{d}x, \\ \hfill \theta \ = \ \theta_{\partial\Omega} \ \text{ in } \ \partial\Omega. \end{cases}$$

We consider the Lagrangian $\mathcal{L}$ defined for all $\phi \in V_0$ by

$$\mathcal{L}(\theta, \alpha, \phi) = \mathcal{J}(\alpha) + \int_\Omega \theta\phi \,\mathrm{d}x + \int_\Omega a\nabla\theta \cdot \nabla\phi \,\mathrm{d}x + \lambda \int_0^1 \int_{\alpha(x_1)}^1 \phi \,\mathrm{d}x - \int_\Omega b\phi \,\mathrm{d}x, \tag{85}$$

$\theta(\alpha)$ being the solution to $(PV)_6$. We solve the equation

$$\left(\frac{\partial \mathcal{L}}{\partial \theta}\big(\theta(\alpha), \alpha, p\big), \delta\theta\right) = 0, \quad \forall\, \delta\theta \in V_0 \tag{86}$$

to determine the adjoint state $p(\alpha)$. Then we get

$$\int_\Omega p(\alpha)\,\phi \,\mathrm{d}x \ + \ \int_\Omega a\nabla p(\alpha) \cdot \nabla\phi \,\mathrm{d}x$$
$$= \int_0^1 \int_{\alpha(x_1)}^1 \big(\theta_c - \theta(\alpha)\big)^+ \phi \,\mathrm{d}x - \int_0^1 \int_0^{\alpha(x_1)} \big(\theta(\alpha) - \theta_c\big)^+ \phi \,\mathrm{d}x, \tag{87}$$

and the adjoint problem is given by

$$(P_a)\quad \begin{cases} \text{Find } \ p \in V_0 \ \text{ such that } \ \forall \phi \in V_0, \\ \displaystyle\int_\Omega p\phi \,\mathrm{d}x + \int_\Omega a\nabla p \cdot \nabla\phi \,\mathrm{d}x \\ \displaystyle\qquad = -\int_0^1 \int_0^{\alpha(x_1)} (\theta - \theta_c)^+ \,\phi \,\mathrm{d}x + \int_0^1 \int_{\alpha(x_1)}^1 (\theta_c - \theta)^+ \,\phi \,\mathrm{d}x. \end{cases}$$

Set

$$J'(\alpha) = \frac{\partial \mathcal{L}(\theta(\alpha), \alpha, p(\alpha))}{\partial \alpha}. \tag{88}$$

If $\theta(\alpha)$ is the solution to the state problem, then

$$\mathcal{J}(\alpha) = \mathcal{L}\big(\theta(\alpha), \alpha, p\big), \quad \forall p \in V_0.$$

In particular, for $p = p(\alpha)$ we get

$$\big(\nabla \mathcal{J}(\alpha), \delta\alpha\big) = \left(\frac{\partial\, \mathcal{L}}{\partial \alpha}\big(\theta(\alpha), \alpha, p(\alpha)\big), \delta\alpha\right). \tag{89}$$

Therefore

$$\begin{aligned}\left(\frac{\partial\, \mathcal{L}(\theta(\alpha), \alpha, p(\alpha))}{\partial \alpha}, \delta\alpha\right) \;=\; & \frac{1}{2}\int_0^1 \Big[\big(\theta\left(x_1, \alpha(x_1)\right) - \theta_c\big)^+\Big]^2 \,\delta\alpha(x_1)\,\mathrm{d}x_1 \\ & - \frac{1}{2}\int_0^1 \Big[\big(\theta_c - \theta\big(x_1, \alpha(x_1)\big)\big)^+\Big]^2 \,\delta\alpha(x_1)\,\mathrm{d}x_1 \\ & - \lambda \int_0^1 p\big(x_1, \alpha(x_1)\big)\,\delta\alpha(x_1)\,\mathrm{d}x_1.\end{aligned}$$

Then

$$\begin{aligned}\nabla \mathcal{J}(\alpha) \;=\; & \frac{1}{2}\Big[\big(\theta\big(x_1, \alpha(x_1)\big) - \theta_c\big)^+\Big]^2 - \frac{1}{2}\Big[\big(\theta_c - \theta\big(x_1, \alpha(x_1)\big)\big)^+\Big]^2 \\ & - \lambda p\big(x_1, \alpha(x_1)\big).\end{aligned} \tag{90}$$

6.2.3. Algorithm

Let ω be a real parameter such that $\omega > 0$, and let an initial free boundary α^0 be given. The optimization method considered consist in generating a sequence $(\alpha^k)_{k>0}$ with the following iterations:

$$\alpha^{k+1} = \alpha^k - \omega\, u^k, \tag{91}$$

where $u^k = u(\alpha^k) = \partial\mathcal{J}/\partial\alpha^k$. If we write $\theta^k = \theta\left(\alpha^k\right)$ and $p^k = p\left(\alpha^k\right)$, then

$$u^k = \frac{1}{2}\Big[\big(\theta^k - \theta_c\big)^+\Big]^2 - \frac{1}{2}\Big[\big(\theta_c - \theta^k\big)^+\Big]^2 - \lambda p^k, \tag{92}$$

where θ^k is the unique solution to the problem

$$P\left(\Omega_L^k\right) \quad \begin{cases} \text{Find } \theta^k \in V \text{ such that} \\ \theta^k - \nabla\cdot\big(a\nabla\theta^k\big) \;=\; -\lambda\,\chi_{\Omega_L(\alpha^k)} + b \quad \text{in } \Omega, \\ \qquad\qquad\qquad \theta^k \;=\; \theta_{\partial\Omega} \qquad\qquad\qquad \text{on } \partial\Omega, \end{cases}$$

and p^k is the adjoint state, associated with θ^k, the unique solution to the problem

$$\left(P_a^k\right) \begin{cases} \text{Find } p^k \in V \text{ such that} & \\ p^k - \nabla \cdot \left(a \nabla p^k\right) = \left(\chi_{\Omega_L(\alpha^k)} - 1\right)\left(\theta^k - \theta_c\right)^+ & \\ \qquad\qquad + \chi_{\Omega_L(\alpha^k)}\left(\theta_c - \theta^k\right)^+ & \text{in } \Omega, \\ \qquad\qquad p^k = 0 & \text{on } \partial\Omega. \end{cases}$$

Algorithm:

Step 0. Input θ^0, α^0, the maximal number of iterations $k_{\max}$, the coefficient ω, the precision for temperature ε and that for the free boundary EPS.

Step 1. Given α^k and $\chi_{\Omega_L(\alpha^k)}$, compute θ^k, the solution to the state Problem $P\left(\Omega_L^k\right)$.

Step 2. Compute p^k, the adjoint state associated with θ^k, the solution to Problem $\left(P_a^k\right)$.

Step 3. Compute the gradient u^k by using (92).

Step 4. Test:

$$\text{if } \left\|\theta^k - \theta^{k-1}\right\| < \varepsilon \text{ or } \left\|u^k\right\| < \text{ EPS or } k > k_{\max} \text{ then } \alpha_{\text{opt}} = \alpha^k,$$

$$\text{otherwise set } \alpha^{k+1} = \alpha^k - \omega u^k \text{ and return to Step 1.}$$

Solution of the partial differential equations under consideration is performed by a standard Finite Element Method (FEM): the region Ω is partitioned using a uniform grid involving steps $h_1 = 1/N_1$, $h_2 = 1/N_2$ and nodes $P_{i,j} = ((i-1)h_1, (j-1)h_2)$ for $1 \leq i \leq N_1$ and $1 \leq j \leq N_2$. A triangular mesh is generated by the diagonals connecting $P_{i+1,j}$ to $P_{i,j+1}$. The functions are approximated by piecewise constant ones on each triangle. For example, α and θ are approximated by piecewise constant functions having the values α_{ij} and θ_{ij} at $P_{i,j}$, respectively. Such a method is standard and will not be detailed here. We limit ourselves to the observation that the FEM reduces Problems $(P(\Omega_L))$ and (P_a) to a linear system. In the numerical experiments, solutions to all the linear systems were obtained using an iterative method of relaxation.

6.3. Numerical Experiments

In order to obtain situations where the exact solution is known, we consider an additional source term g on the right-hand side of the heat equation related to Problem (P_1). We consider the situation where $T = 2$, $\lambda = 1$, $c_s = 11$, $c_l = 10$, $\theta_c = 0$,

$$g(x_1, x_2, t) = \begin{cases} \exp(-t) - 4c_s & \text{if } x_1^2 + x_2^2 - \exp(-t) > 0, \\ \exp(-t) - 4c_l & \text{otherwise,} \end{cases} \tag{93}$$

and $\theta_0(x_1, x_2, t) = x_1^2 + x_2^2 - \exp(-t)$. In this case, the exact representation of the free boundary is given by

$$\alpha(x_1, x_2, t) = \sqrt{\exp(-t) - x_1^2} - x_2, \tag{94}$$

which is a solution to the equation $\theta_0(x_1, x_2, t) = 0$. We denote by $S(t)$ the exact free boundary at time t defined by

$$S(t) = \big\{x = (x_1, x_2) \in \Omega \mid \alpha(x_1, x_2, t) = 0\big\}. \tag{95}$$

For these methods, we consider the following choices:

- $k(n)$ denotes the last iteration number at time t_n. The total number of iterations for the whole solution on $[0, T]$, k_{tot} and the maximum number of iterations for a time step $k_{\max}$ are respectively given by

$$k_{\text{tot}} = \sum_{n=1}^{N} k(n), \quad k_{\max} = \max_{1 \le n \le N} k(n). \tag{96}$$

- The free boundary $S(t_n)$ at time t_n is numerically determined as follows: Let α^0 be an initial free boundary. Compute

$$\alpha^{k+1} = \alpha^k - \omega\, u(\alpha^k) \tag{97}$$

  iteratively for $k = 1, \ldots, k(n)$, until getting an approximation of the optimal solution with a given precision. Setting

$$\alpha^{\text{op}} = \alpha^{k(n)}, \tag{98}$$

  we fix $i \in \{1, \ldots, N_1\}$ and determine $j \in \{1, \ldots, N_2\}$ such that

$$\alpha_{ij}^{k(n)} < 0 < \alpha_{ij+1}^{k(n)}. \tag{99}$$

  The front pass at a point of $[P_{ij}, P_{ij+1}]$ that we approximate by the point $P_{ij+\frac{1}{2}}$ is

$$S_{ij} = P_{ij+\frac{1}{2}} = \big((i-1)h_{x_1}, (j-1/2)h_{x_2}\big). \tag{100}$$

  $S(t_n)$ is then obtained by linear interpolation from the points S_{ij} when $i = 1, \ldots, N_1$.

- Consider

$$ef_{ij}(n) = \big|\alpha_{ij}^{k(n)} - \alpha(P_{ij}, t_n)\big|. \tag{101}$$

The absolute error in the position of the free boundary is controlled by

$$ef(n) = \left(h_1 h_2 \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} ef_{ij}(n)^2\right)^{1/2}. \tag{102}$$

The global behaviour on $[0,T]$ is controlled by its mean on the global calculation, i.e.

$$ef_2 = \frac{1}{N} \sum_{n=1}^{N} ef(n). \tag{103}$$

- In the same way, write

$$et_{ij}(n) = \left|\theta_{ij}^{k(n)} - \theta(P_{ij}, t_n)\right|. \tag{104}$$

The absolute error in the field of temperatures is controlled by

$$et(n) = \left(h_1 h_2 \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} et_{ij}(n)^2\right)^{1/2}. \tag{105}$$

The global behaviour on $[0,T]$ is controlled by its mean on the global calculation:

$$et_2 = \frac{1}{N} \sum_{n=1}^{N} et(n). \tag{106}$$

- We shall also present the final values of the mean-square norm of the gradient

$$e_2 = \frac{1}{N} \sum_{n=1}^{N} e(n), \tag{107}$$

where

$$e(n) = \left(h_1 h_2 \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \left(u\left(\alpha_{ij}^{k(n)}\right)\right)^2\right)^{1/2}. \tag{108}$$

We analyze the influence of the mesh and the coefficient ω, before giving some results concerning the field of temperatures and the free-boundary errors.

Table 1. Results for the mesh $(20 \times 10P)$.

P	1	2	3	4	5	6	7
et_2	3.3×10^{-3}	3.5×10^{-3}	3.5×10^{-3}	3.5×10^{-3}	3.5×10^{-3}	3.5×10^{-3}	3.6×10^{-3}
ef_2	8.3×10^{-2}	7.9×10^{-2}	7.6×10^{-2}	7.4×10^{-2}	7.4×10^{-2}	7.4×10^{-2}	7.4×10^{-2}
e_2	8.0×10^{-1}	8.3×10^{-1}	8.4×10^{-1}	8.0×10^{-1}	8.0×10^{-1}	8.2×10^{-1}	8.1×10^{-1}
$k_{\max}$	20	20	20	20	20	20	20

Table 2. Variation of the coefficient ω for the mesh (20×50).

ω	0.1	1	5	10	20	30	40
et_2	1.8×10^{-2}	5.8×10^{-3}	2.1×10^{-3}	2.2×10^{-3}	3.5×10^{-3}	4.2×10^{-3}	4.6×10^{-3}
ef_2	3.4×10^{-1}	1.0×10^{-1}	4.1×10^{-2}	4.8×10^{-2}	7.4×10^{-2}	9.6×10^{-2}	1.0×10^{-1}
e_2	3.32	1.5×10^{-1}	1.0×10^{-2}	3.8×10^{-1}	8.0×10^{-1}	1.0	1.1
$k_{\max}$	20	20	20	20	20	20	20

In the simulations, we considered the time step $\tau = 0.1$, $T = 4$, $k_{\max} = 20$, prec $= 1.0$E-5. The regularization parameter was EPS $= 1.0$E-3. The relaxation method involved in the FEM used $\mu = 0.1$, precision $\text{prec}_R = 1.0$E-5 and the maximum number of iterations $M_{\max} = 1000$.

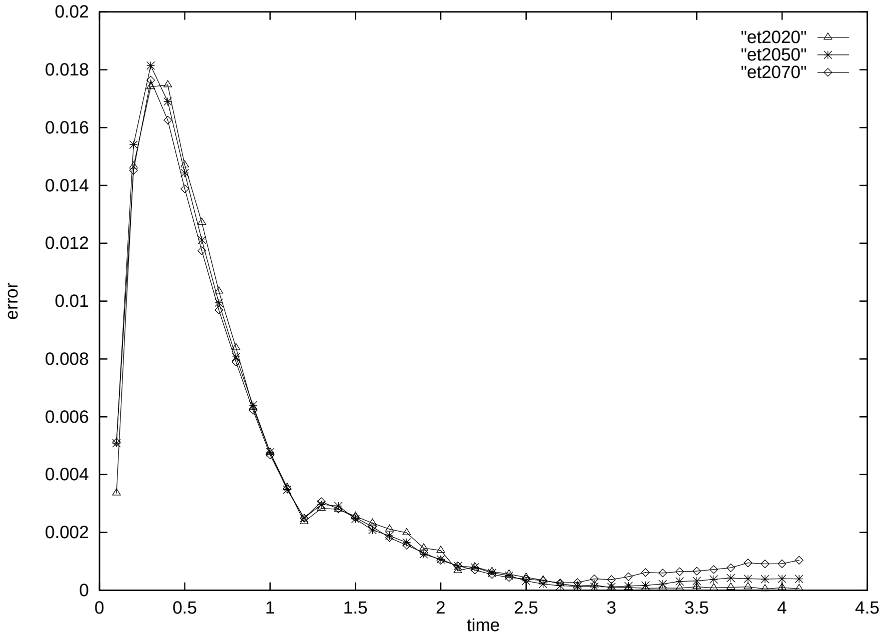


Fig. 3. Mean-square error of the temperatures while varying the mesh ($\omega = 20$).

From the numerical experiments, the following conclusions can be drawn:

- According to Table 1, the tests involving different meshes show that their influence is minor on both the error in the field temperature (Fig. 3) and that in the free boundary (Fig. 4).
- In Figs. 5 and 6, we consider the convergence of the errors in the field of the temperatures and the evaluation of the free boundary with respect to the coefficient ω for the mesh 20×50 (see Table 2). Note that $\omega = 5$ leads to better convergence for both the errors in the intervals $[0, 2.4]$ and $[0, 1.4]$, respectively, and $\omega = 20$ in the intervals $[2.4, 4]$ and $[1.4, 4]$.

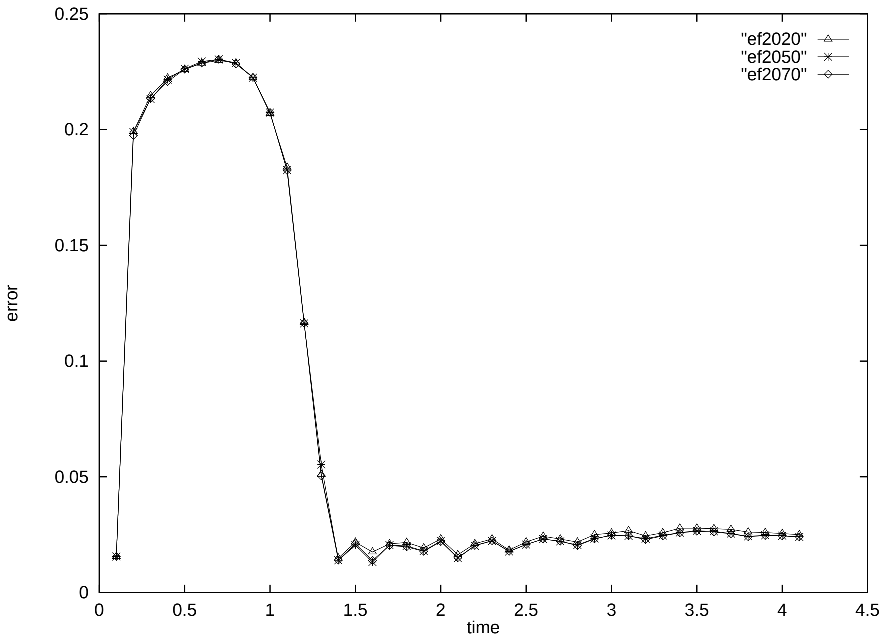


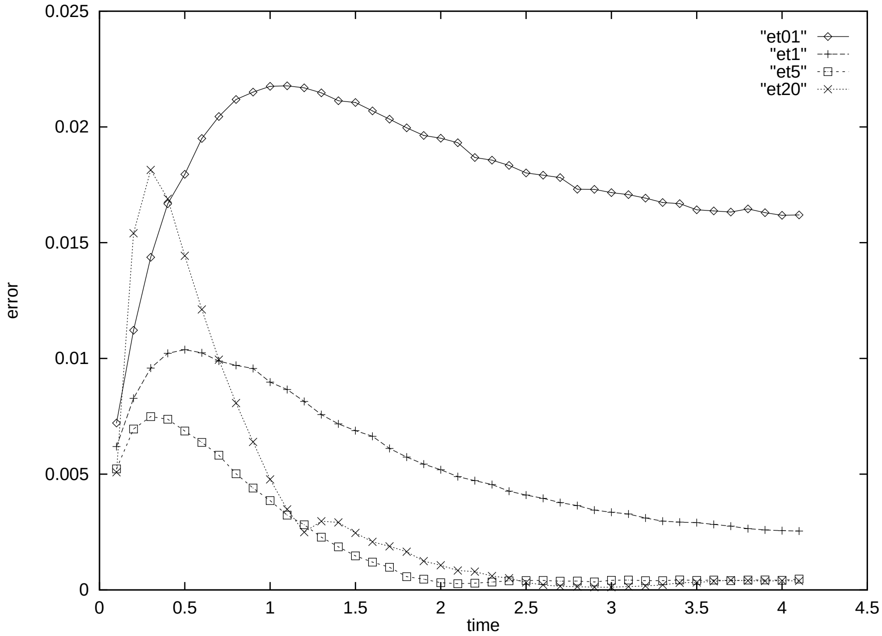
Fig. 4. Mean-square error of the free boundary while varying the mesh ($\omega = 20$).

- In Fig. 7, we present the computed and exact positions of the free boundary for the mesh 20×50 and the coefficient $\omega = 20$.
- The evolution of the cost function and the gradient versus the number of iterations is established in Figs. 8 and 9, respectively.

7. Conclusion

We have considered a two-phase Stefan model for solidification/melting situations involving a critical temperature θ. This model assumes that the two phases are separated by an unknown free boundary, and leads to evolution equations describing the temperature θ of the material and the moving boundary. The major difficulty in a direct problem is the fact that the unknown boundary affects explicitly the equations for the thermal state of the system. This difficulty was overcome by a reformulation of the problem: We characterized the different regions using the sign of an unknown function α. Then we introduced the characteristic function of the region $\alpha > 0$ that transformed the initial problem into a partial differential equation valid on the whole cavity occupied by the material coupled to a scalar equation connecting the signs of α and $\theta - \theta_c$.

The stability and convergence results of the proposed scheme for the temporal semi-discretization of the new formulation were established. Then we suggested a



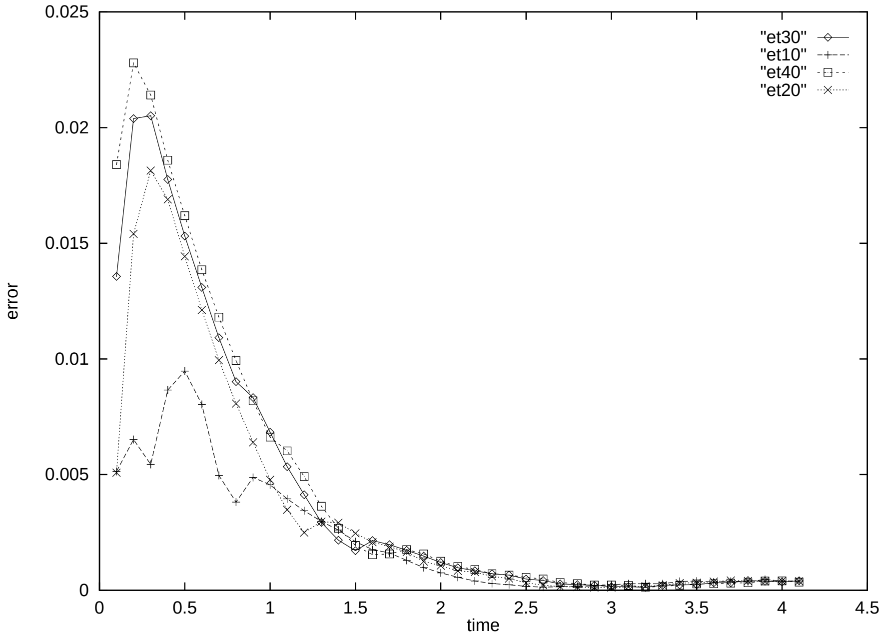
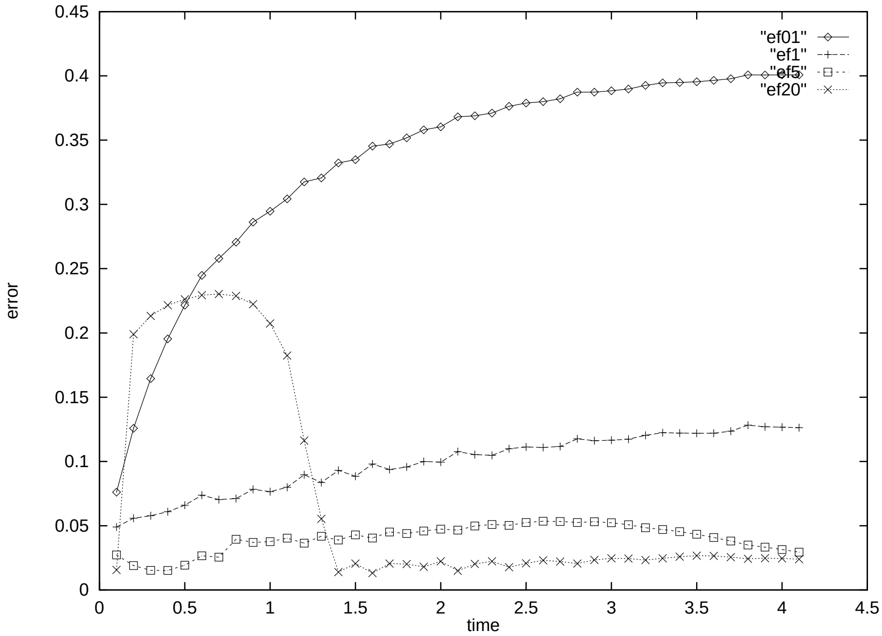


Fig. 5. Mean-square error of the temperatures while varying the coefficient ω for the mesh 20×20.



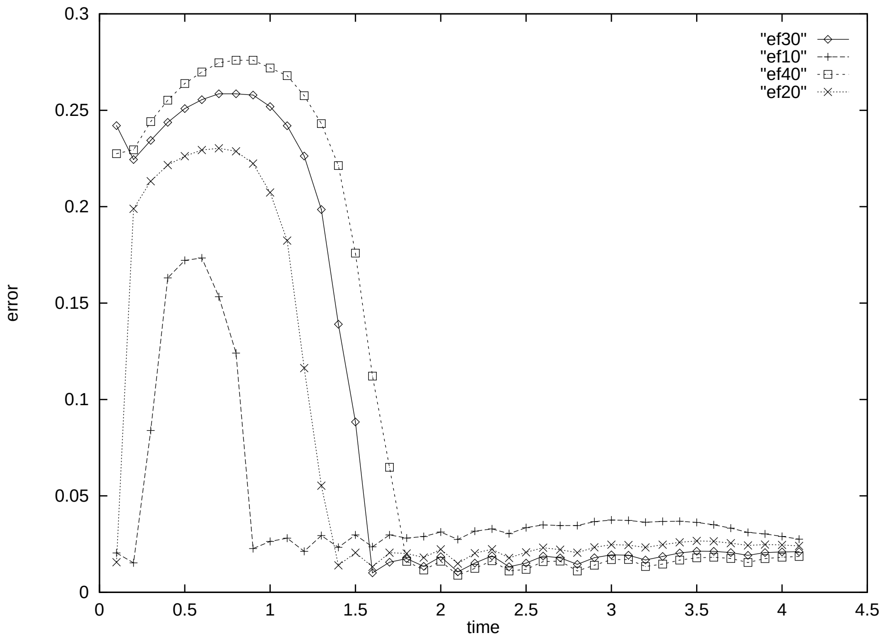


Fig. 6. Mean-square error of the free boundary while varying the coefficient ω for the mesh 20×50.

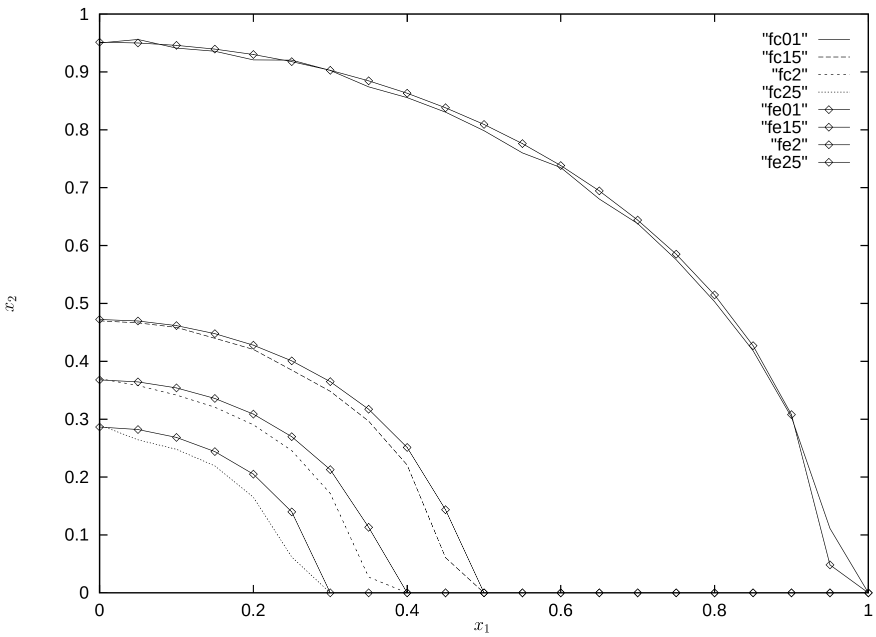


Fig. 7. Computed and exact positions of the free boundary for the mesh 20×50 and the coefficient $\omega = 20$.

numerical method based on domain optimization techniques which were tested in a simple situation considered in (Humeau and Souza del Cursi, 1993). We proved the existence of an optimal domain and a shape gradient. The computations of this gradient were performed using the material derivative and duality methods.

Introduction of specialized methods for discretization in time may lead to a better method. The numerical methods can be simply extended to mixed boundary conditions, even though the question of the uniqueness of solutions for general mixed boundary conditions is still open.

References

Baiocchi C., Comincioli V., Magenes E. and Pozzi G.A. (1973): *Free boundary problems in the theory of fluid flow through porous media. Existence and uniqueness theorems.* — Annali Mat. Pura App., Vol.4, No.97, pp.1–82.

Baiocchi C. (1977): *Problèmes à frontière libre en hydraulique: milieu non homogène.* — Annali della Scuola Norm. Sup. di Pisa, Vol.28, pp.429–453.

Ciavaldini J.F. (1972): *Résolution numérique d'un problème de Stefan à deux phases.* — Ph.D. Thesis, Rennes, France.

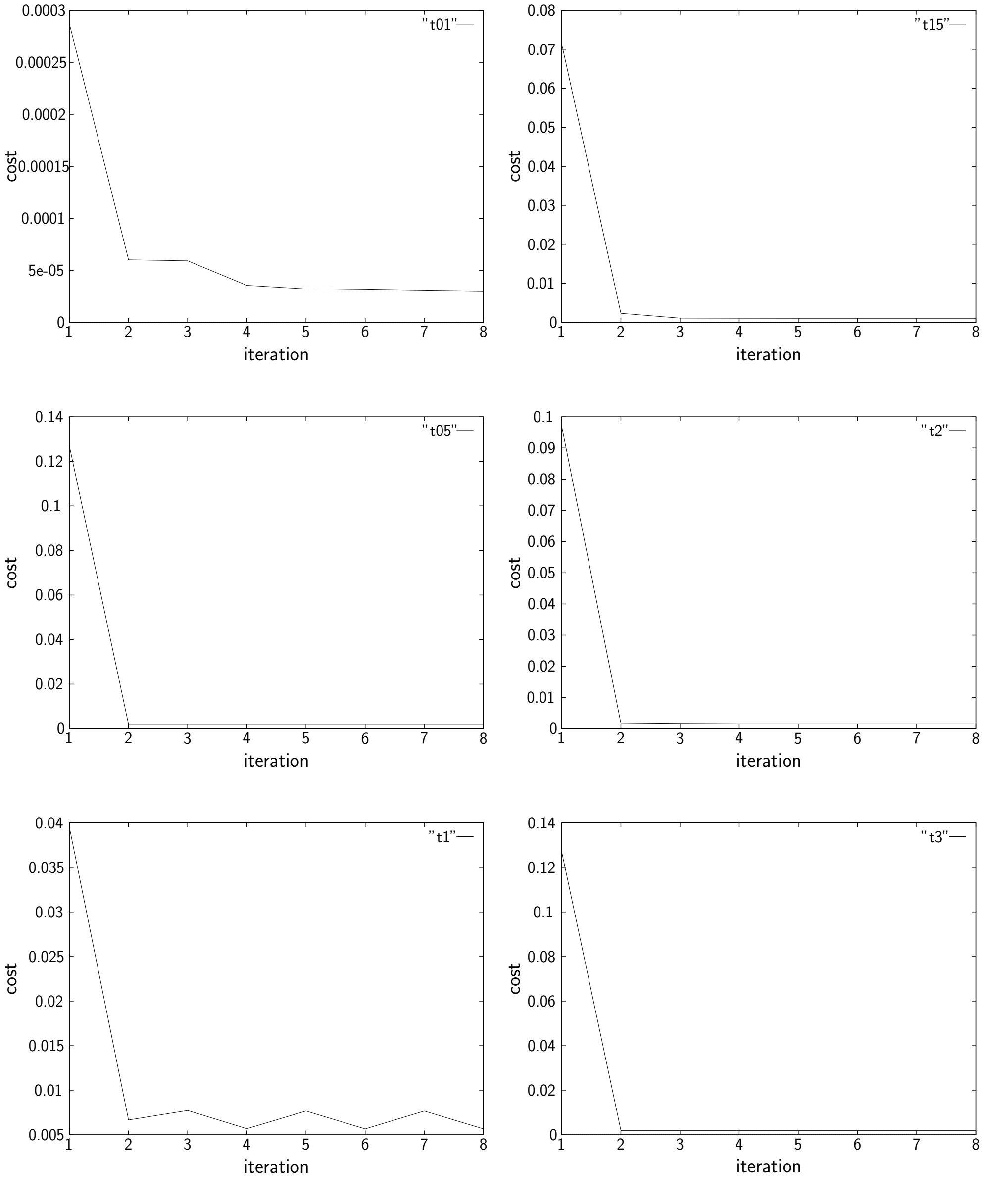


Fig. 8. Evolution of the cost versus iterations for the mesh 20×50 and the coefficient $\omega = 20$.

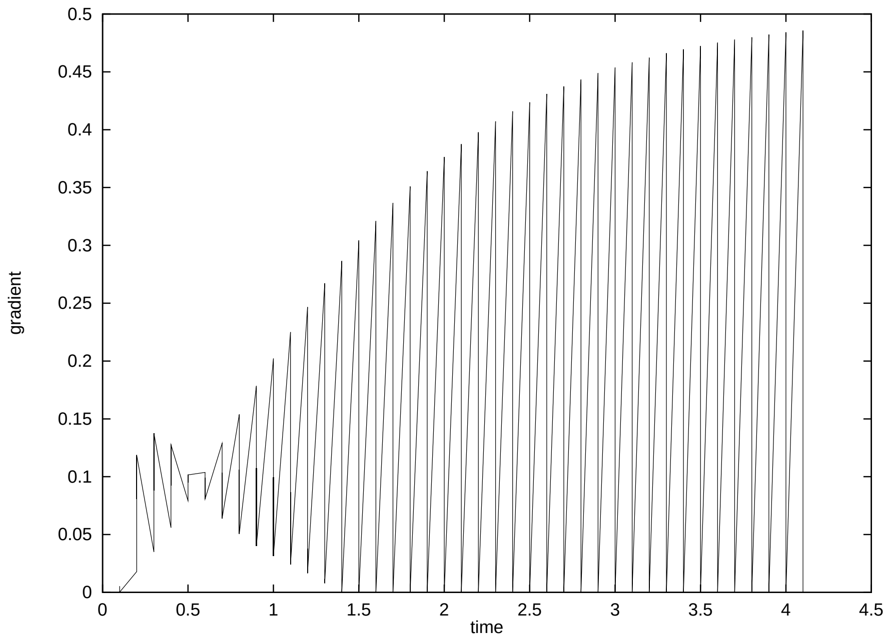


Fig. 9. Time evolution of the gradient for the mesh 20×50 and the coefficient $\omega = 20$.

El Bagdouri M. (1987): *Commande optimale d'un système thermique non-lineaire.* — Thèse de Doctorat d'Etat és-Sciences, Ecole Nationale Supérieure de Mécanique, Université de Nantes.

Haggouch I. (1997): *Résolution d'un problème de Stefan à deux phases par la méthode d'optimisation de forme.* — Ph.D. Thesis, Rabat, Morocco.

Haslinger J. and Neittaanmäki P. (1988): *Finite Element Approximation for Optimal Shape Design. Theory and Application.* — New York: Wiley.

Humeau J.P. and Souza del Cursi J.E. (1993): *Regularisation and numerical resolution of a two-dimensional Stefan problem.* — J. Math. Syst. Estim. Contr., Vol.3, No.4, pp.473–497.

Lions J.L. (1968): *Contrôle Optimal d'un Système Gouverné par des Équations aux Dérivées Partielles.* — Paris: Dunod.

Lions J.L. (1969): *Quelques Méthodes de Résolution des Problèmes aux Limites Non Linéaires.* — Paris: Dunod.

Lyaghfouri A. (1996): *The inhomogeneous dam with linear Darcy's law and Dirichlet boundary conditions.* — Math. Models Meth. Appl. Sci., Vol.6, No.8, pp.1051–1077.

Nochetto R.H., Paolin M. and Verdi C. (1991): *An adaptive finite element method for two phase Stefan problems in two space dimension, Part 1: Stability and error estimates.* — Math. Comp., Vol.57, No.57, pp.73–108, S1–S11 (supplement); *Part 2: Implementation and Numerical Experiments.* — SIAM J. Sci. Stat. Comput., Vol.12, No.5, pp.1207–1244.

Peneau S. (1995): *Contrôle optimal et optimisation de forme dans des problèmes à frontière libre. Application à un système thermique avec changement de phase.* — Ph.D., Ecole Central de Nantes, France.

Pironneau O. (1983): *Optimal Shape Design for Elliptic Systems.* — Berlin: Springer.

Raviart P.A. and Girault V. (1981): *Finite Element Approximation of the Navier-Stokes Equations.* — Berlin: Springer.

Rodrigues J.F. (1980): *Sur la cristallisation d'un métal en coulée continue par des méthodes variationnelles.* — Ph.D. Thesis, Université Paris 6.

Saguez C. (1980): *Contrôle optimal de systèmes à frontière libre.* — Ph.D. Thesis, Université de Technologie de Compiègne, France.

Srunk and Friedman A. (1994): *Variational and Free Boundary Problems.* — Berlin: Springer.

Zolésio J.P. (1981): *The material derivative (or speed method) for shape optimisation*, In: Optimisation of Parameter Structures, Vol.II (E.J. Haug and J. Cea, Eds.). — Alphen aan den Rijn, the Netherlands: Sijthoff, pp.1098–1151.

Zolésio J.P. (1979): *Identification de domaines par déformations.* — Thèse d'Etat, Université de Nice, France.

Received: 10 July 2000
Revised: 17 June 2000
Re-revised: 24 May 2001