Mathematical Models and Methods in Applied Sciences

A 3D Shape Optimization Problem in Heat Transfer: Analysis and Approximation via BEM

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Received (Day Month Year)
Revised (Day Month Year)
Communicated by (xxxxxxxxxx)

In this paper an optimal shape control problem dealing with heat transfer in enclosures is studied. We model an enclosure heated by a flame surface (taking account of radiation, conduction and convection effects), and we try to find an *optimal flame shape* which minimizes some cost functional defined on the temperature field. This kind of problem arises in industrial furnaces optimization, being *temperature uniformity* one of the most important aspects in industrial plant analysis and design. Analytical results (smoothness of the control-to-state mapping, existence of an optimal shape in a certain admissible class) as well as numerical optimization results by the *boundary element method* are obtained; we employ the *gradient method* to optimize the flame shape, exploiting the *adjoint equation* associated with the state equation and the cost function.

Keywords: optimal control; shape optimization; heat transfer; boundary element methods.

AMS Subject Classification: 49K20, 80M15

1. Introduction

In the setting of ceramic industry, one of the most important aspects of production process is *temperature control* in furnaces. In order to have a good product, one has to fulfill several specification on the temperature field within the furnace. If the temperature oscillates too much, or it doesn't match a desired thermal profile, the processed material can be damaged.

There is a large number of parameters which affects the temperature within a furnace: in this paper, we focus on the influence of the flames, generated by the burners, and we consider the dependence of the temperature on the *flame shape*, that we define as an isothermal surface (at high temperature). Roughly speaking, the aim of this work is to study the following optimization problem: *find an optimal flame shape in order that the temperature on internal walls surfaces in a given furnace is as close as possible to a prescribed temperature field.*

Let us consider a bounded domain $\Omega \in \mathbb{R}^3$. Physically, Ω consists in the furnace wall's firebricks: in this region there are no heat sources and the temperature is an harmonic function (by Fourier law). At the boundary $\partial\Omega$, we consider convective and radiative conditions on the heat flux; radiative fluxes, however, are important only on internal hot surfaces, thus we decompose $\partial\Omega$ in two disjoint parts Γ_{in} and Γ_{en}, where Γ_{in} is the internal hot surface, Γ_{ex} is the external cold one, and radiation is considered only on Γ_{in}. The flame surface is denoted with $\Gamma_f(\rho)$, where ρ is the *control* parameter, that is typically a function defining the surface to be optimized. The surface $\Gamma_f(\rho)$ is not part of the boundary $\partial\Omega$, it is a control surface over which we consider radiation toward the inner furnace boundary Γ_{in}.

We assume that the following quantity are known:

- the convection coefficients h_{in} on the internal surface and h_{ex} on the external one. We shall assume $h_{in} \geq 0$, $h_{ex} \geq 0$ and that a number $h_{inf} > 0$ exists such that $h_{in} > h_{inf}$, at least on an open subset of Γ_{in};
- the temperature u_{in} of combustion gases flowing on Γ_{in} and the environment temperature u_{ex} on Γ_{ex};
- the constant flame temperature $u_f > 0$;
- the wall emissivity ε; We shall assume that $0 < \varepsilon_0 \leq \varepsilon \leq \varepsilon_1 < 1$ on Γ_{in} for some constants ε_0 and ε_1;
- the flame emissivity $\varepsilon_f > 0$ (constant).

All these functions except emissivity are assumed in $L^{\inf}(\Gamma_k)$, with $k = in, ex$, and except emissivity they are normalized : the scaling of correspondent physical quantities is described in Table 1.

Taking account of conduction, convection and radiation for the evaluation of heat fluxes at the boundary, the temperature u satisfies the following differential problem:

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega; \\ -\partial u/\partial n = h_{ex}\ (u - u_{ex}) & \text{on } \Gamma_{ex}; \\ -\partial u/\partial n = h_{ex}\ (u - u_{in})\ +\ q & \text{on } \Gamma_{in}, \end{cases} \tag{1.1}$$

where u is the temperature and q is the radiative component of heat flux.

The radiation equation for q (for a general approach to radiation heat transfer

Table 1.

Physical quantity	Non-dimensional quantity	Scaling
temperature $\tilde{u}$	u	$u = \frac{\tilde{u}}{T_0}$
convection coefficient $\tilde{h}$	h	$h = \frac{L_0}{k}\tilde{h}$
Stefan constant $\tilde{\sigma}$	σ	$\sigma = \frac{L_0 T_0^3}{k}\tilde{\sigma}$
radiative heat flux $\tilde{q}$	q	$q = \frac{L_0}{kT_0}\tilde{q}$

Note: Here k is the *thermal conductivity* in Ω, which is assumed constant, L_0 is some reference length, and T_0 is some reference temperature.

see Modest[5]) is:

$$\begin{aligned} \sigma u^4(x) - \sigma \int_{\Gamma_{in}} K_0(x,y)u^4(y)\, \mathrm{d}\Gamma(y) = \\ = \frac{1}{\varepsilon(x)}q(x) - \int_{\Gamma_{in}} K_0(x,y)\frac{1-\varepsilon(y)}{\varepsilon(y)}q(y)\, \mathrm{d}\Gamma(y) + \\ + \sigma\varepsilon_f u_f^4 \int_{\Gamma_f(\rho)} K_0(x,y)\, \mathrm{d}\Gamma(y), \qquad x \in \Gamma_{in}. \end{aligned} \tag{1.2}$$

where σ is the normalized *Stefan constant* of radiation (see again table 1), and K_0 is radiation integral kernel, defined by

$$K_0(x,y) = \frac{\cos\phi_x \cos\phi_y}{\pi|x-y|^2}\alpha(x,y), \tag{1.3}$$

being

$$\alpha(x,y) = \begin{cases} 1 & \text{if } x \text{ can be seen from } y \\ 0 & \text{otherwise} \end{cases}.$$

In eq. (1.3) we denote by $\phi_x = \frac{n(x)\cdot(y-x)}{|x-y|}$ the angle between the outer normal $n(x)$ at $x \in \Gamma_{in}$ and the $y-x$ line, and analogously $\phi_y = \frac{n(y)\cdot(x-y)}{|y-x|}$ (see fig. 1). The kernel K_0 is positive and symmetric.

Let we write the flame radiative contribution as an operator dependent by the shape control parameter:

$$\mathcal{F}(\rho)(x) := \varepsilon_f u_f^4 \int_{\Gamma_f(\rho)} K_0(x,y)\, \mathrm{d}\Gamma(y), \qquad x \in \Gamma_{in}. \tag{1.4}$$

In this paper we consider convex flames shapes enclosed by a concave inner wall surface Γ_{in}, so we suppose that given $x \in \Gamma_{in}$ and $y \in \Gamma_f$, x is seen from y (i.e. $\alpha(x,y) = 1$) iff each point lies in the positive semi-space defined by the normal in the other one, that is $0 \le \phi_x < \pi/2$ and $0 \le \phi_y < \pi/2$. So:

$$\alpha(x,y) = \begin{cases} 1 & \text{if } K_0(x,y) > 0 \\ 0 & \text{otherwise} \end{cases}, \quad \forall x \in \Gamma_{in},\ y \in \Gamma_f. \tag{1.5}$$

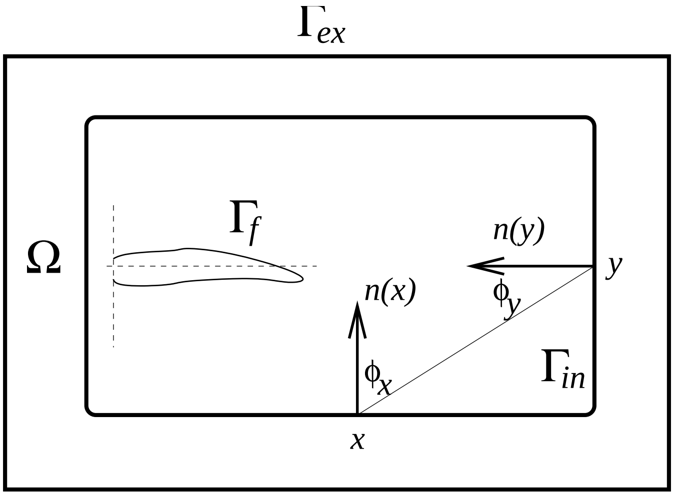

Fig. 1. An enclosure.

We consider polar coordinates parametrization for the flame surface $\Gamma_f(\rho)$ (see fig. 2). Therefore, the shape parameter $\rho = \rho(\varphi, \vartheta)$ is the flame radial coordinate, which depends by the angular coordinates φ and ϑ; that is, the parametric equation of $\Gamma_f(\rho)$ is

$$y = y(\varphi, \vartheta) = y_0 + \rho(\varphi, \vartheta)\mathbf{u}_\rho(\varphi, \vartheta), \qquad (\varphi, \vartheta) \in Q, \tag{1.6}$$

where y_0 is the center of polar system for the flame surface, $\mathbf{u}_\rho$ is the radial unit vector, and $Q = (0, \pi)^2$. Using equation (1.6) for change the integration variables in (1.4), thanks to (1.5), we obtain the following form for the operator $\mathcal{F}$:

$$\mathcal{F}(\rho)\ (x) \ = \ \int_Q [L(x;\ \rho,\ \rho_\varphi,\ \rho_\vartheta,\ \varphi,\ \vartheta)]^+ \, \mathrm{d}\varphi \mathrm{d}\vartheta, \tag{1.7}$$

where

$$[t]^+ := \begin{cases} t & \text{if } t \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

Calculations show that L is defined by

$$L \ = \ \varepsilon_f u_f^4 \ \frac{(y-x) \cdot n(x)\ (x-y) \cdot v}{\pi \ \mid y - x \mid^4}. \tag{1.8}$$

where y is given by (1.6) and

$$v := \sin\varphi\ \rho^2 \mathbf{u}_\rho(\varphi, \vartheta) - \sin\varphi\ \rho\ \rho_\varphi \mathbf{u}_\varphi(\varphi, \vartheta) - \rho\ \rho_\vartheta \mathbf{u}_\vartheta(\varphi, \vartheta)$$

is a normal vector on Γ_f (see fig. 2), being $\mathbf{u}_\varphi$ the φ unit vector and $\mathbf{u}_\vartheta$ the ϑ unit vector in the polar coordinates.

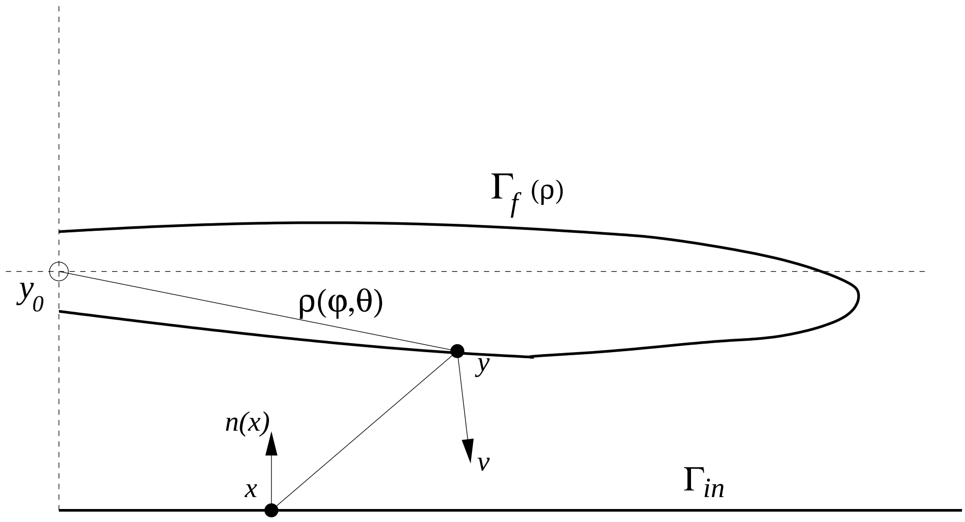

Fig. 2. A parametrized flame surface.

In our optimization problem, the aim is to minimize a *cost functional* J defined as

$$J = \int_{\Gamma_{in}} (u - u_d)^2 \omega \ \mathrm{d}\Gamma, \tag{1.9}$$

where u_d is the desired temperature on Γ_{in}, and $\omega \geq 0$ is a weight function. In order to use standard gradient-based algorithms to find the optimal flame shape, we are interested in first (Fréchet) derivative of J with respect to the control ρ:

$$J'(\rho)[\delta\rho] = 2 \int_{\Gamma_{in}} (u - u_d) u'(\rho)[\delta\rho] \omega \ \mathrm{d}\Gamma, \tag{1.10}$$

and especially we will focus on differentiability of J; we will also introduce an adjoint equation to compute J', and we will consider numerical methods of optimization for our problem.

2. Preliminary results

Let us introduce the integral radiation operators $\mathcal{K}_0$ and $\mathcal{K}_\varepsilon$:

$$(\mathcal{K}_0 f)\ (x) = \int_{\Gamma_{in}} K_0(x, y) f(y) \ \mathrm{d}\Gamma(y); \tag{2.11}$$

$$(\mathcal{K}_\varepsilon f)\ (x) = \int_{\Gamma_{in}} K_\varepsilon(x, y) f(y) \ \mathrm{d}\Gamma(y), \text{ being:} \tag{2.12}$$

$$K_\varepsilon(x, y) = (1 - \varepsilon(y))\ K_0(x, y). \tag{2.13}$$

The mathematical analysis of radiative models, (equations (1.1) and (1.2)) has been investigated by various papers (see Perret and Witomski[8], Monnier and Vila[6], and

Chenais, Monnier and Vila[2]). This work is substantially based on the paper of Perret and Witomski[8], but we add to the model the control parameter ρ via the flame radiation operator $\mathcal{F}(\rho)$. Some basic properties of radiation integral kernels, stated by Perret and Witomski[8], are recalled below: we denote by $\mathcal{L}(X;Y)$ the Banach space of bounded linear operators from X to Y, where X, Y are Banach spaces, and we set $\mathcal{L}(X) = \mathcal{L}(X;X)$.

Proposition 2.1. *We have* $\forall p \in [1,\infty]$*:*

a) $\mathcal{K}_\varepsilon \in \mathcal{L}(L^p(\Gamma_{in}))$, $\quad \|\mathcal{K}_\varepsilon\|_{\mathcal{L}(L^p(\Gamma_{in}))} \leq 1-\varepsilon_0$;
b) $\exists\ (\mathcal{I}-\mathcal{K}_\varepsilon)^{-1} \in \mathcal{L}(L^p(\Gamma_{in}))$*, and:* $\|(\mathcal{I}-\mathcal{K}_\varepsilon)^{-1}\|_{\mathcal{L}(L^p(\Gamma_{in}))} \leq \frac{1-\varepsilon_0}{\varepsilon_0}$.

Moreover, $\forall p \in [1,\infty]$*:*

c) $\mathcal{K}_0 \in \mathcal{L}(L^p(\Gamma_{in}))$, $\quad \|\mathcal{K}_0\|_{\mathcal{L}(L^p(\Gamma_{in}))} \leq 1$.

Proposition 2.2. *An integral kernel* $H_\varepsilon \in L^1(\Gamma_{in}\times\Gamma_{in})$ *exists, such that*

$$H_\varepsilon(x,y) \geq 0 \quad \text{in } \Gamma_{in}\times\Gamma_{in};$$
$$(\mathcal{I}-\mathcal{K}_\varepsilon)^{-1} = \mathcal{I}+\mathcal{H}_\varepsilon,$$

being $\mathcal{H}_\varepsilon$ *the integral operator with kernel* H_ε*. Moreover:*

$$\|\mathcal{H}_\varepsilon\|_{\mathcal{L}(L^p(\Gamma_{in}))} \leq \frac{1}{\varepsilon_0}\ \forall p \in [1,\infty].$$

To describe the properties of the $\mathcal{F}(\rho)$ operator, we choice a suitable functional space for the shape parameter ρ. We assume the control ρ belong to $W^{1,\infty}(Q)$, being $Q=(0,\pi)^2$, and we consider some constraints on the class of admissible shapes $\Gamma_f(\rho)$. First of all, we assume two bounds: a maximum control ρ_{max} and a minimum control ρ_{min}, such that

$$c < \rho_{min} \leq \rho \leq \rho_{max} < C \quad \text{ in } Q, \tag{2.14}$$

where $c>0$ and $C>0$ are constants. This means that an admissible flame shape is confined between a maximum and a minimum one. Besides, we assume that admissible shapes have some *convexity* properties, in order to have existence of an optimum, as we will see. We say that a function $r:(0,\pi)\to\mathbb{R}^+$ is *convex in the polar sense* (CPS) if $\forall\theta_1,\theta_2\in(0,\pi)$ and $\forall\theta\in(\theta_1,\theta_2)$, the radius $r(\theta)$ is greater or equal to the corresponding radial coordinate for the line between $(\theta_1, r(\theta_1))$ and $(\theta_2, r(\theta_2))$. That is, r is CPS if the set (described by polar coordinates) $\{(\rho,\theta): 0\leq\rho\leq r(\theta), 0\leq\theta\leq\pi\}$ is convex. Formally:

Definition 2.1. We say that r is CPS if $\forall\theta\in(\theta_1,\theta_2)$:

$$r(\theta) \geq \frac{r_1 r_2 \sin(\theta_2-\theta_2)}{r1\sin(\theta-\theta_1)+r2\sin(\theta_2-\theta)}, \tag{2.15}$$

being $r_1=r(\theta_1)$ and $r_2=r(\theta_2)$. If this inequality is *strict*, we say that r is *strictly convex* in a polar sense (SCPS).

In the cartesian case, convex functions have "good" properties of differentiability, and their derivatives are estimated by upper and lower bounds in the form of finite difference: B. Kawohl[3] used these properties for obtain, among other results, existence of an optimal convex shape in the Newton problem of the body with minimum drag. This is a problem from calculus of variations: we follow the same idea in our optimal control framework, exploiting the following properties:

Proposition 2.3. *Let* $r = r(\theta) : \ [0, \pi] \to \mathbb{R}^+$ *be a continuous CPS function, and set*

$$m(\theta, \epsilon) = r(\theta) \frac{r(\theta + \epsilon) \cos \epsilon \ - \ r(\theta)}{r(\theta + \epsilon) \sin \epsilon}.$$

Then

(a) $m(\theta, \epsilon)$ *is monotone non-decreasing (*$m(\theta, -\epsilon)$ *is monotone non-increasing) with respect to* $\epsilon > 0$*;*
(b) r *have left and right derivatives everywhere, is differentiable almost everywhere, and if* $\theta \in (0, \pi)$ *is a point in which* r *is differentiable we have* $\forall \epsilon_1, \epsilon_2 > 0$ *such that* $0 \le \theta - \epsilon_1 < \theta + \epsilon_2 \le \pi$*:*

$$m(\theta, \epsilon_2) \ \le \ r'(\theta) \ \le \ m(\theta, -\epsilon_1). \tag{2.16}$$

Proof. The proof is analogous at the one of the well-known convex function properties in cartesian coordinates: we consider only the first statement because the second immediately follow from it. Let $\theta \in (0, \pi)$ and $\epsilon > \epsilon' > 0$; we have

$$m(\theta, \epsilon') \ = \ r(\theta) \left(\frac{\cos \epsilon'}{\sin \epsilon'} - \frac{r(\theta)}{r(\theta + \epsilon') \sin \epsilon'} \right),$$

so by (2.15) applied for $r(\theta + \epsilon')$

$$m(\theta, \epsilon') \ \ge \ r(\theta) \left(\frac{\cos \epsilon'}{\sin \epsilon'} - \frac{r(\theta) \sin \epsilon' + r(\theta + \epsilon) \sin(\epsilon - \epsilon')}{r(\theta + \epsilon) \sin \epsilon' \sin \epsilon} \right).$$

Elementary calculations show that the right hand side of this equation is equal to $m(\theta, \epsilon)$; therefore, $m(\theta, \epsilon)$ is non-increasing with respect to $\epsilon > 0$. Similarly, one can show that $m(\theta, -\epsilon)$ is non-decreasing. □

Now we can introduce the class of admissible shape controls, which we call R_{ad}. Our results concerning the smoothness of the control-to-state map will be stated in the following admissible class:

$$\begin{aligned} R_{ad} := \Big\{ \ & W^{1,\infty}(Q) \ni \rho = \rho(\varphi, \vartheta) : \ \rho_{min} < \rho < \rho_{max}, \\ & \rho \text{ is SCPS with resp. to } (\varphi, \vartheta) \Big\}, \end{aligned} \tag{2.17}$$

while we will show the existence of an optimum for the sets

$$R_{ad}^M := \Big\{ \rho \in W^{1,\infty}(Q), \ \rho_{min} \le \rho \le \rho_{max}, \ \left| \frac{\partial \rho}{\partial n} \right| \le M \text{ on } \partial Q \Big\}, \tag{2.18}$$

for a given $M > 0$ (we remark that for a SCPS function ρ on Q the left and right derivatives exist everywhere, therefore the normal derivative $\partial\rho/\partial n$ is well-defined on ∂Q). We also assume

$$d_0 = \inf_{\rho \in R_{ad}} \operatorname{dist}\{\Omega, \Gamma_f(\rho)\} > 0, \tag{2.19}$$

that is admissible flames are uniformly distant from the walls.

In the sequel, the derivatives of a functional $F(u): X \to Y$ evaluated in $u \in X$ will be denoted by $F'(u)[h] \in \mathcal{L}(X; Y)$, $F''(u)[h_1, h_2] \in \mathcal{L}(X \times X; Y)$, and so on. We also indicate by $\mathrm{Lip}(X; Y)$ the Banach space of Lipschitz functions from X to Y, being X and Y Banach spaces. We have that R_{ad} is an open set in $W^{1,\infty}(Q)$, and on this admissible class the operator $\mathcal{F}$ has the following properties:

Proposition 2.4. *$\mathcal{F}$ is Fréchet differentiable from $R_{ad} \subset W^{1,\infty}(Q)$ to $L^2(\Gamma_{in})$, and has first variation defined by*

$$\mathcal{F}'(\rho)[h] \;=\; \int_Q \left(L_\rho\ h + L_{\rho_\varphi}\ h_\varphi + L_{\rho_\vartheta}\ h_\vartheta\right) \chi_+(L)\ \mathrm{d}\varphi \mathrm{d}\vartheta, \tag{2.20}$$

where $h \in W^{1,\infty}(Q)$, and

$$\chi_+(t) = \begin{cases} 0 \text{ if } t \leq 0 \\ 1 \text{ otherwise.} \end{cases}$$

$\mathcal{F}'$ is lipschitz with respect to ρ, that is:

$$\mathcal{F}' \in \mathrm{Lip}\left(R_{ad};\ \mathcal{L}(W^{1,\infty}(Q);\ L^2(\Gamma_{in}))\right).$$

Proof. We define, given $\rho \in R_{ad}$ and $x \in \Gamma_{in}$,

$$L^\rho := L(x; \rho, \rho_\varphi, \rho_\vartheta, \varphi, \vartheta).$$

First, we claim that L^ρ, as a function of (φ, ϑ), is almost everywhere $\neq 0$. In fact, if the previous statement was not true, there will be an open subset S of $\Gamma_f(\rho)$ such that $(y - x) \cdot n(x) = 0$ for $y \in S$ or $(y - x) \cdot v = 0$ for $y \in S$ (see eq. (1.8)). One can see that ρ cannot be SCPS in both cases, because S will be necessarily plane.

Now, by eq. (1.8) and (2.19) we have that L is regular with respect to ρ, ρ_φ, ρ_ϑ. Thus, for $h \in W^{1,\infty}(Q)$ and $\mathbb{R} \ni t \to 0$, we have

$$\lim_{t \to 0} \frac{[L^{\rho+th}]^+ - [L^\rho]^+}{t} \;=\; \left(L^\rho_\rho\ h + L^\rho_{\rho_\varphi}\ h_\varphi + L^\rho_{\rho_\vartheta}\ h_\vartheta\right) \chi_+(L^\rho), \tag{2.21}$$

for almost all $(\varphi, \vartheta) \in Q$. One can check in (1.8) that L is lipschitz with respect to ρ, ρ_φ and ρ_ϑ uniformly for $\rho \in R_{ad}$ and $x \in \Gamma_{in}$: so, by Lebesgue theorem applied to (2.21), we can state that $\forall x \in \Gamma_{in}$

$$\lim_{t \to 0} \frac{\mathcal{F}(\rho + th)(x) - \mathcal{F}(\rho)(x)}{t} \;=\; \int_Q \left(L_\rho\ h + L_{\rho_\varphi}\ h_\varphi + L_{\rho_\vartheta}\ h_\vartheta\right) \chi_+(L)\ \mathrm{d}\varphi \mathrm{d}\vartheta,$$

and then in the same way we obtain the existence of the first variation of $\mathcal{F}$:

$$\lim_{t \to 0} \frac{\mathcal{F}(\rho\ +\ th)\ -\ \mathcal{F}(\rho)}{t} \;=\; \mathcal{F}'(\rho)[h] \quad \text{in } L^2(\Gamma_{in}),$$

where $\mathcal{F}'(\rho)[h]$ is defined by eq. (2.20). The boundedness of $\mathcal{F}'(\rho)[\cdot]$ is trivial. Exploiting the uniform lipschitzianity of L with respect to ρ, ρ_φ and ρ_ϑ it is easy to prove that $\mathcal{F}'(\cdot)[h]$ is continuous as operator from R_{ad} to $L^2(\Gamma_{in})$: so $\mathcal{F}$ is Fréchet-differentiable. $\square$

3. State equation

We follow Perret and Witomsky[8] considering a truncation method for handling the nonlinearity introduced by the radiation model: they use upper and lower solutions to achieve well-posedness of the state equation. Our choice for the upper bound for the temperature must take in account the flame contribution, so we set

$$u_{sup} \;=\; \max\left\{ \sup u_{ex},\ \sup\left(u_{in} \;+\; \sigma\, \frac{\varepsilon_1}{h_{in}\varepsilon_0} u_f^4 \right) \right\}. \tag{3.22}$$

¿From our assumptions it follows that $0 < u_{sup} < +\infty$. We can introduce a truncation function $\tau \in C^\infty(\mathbb{R})$, such that:

τ and his derivatives are *bounded* ;
τ is *strictly increasing* ;
$\forall t \in [0, u_{sup}] :\ \tau(t) = t.$

By the Propositions 2.1 and 2.2 we can define the operator:

$$q(u,\ \rho) \;=\; \sigma\, \varepsilon\, (\mathcal{I} + \mathcal{H}_\varepsilon)\Big(\ (\mathcal{I} - \mathcal{K}_0)\tau(u)^4 \;-\; \mathcal{F}(\rho)\ \Big). \tag{3.23}$$

With this definition we consider q as the solution of the radiation equation (1.2) for a given temperature u such that $0 \le u \le u_{sup}$, and a given control $\rho \in R_{ad}$. If $u \in H^1(\Omega)$, then the trace of u on Γ_{in} is in $H^{1/2}(\Gamma_{in}) \hookrightarrow L^2(\Gamma_{in})$, so $\tau(u)^4 \in L^\infty(\Gamma_{in})$ and q is well-defined as *non-linear integral operator* from $H^1(\Omega) \times R_{ad}$ to $L^\infty(\Gamma_{in})$.

The state equation for the temperature distribution in the furnace's walls is the following one:

given a control $\rho \in R_{ad}$, find $u = u(\rho) \in H^1(\Omega)$, $0 \le u \le u_{sup}$, such that:

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega, \\ -\partial u/\partial n = h_{ex}\ (u - u_{ex}) & \text{on } \Gamma_{ex}, \\ -\partial u/\partial n = h_{in}\ (u - u_{in}) \;+\; q(u,\ \rho) & \text{on } \Gamma_{in}. \end{cases} \tag{3.24}$$

Given $\nu > 0$, we seek a fixed point for the operator $M_\nu :\ H^1(\Omega) \to H^1(\Omega)$, where $u = M_\nu v$ is defined by

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \\ -\partial u/\partial n \;-\; \nu u = -\,\nu v \;+\; h_{ex}\ (v - u_{ex}) & \text{on } \Gamma_{ex} \\ -\partial u/\partial n \;-\; \nu u = -\,\nu v \;+\; h_{in}\ (v - u_{in}) \;+\; q(v,\ \rho) & \text{on } \Gamma_{in} \end{cases} \tag{3.25}$$

Following Perret and Witomski[8], it turns out that M_ν is compact and, for ν sufficiently great, it is monotone non-increasing, $\underline{u} = 0$ is an under-solution, and $\overline{u} = u_{sup}$ is an upper-solution. Therefore we achieve existence and uniqueness of the solution u for the state equation (3.24), being $0 \le u \le u_{sup}$. Moreover, the control-to-state mapping is C^1: we will prove this claim by the implicit function theorem in Banach spaces and a smoothness result for the q operator.

Lemma 3.1. *The mapping* $F: \; u \mapsto F(u) = \tau(u)^4$ *is Fréchet-differentiable from* $H^1(\Omega)$ *to* $L^2(\Gamma_{in})$. *His first variation*

$$F'(u)[h] \;=\; 4\tau(u)^3\tau'(u)h$$

is lipschitz, that is

$$F' \;\in\; \mathrm{Lip}\left(H^1(\Omega);\; \mathcal{L}(H^1(\Omega);\; L^2(\Gamma_{in}))\right).$$

Proof. The linear mapping $H^1(\Omega) \longrightarrow H^{1/2}(\Gamma_{in}) \longrightarrow L^2(\Gamma_{in})$ is continuous, thus it is Fréchet differentiable from $H^1(\Omega)$ to $L^2(\Gamma_{in})$. Therefore, we need only to prove the smoothness of F from $L^2(\Gamma_{in})$ to $L^2(\Gamma_{in})$. We have, for $u, h \in L^2(\Gamma_{in})$ and $\mathbb{R} \ni t \to 0$:

$$\frac{\tau(u+th)^4 - \tau(u)^4}{t} \longrightarrow 4\tau(u)^3\tau'(u)h \quad \text{point-wise on } \Gamma_{in}. \tag{3.26}$$

But τ and his derivatives are bounded, so τ^4 is lipschitz, and there is $L > 0$ such that

$$\left|\frac{\tau(u+th)^4 - \tau(u)^4}{t}\right| \leq L|h|.$$

Therefore, by the Lebesgue theorem, the limit (3.26) also holds in $L^2(\Gamma_{in})$ norm, and F has first variation $F'(u)[h] = 4\tau(u)^3\tau'(u)h$. Clearly, $F'(u)[\cdot]$ is linear and continuous from $L^2(\Gamma_{in})$ to $L^2(\Gamma_{in})$. The function $4\tau(\cdot)^3$ is lipschitz; let $C > 0$ his lipschitz norm. We have $\|F'(u) - F'(v)\|_{\mathcal{L}(L^2(\Gamma_{in}))} \leq C\|u - v\|_{L^2(\Gamma_{in})}$, so F' is lipschitz with respect to u. From this it follows that F is Fréchet differentiable. □

By the lemma 3.1, proposition 2.4 and the continuity of the linear integral radiation operators (proposition 2.1 and 2.2), we have immediately this result:

Proposition 3.1. *The operator* $q = q(u, \rho)$ *defined by (3.23) is Fréchet-differentiable with respect to his arguments. The derivatives are:*

$$q_u \;=\; q_u(u)[\delta u] = 4\;\sigma\;\varepsilon\;(\mathcal{I} + \mathcal{H}_\varepsilon)(\mathcal{I} - \mathcal{K}_0)(\tau(u)^3\tau'(u)\;\delta u), \tag{3.27}$$

$$q_\rho \;=\; q_\rho(\rho)[\delta\rho] = -\sigma\;\varepsilon\;(\mathcal{I} + \mathcal{H}_\varepsilon)\mathcal{F}'(\rho)[\delta\rho], \tag{3.28}$$

and we have:

$$q_u \in \mathrm{Lip}\Big(H^1(\Omega);\; \mathcal{L}(H^1(\Omega);\; L^2(\Gamma_{in}))\Big),$$
$$q_\rho \in \mathrm{Lip}\Big(R_{ad};\; \mathcal{L}(W^{1,\infty}(Q);\; L^2(\Gamma_{in}))\Big).$$

Now we can show that the temperature u is a smooth function of the control shape parameter ρ. First of all, we introduce the weak formulation of the state equation. Let we consider the following operator $G : H^1(\Omega) \times R_{ad} \rightarrow H^1(\Omega)^*$, where $H^1(\Omega)^*$ is the dual space of $H^1(\Omega)$:

$$\begin{aligned} G(u,\ \rho)\cdot\lambda = \int_\Omega \nabla u\cdot\nabla\lambda\ \mathrm{d}\Omega\ -\ \int_{\Gamma_{ex}} h_{ex}(u-u_{ex})\lambda\ \mathrm{d}\Gamma\ - \\ -\ \int_{\Gamma_{in}} h_{in}(u-u_{in})\lambda\ \mathrm{d}\Gamma\ -\ \int_{\Gamma_{in}} q(u,\ \rho)\lambda\ \mathrm{d}\Gamma. \end{aligned} \tag{3.29}$$

The operator G is non-linear with respect to the state u and the control ρ; moreover it values are bounded linear functionals on the test functions $\lambda \in H^1(\Omega)$. The weak formulation of (3.24) is

$$G(u,\rho) = 0 \qquad \text{in } H^1(\Omega)^*. \tag{3.30}$$

We want to apply the implicit function theorem to (3.30) for obtain the smoothness of the mapping $u = u(\rho)$. By the isometry of a Hilbert space and his dual space, exploiting the proposition 3.1 for the non-linear term in (3.29), we can claim that G is Fréchet-differentiable with respect all his arguments. His Fréchet derivatives are:

$$\begin{aligned} G_\rho\ &=\ G_\rho(\rho)[\delta\rho]\cdot\lambda = -\int_{\Gamma_{in}} q_\rho(\rho)[\delta\rho]\ \lambda\ \mathrm{d}\Gamma; \\ G_u\ &=\ G_u(u)[\delta u]\cdot\lambda = \int_\Omega \nabla\delta u\cdot\nabla\lambda\ \mathrm{d}\Omega\ -\ \int_{\Gamma_{ex}} h_{ex}\ \delta u\ \lambda\ \mathrm{d}\Gamma\ - \\ &\qquad -\ \int_{\Gamma_{in}} h_{in}\ \delta u\ \lambda\ \mathrm{d}\Gamma - \int_{\Gamma_{in}} q_u(u)[\delta u]\ \lambda\ \mathrm{d}\Gamma. \end{aligned} \tag{3.31}$$

We can prove (theorem 3.1) that the linear operator $G_u(u)^{-1}$ exists and it is bounded from $H^1(\Omega)^*$ to $H^1(\Omega)$; by the implicit function theorem (see V. Khatskevitch and D. Shoiykhet[4]) it follows that the control-to-state mapping is smooth, and his Fréchet derivative is the solution of the following equation:

$$G_u(u(\rho))\Big[u'(\rho)[\delta\rho]\Big] + G_\rho(\rho)[\delta\rho] = 0. \tag{3.32}$$

So we have:

Theorem 3.1. *The control-to-state mapping*

$$u = u(\rho) : \quad R_{ad} \longrightarrow H^1(\Omega)$$

is Fréchet-differentiable, and given $\delta\rho \in W^{1,\infty}(Q)$ we have $u'(\rho)[\delta\rho] = \delta u$, where:

$$\begin{cases} \quad -\Delta\ \delta u = 0 & \text{in } \Omega, \\ -(\partial/\partial n)\ \delta u = h_{ex}\ \delta u & \text{on } \Gamma_{ex}, \\ -(\partial/\partial n)\ \delta u = h_{in}\ \delta u\ +\ q_u(u)[\delta u]\ +\ q_\rho(\rho)[\delta\rho] & \text{on } \Gamma_{in}. \end{cases} \tag{3.33}$$

Proof. The problem (3.33) is the strong formulation of the linear variational problem (3.32). We assert that:

$$\int_{\Gamma_{in}} q_u(u)[\lambda]\ \lambda\ \mathrm{d}\Gamma\ \geq\ 0 \quad \forall\lambda \in H^1(\Omega). \tag{3.34}$$

Let us define $\beta(u) = \tau(u)^3\tau'(u)$; by proposition 2.1 we have $\|\mathcal{K}_0\| \leq 1$, $\|\mathcal{K}_\varepsilon\| < 1$, so $\mathcal{I} - \mathcal{K}_0$ and $\mathcal{I} - \mathcal{K}_\varepsilon$ are defined positive with respect the scalar product in $L^2(\Gamma_{in})$, and also $(\mathcal{I}-\mathcal{K}_\varepsilon)^{-1} = \mathcal{I}+\mathcal{H}_\varepsilon$ it is. Moreover, consider the bounded positive function $\beta(u) = 4\sigma\tau(u)^3\tau'(u)$; the operator $\beta(u)\mathcal{I}$ is evidently positive semidefinite. So, being (see eq. (3.27) q_u defined as

$$q_u(u)[\cdot] \;=\; (\mathcal{I} + \mathcal{H}_\varepsilon)\;(\mathcal{I} - \mathcal{K}_0)\;\beta(u)\mathcal{I}$$

it is positive semidefinite, as composition of positive semidefinite operators; therefore, (3.34) is proved. The ellipticity of problem 3.33 follows, by our assumptions on h. So, by the Lax-Milgram theorem $G_u(u)[\cdot]$ has bounded inverse operator, and from the implicit function theorem we obtain the smoothness of the control-to-state mapping. □

4. Adjoint equation and first variation of the cost function

We will now introduce the Lagrangian function for our optimal control problem. By stationarity conditions for the Lagrangian, we will find an adjoint equation, which is a classical tool for the computation of the cost function gradient.

Let us recall that our aim is to minimize the cost functional J defined by (1.9). Consider the Lagrangian functional $\mathscr{L} : H^1(\Omega) \times H^1(\Omega) \times R_{ad} \to \mathbb{R}$, in which the test function λ play the role of Lagrange multiplier associated to the constraint given by the state equation (3.30):

$$\mathscr{L}(u, \rho, \lambda) \;=\; J(u) \;+\; G(u, \rho) \cdot \lambda. \tag{4.35}$$

The first-order stationarity conditions for the minimization problem (5.42) are:

$$\mathscr{L}_\lambda(u^o, \rho^o, \lambda^o)[\delta\lambda] = G(u^o, \rho^o) \cdot \delta\lambda = 0 \quad \forall\; \delta\lambda \in H^1(\Omega); \tag{4.36}$$
$$\mathscr{L}_u(u^o, \rho^o, \lambda^o)[\delta u] = J_u(u^o)[\delta u] + G_u(u^o)[\delta u] \cdot \lambda^o = 0 \quad \forall\; \delta u \in H^1(\Omega); \tag{4.37}$$
$$\mathscr{L}_\rho(u^o, \rho^o, \lambda^o)[\delta\rho] = G_\rho(\rho^o)[\delta\rho] \cdot \lambda^o = 0 \quad \forall\; \delta\rho \in W^{1,\infty}(Q), \tag{4.38}$$

where we have used the differentiability properties from the former section. This is a system of three coupled non-linear variational equations; the (4.36) is the weak formulation of the *state equation*, the (4.37) is the weak formulation of the associate *adjoint equation*, and the (4.38) is the *gradient equation*. We will show that given $u \in H^1(\Omega)$, the adjoint equation is well-posed and there is a unique *adjoint state* $\lambda = \lambda(u)$ which solve $J_u(u)[\delta u] + G_u(u)[\delta u] \cdot \lambda = 0\; \forall\; \delta u \in H^1(\Omega)$. Thanks to the adjoint state λ associated to a given u, using equation (3.32), we can compute the first variation of the cost function J defined by (1.10), as

$$J'(\rho)[\delta\rho] = \mathscr{L}_\rho(\lambda, u, \rho) = -\int_{\Gamma_{in}} q_\rho(\rho)[\delta\rho]\;\lambda\;\mathrm{d}\Gamma, \tag{4.39}$$

which is a classical result in optimization. This expression is helpful on the numerical point of view, because for each $\delta\rho$, the expression (1.10) would require the solution of the integral-differential problem (3.33) for computing J'; this trouble is avoided using the adjoint state approach.

Let us consider our adjoint problem.

Theorem 4.1. *Given $\rho \in R_{ad}$, consider the solution $u = u(\rho)$ of the state equation (4.36). It exists a unique $\lambda \in H^1(\Omega)$ such that:*

$$J_u(u)[\delta u] + G_u(u)[\delta u] \cdot \lambda = 0 \ \forall \ \delta u \in H^1(\Omega),$$

which is the weak formulation of the adjoint problem:

$$\begin{cases} -\Delta \ \lambda = 0 & \text{in } \Omega \\ -(\partial/\partial n) \ \lambda = h_{ex} \ \lambda & \text{on } \Gamma_{en} \\ -(\partial/\partial n) \ \lambda = h_{in} \ \lambda \ + \ \eta(u)[\lambda] \ + \ 2\omega(u - u_d) & \text{on } \Gamma_{in} \end{cases} \tag{4.40}$$

being $\eta(u)[\cdot]$ the adjoint integral operator of $q_u(u)[\cdot]$ with respect to the $L^2(\Gamma_{in})$ duality:

$$\eta(u)[\lambda] \ = \ 4 \ \sigma \ \tau(u)^3 \ (\mathcal{I} - \mathcal{K}_0)(\mathcal{I} - \mathcal{K}_\varepsilon^*)^{-1}(\varepsilon \ \lambda). \tag{4.41}$$

Proof. In the proof of theorem 3.1, we have shown that $q_u(u)[\cdot]$ is positive semidefinite with respect the scalar product in $L^2(\Gamma_{in})$. Being $\eta(u) = q_u(u)[\cdot]^*$, $\eta(u)$ is also positive semidefinite. Thus, in the same way we obtain that problem (4.40) is well posed by the Lax-Milgram theorem. We remark that, by (2.12), (2.13) and thanks to the symmetry of the kernel $K_0(x, y)$, the adjoint operator $\mathcal{K}_\varepsilon^*$ is defined by

$$(\mathcal{K}_\varepsilon^* f) \ (x) \ = \ (1 - \varepsilon(x)) \int_{\Gamma_{in}} K_0(x, y) f(y) \ \mathrm{d}\Gamma(y).$$

□

5. Existence of an optimal flame shape

Let us state the optimal shape control problem in the subset $R_{ad}^M \subset R_{ad}$ defined by (2.18): *find $\rho^o \in R_{ad}^M$ such that*

$$J(u^o) \leq J(u(\rho)) \quad \forall \rho \in R_{ad}^M, \tag{5.42}$$

being $u^o = u(\rho^o)$.

We will show that at least one optimal admissible flame shape exists, exploiting the SCSP-property of the admissible controls. The idea of Kawohl[3] is adapted in our optimal control setting.

Theorem 5.1. *The optimization problem (5.42) has (at least) a solution $\rho^o \in R_{ad}^M$.*

Proof. Being $J \geq 0$, it exists a minimizing sequence $\{\rho_n\}$. We claim that a subsequence ρ_{n_k} exists such that $\rho_{n_k} \to \rho^o \in R_{ad}^M$ in $W^{1,\infty}(Q)$, and:

$$\mathcal{F}(\rho_{n_k}) \to \mathcal{F}(\rho^o) \quad \text{in } L^2(\Gamma_{in}). \tag{5.43}$$

This implies $u(\rho_{n_k}) \to u(\rho^o)$ in $H^1(\Omega)$ by the well-posedness of the state equation, so we have

$$\inf_{\rho \in R_{ad}} J(u(\rho)) \ = \ \lim_{k \to \infty} J(u(\rho_{n_k})) \ = \ J(\rho^o),$$

and ρ^o is an optimal control.
Let us construct the sub-sequence ρ_{n_k}. Every $\rho_n(\varphi,\vartheta)$ is SCPS with respect of φ and ϑ: so we can apply the proposition 2.3-*(b)* with $\epsilon_1=\varphi$ and $\epsilon_2=\pi-\varphi$ to obtain

$$m_1^k(\varphi,\vartheta) := \rho_{n_k}(\varphi,\vartheta)\frac{\rho_{n_k}(\pi,\vartheta)\cos(\pi-\varphi)-\rho_{n_k}(\varphi,\vartheta)}{\rho_{n_k}(\pi,\vartheta)\sin(\pi-\varphi)} \le \frac{\partial}{\partial\varphi}\rho_{n_k}(\varphi,\vartheta) \le$$
$$\le \rho_{n_k}(\varphi,\vartheta)\frac{\rho_{n_k}(\varphi,\vartheta)-\rho_{n_k}(0,\vartheta)\cos\theta}{\rho_{n_k}(0,\vartheta)\sin\theta} =: m_2^k(\varphi,\vartheta),$$

for $(\varphi,\vartheta)\in(0,\pi)^2$. Being $\rho_{min}<|\rho_{n_k}|<\rho_{max}$, m_1^k and m_2^k are uniformly bounded in each compact set in Q. Moreover, they have a continuous extension to the whole $Q=[0,\pi]^2$, since

$$\lim_{\varphi\to\pi} m_1^k(\varphi,\vartheta) = \rho_{n_k}(\varphi,\vartheta)\frac{\partial}{\partial\varphi}\rho_{n_k}(\pi,\vartheta), \qquad \lim_{\varphi\to 0} m_2^k(\varphi,\vartheta) = \rho_{n_k}(\varphi,\vartheta)\frac{\partial}{\partial\varphi}\rho_{n_k}(0,\vartheta),$$

and thanks to $\rho_{n_k}\in R_{ad}^M$ we have $|\frac{\partial}{\partial\varphi}\rho_{n_k}(\pi,\vartheta)|\le M$, $|\frac{\partial}{\partial\varphi}\rho_{n_k}(0,\vartheta)|\le M$.

The same is true for the ϑ-partial derivative; so the sequence $\{\rho_n\}$ is uniformly bounded in $W^{1,\infty}(Q)$. By the Ascoli-Arzelà theorem, subsequence $\{\rho_{n_k}\}$ exists such that $\rho_{n_k}\to\rho^o$ *uniformly* in every compact set in Q. Therefore ρ^o is continuous, it is SCPS and such that $\rho_{min}<\rho^o<\rho_{max}$, $|\partial\rho^o/\partial n|\le M$ on ∂Q. Thanks to proposition 2.3, ρ^o is almost everywhere differentiable with bounded derivatives in every compact in Q, so $\rho^o\in R_{ad}^M$.

By (2.16), we obtain, for points (φ,ϑ) in which ρ_{n_k} is differentiable:

$$\rho_{n_k}(\varphi,\vartheta)\frac{\rho_{n_k}(\varphi+\epsilon,\vartheta)\cos\epsilon-\rho_{n_k}(\varphi,\vartheta)}{\rho_{n_k}(\varphi+\epsilon,\vartheta)\sin\epsilon} \le \frac{\partial}{\partial\varphi}\rho_{n_k}(\varphi,\vartheta) \le$$
$$\le \rho_{n_k}(\varphi,\vartheta)\frac{\rho_{n_k}(\varphi,\vartheta)-\rho_{n_k}(\varphi-\epsilon,\vartheta)\cos\epsilon}{\rho_{n_k}(\varphi-\epsilon,\vartheta)\sin\epsilon}. \tag{5.44}$$

For almost all $(\varphi,\vartheta)\in Q$ *all* the functions ρ_{n_k}, ρ^o are differentiable; for those points, when $k\to\infty$ we get:

$$\rho^o(\varphi,\vartheta)\frac{\rho^o(\varphi+\epsilon,\vartheta)\cos\epsilon-\rho^o(\varphi,\vartheta)}{\rho^o(\varphi+\epsilon,\vartheta)\sin\epsilon} \le \liminf \frac{\partial}{\partial\varphi}\rho_{n_k}(\varphi,\vartheta) \le$$
$$\le \limsup \frac{\partial}{\partial\varphi}\rho_{n_k}(\varphi,\vartheta) \le \rho^o(\varphi,\vartheta)\frac{\rho^o(\varphi,\vartheta)-\rho^o(\varphi-\epsilon,\vartheta)\cos\epsilon}{\rho^o(\varphi-\epsilon,\vartheta)\sin\epsilon},$$

and so for $\epsilon\to 0$:

$$\exists \lim_{k\to\infty}\frac{\partial}{\partial\varphi}\rho_{n_k}(\varphi,\vartheta) = \frac{\partial}{\partial\varphi}\rho^o(\varphi,\vartheta).$$

The same is true for the ϑ derivative: it follows that $\nabla\rho_{n_k}(\varphi,\vartheta)\to\nabla\rho^o(\varphi,\vartheta)$ for almost all $(\varphi,\vartheta)\in Q$. So, for almost all $(\varphi,\vartheta)\in Q$:

$$\lim_{k\to\infty}\left[L(x;\rho_{n_k},\frac{\partial\rho_{n_k}}{\partial\varphi},\frac{\partial\rho_{n_k}}{\partial\vartheta},\varphi,\vartheta)\right]^+ = \left[L(x;\rho^o,\frac{\partial\rho^o}{\partial\varphi},\frac{\partial\rho^o}{\partial\vartheta},\varphi,\vartheta)\right]^+.$$

Using two times the Lebesgue theorem, (5.43) is proved. □

6. BEM discretization of state and adjoint equations

We will present some numerical results for the problem of finding an optimal flame shape. The main minimization algorithm we use for our optimization purpose is the *gradient method*, with some well-known search-line procedures[a]. Our results are obtained by means of a Fortran90 code that gets approximate solutions of the state and the adjoint equations, using a discretization of the expression (4.39) to compute the gradient of the cost function J with respect to the degrees of freedom of the flame surface. Both the state and adjoint equations are potential equations with integral boundary conditions, so it is very suitable to reformulate them as *boundary integral equations* and use the *boundary element method* (BEM). The application of BEM for our state equation is accurately studied in the papers of Nowak[7], and Bialecki[1], so we just recall it shortly. For $x, y \in \partial\Omega$ we set:

$$u^*(x,y) \;:=\; E(x,y), \qquad q^*(x,y) \;:=\; -\frac{\partial E(x,y)}{\partial n(y)},$$

where E is the fundamental solution for the laplacian, which is in 3D defined as:

$$E(x,y) = \frac{1}{4\pi}\,\frac{1}{\mid x-y \mid}.$$

In the analysis of the state problem, we considered the operator $q = q(u,\rho)$ by implicitly solving the radiation equation (1.2). Now we consider the state equation (1.1) and the radiation equation (1.2), as a system with u and q as unknowns. Reformulating (1.1) as a boundary integral equations, we have:

$$\begin{aligned} c(x)\;u(x) = &\int_{\partial\Omega} q^*(x,y)\;u(y)\;\mathrm{d}\Gamma(y)\;\; - \\ &- \int_{\Gamma_{ex}} u^*(x,y)\;h(y)\Big(u(y)-u_{ex}(y)\Big)\;\mathrm{d}\Gamma(y)\;\; - \\ &- \int_{\Gamma_{in}} u^*(x,y)\;\Big(q(y)\;+\;h(y)\big(u(y)-u_{in}(y)\big)\Big)\;\mathrm{d}\Gamma(y) \end{aligned} \qquad (6.45)$$

for $x \in \partial\Omega$, being $c(x) = \int_{\partial\Omega} q^*(x,y)\;\mathrm{d}\Gamma(y)$. The former is an integral equation just like the radiation equation, which we rewrite as

$$\begin{aligned} \sigma u^4(x) - \sigma \int_{\Gamma_{in}} K_0(x,y)\;u^4(y)\;\mathrm{d}\Gamma(y) = &\;\frac{q(x)}{\varepsilon(x)} - \int_{\Gamma_{in}} K_\varepsilon(x,y)\;\frac{q(y)}{\varepsilon(y)}\;\mathrm{d}\Gamma(y)\;\; + \\ &+ \sigma\mathcal{F}(\rho)(x) \end{aligned} \qquad (6.46)$$

for $x \in \Gamma_{in}$.

We can apply the collocation method to discretize the integral equations (6.45) and (6.46), and to find numerical approximations for the temperature u and the

[a]for example the *Armijo's rule*, see Polak[10]; about the gradient method in shape optimization see Pironneau[9].

radiative flux q. Consider the boundary $\partial\Omega$ divided in boundary elements, which we assume quadrilateral:

$$\partial\Omega = \bigcup_k \Gamma^k,$$

and let $\mathbb{QP}_n$ the set of polynomials on the reference square having degree lower or equal to n with respect to each variable. We can define the following discrete spaces on $\partial\Omega$, for the temperature and the heat fluxes:

$$V_u = \Big\{ v \in C(\partial\Omega) : \ v|_{\Gamma^k} \in \mathbb{QP}_{n_u} \ \forall \Gamma^k \Big\},$$
$$V_q = \Big\{ v \in C(\Gamma_{in}) : \ v|_{\Gamma^k} \in \mathbb{QP}_{n_q} \ \forall \Gamma^k \subset \Gamma_{in} \Big\},$$

being n_u (resp. n_q) the polynomial degree of the elements in V_u (resp. V_q). In our code we have chosen bi-quadratic quadrilateral elements ($n_u = 2$, 9 d.o.f.) for the temperature, and constants ($n_q = 2$, 1 d.o.f.) for the fluxes.

We ave also to discretize the control space, which is a subset of $W^{1,\infty}(Q)$. We consider the points $0 = \alpha_1 < \ldots < \alpha_M = \pi$, and the associated finite-dimensional space R of tensor-product of cubic B-splines on the square $Q = (0, \pi)^2$: that is, if $\{B_i(\alpha)\}$ is the cubic B-spline basis associated to the points $\{\alpha_m\}$, the functions $\{B_i(\varphi)B_j(\vartheta)\}$ form a basis of R.

Let x^i, $i = 1, \ldots, N_u = \dim(V_u)$ are the nodal coordinates of the degrees of freedom associated to V_u, and let $\tilde{x}^k$, $k = 1, \ldots, N_q = \dim(V_q)$ the analogous coordinates associated to V_q. The discretized state equation by the collocation method is:

given $\rho \in R$, find $u \in V_u$, $q \in V_q$ such that:

$$\begin{aligned} c(x^i)\ u(x^i) = &\int_{\partial\Omega} q^*(x^i, y)\ u(y)\ \mathrm{d}\Gamma(y)\ - \\ &- \int_{\Gamma_{en}} u^*(x^i, y)\ h_{en}(y)\Big(u(y) - u_{en}(y)\Big)\ \mathrm{d}\Gamma(y)\ - \\ &- \int_{\Gamma_{in}} u^*(x^i, y)\ \Big(q(y)\ +\ h_{in}(y)\big(u(y) - u_{in}(y)\big)\Big)\ \mathrm{d}\Gamma(y) \end{aligned} \quad (6.47)$$

for $i = 1, \ldots, N_u$, and:

$$\begin{aligned} \sigma P u^4(\tilde{x}^k) - \sigma \int_{\Gamma_{in}} K_0(\tilde{x}^k, y)\ P u^4(y)\ \mathrm{d}\Gamma(y) = \\ \frac{q(\tilde{x}^k)}{\varepsilon(\tilde{x}^k)} - \int_{\Gamma_{in}} K_\varepsilon(\tilde{x}^k, y)\ \frac{q(y)}{\varepsilon(y)}\ \mathrm{d}\Gamma(y)\ + \\ +\ \sigma\mathcal{F}(\rho)(\tilde{x}^k), \quad \text{for } k = 1, \ldots, N_q, \end{aligned} \quad (6.48)$$

where P is the projection on V_u (the interpolating function on the mesh nodes), which is introduced to handle the non-linearity. Let $\phi_1, \ldots, \phi_{N_u}$ are the functions of a V_u lagrangian basis, and $\tilde{\phi}_1, \ldots, \tilde{\phi}_{N_u}$ the functions of a V_u one; let

$$u = \sum_i u^i \phi_i, \qquad q = \sum_k q^k \tilde{\phi}_k.$$

We consider the vectors $\mathbf{u} = [u^1, \ldots, u^{N_u}]^T$ and $\mathbf{q} = [q^1, \ldots, q^{N_q}]^T$, and we suppose that the mesh nodes on Γ_{in} are the first N_u^{in} ones, so we can consider the splitting

$$\mathbf{u} \;=\; \begin{bmatrix} \mathbf{u}_{in} \\ \mathbf{u}_{ex} \end{bmatrix},$$

where $\mathbf{u}_{in} = [u^1, \ldots, u^{N_u^{in}}]^T$ are the nodal values on Γ_{in}, and $\mathbf{u}_{ex}$ are the nodal values on Γ_{ex}. Equations (6.47) and (6.48) form a non-linear system for the unknowns $\mathbf{u}$ and $\mathbf{q}$, namely:

$$\begin{cases} \mathbf{A}\mathbf{u} \;+\; \mathbf{B}\mathbf{q} = \mathbf{a}, \\ \mathbf{C}\mathbf{u}_{in}^4 \;+\; \mathbf{D}\mathbf{q} = \mathbf{b}. \end{cases} \tag{6.49}$$

In Nowak[7] there is studied an efficient method to solve the non-linear equations (6.49) by the Newton-Raphson algorithm, after several gaussian eliminations.

Let us note that, in our problem, a flame contribution dependent by the shape is present, which is the term $\mathbf{b} = [b^1, \ldots, b^{N_q}]^T$ in (6.49), defined by

$$b^k = \sigma \mathcal{F}(\rho)(\tilde{x}^k) = \sigma \int_Q \left[L(\tilde{x}^k;\; \rho,\; \rho_\varphi,\; \rho_\vartheta,\; \varphi,\; \vartheta)\right]^+ \; \mathrm{d}\varphi \mathrm{d}\vartheta.$$

Given ρ, this term is computable via numerical quadrature. We can compute the nodal values of the first variation:

$$\delta b_i^k = \sigma \mathcal{F}'(\rho)[h_i](\tilde{x}^k) = \sigma \int_Q \left(L_\rho \; h + L_{\rho_\varphi} \frac{\partial h_i}{\partial \varphi} + L_{\rho_\vartheta} \frac{\partial h_i}{\partial \vartheta} \right) \chi_+(L) \; \mathrm{d}\varphi \mathrm{d}\vartheta,$$

being h_i the i-th element of a spline basis for R.

The adjoint state is also computable via BEM. First, we consider the full integral boundary equations associated with (4.40) and (4.41): for $x \in \partial\Omega$,

$$\begin{aligned} c(x)\; \lambda(x) &= \int_{\partial\Omega} \left\{ q^*(x,y)\lambda(y) \;-\; u^*(x,y) \left(-\frac{\partial \lambda(y)}{\partial n} \right) \right\} \; \mathrm{d}\Gamma(y) \\ &= \int_{\partial\Omega} q^*(x,y)\; \lambda(y)\; \mathrm{d}\Gamma(y) \;- \\ &\quad - \int_{\Gamma_{ex}} u^*(x,y)\; h_{ex}(y)\eta(y)\; \mathrm{d}\Gamma(y) \;- \\ &\quad - \int_{\Gamma_{in}} u^*(x,y) \; \Big(\eta(y) \;+\; 2\omega(u - u_d) \;+ h_{in}(y)\lambda(y) \Big) \; \mathrm{d}\Gamma(y), \end{aligned} \tag{6.50}$$

being

$$\eta = 4\sigma\tau(u)^3 \, (\mathcal{I} - \mathcal{K}_0) \, \xi, \tag{6.51}$$

where $\xi \in L^2(\Gamma_{in})$ is solution of

$$(\mathcal{I} - \mathcal{K}_\varepsilon^*) \, \xi = \varepsilon\lambda. \tag{6.52}$$

Equations (6.50), (6.51), (6.52) are three boundary integral equations for the unknown λ and the auxiliary unknowns η e ξ; we discretize them by means of the collocation method. So we have the following discrete adjoint problem:

find $\lambda \in V_u$, $\eta \in V_q$, *and* $\xi \in V_q$ *such that:*
for $i = 1, \ldots, N_u$:

$$\begin{aligned} c(x^i)\ \lambda(x^i) = & \int_{\partial\Omega} q^*(x^i, y)\ \lambda(y)\ \mathrm{d}\Gamma(y)\ - \\ & - \int_{\Gamma_{en}} u^*(x^i, y)\ h_{ex}(y)\lambda(y)\ \mathrm{d}\Gamma(y)\ - \\ & - \int_{\Gamma_{in}} u^*(x^i, y)\ \Big(\eta(y)\ +\ 2\omega(u(y) - u_d(y))\ + h_{in}(y)\lambda(y)\Big)\ \mathrm{d}\Gamma(y), \end{aligned} \tag{6.53}$$

for $k = 1, \ldots, N_q$:

$$\eta(\tilde{x}^k) = 4\sigma u(\tilde{x}^k)^3 \Big(\xi(\tilde{x}^k)\ -\ \int_{\Gamma_{in}} K_0(\tilde{x}^k, y)\xi(y)\ \mathrm{d}\Gamma(y)\Big), \tag{6.54}$$

for $i = 1, \ldots, N_u^{in}$:

$$\frac{1}{\varepsilon(x^i)}\xi(x^i) - \int_{\Gamma_{in}} \frac{K_\varepsilon(y, x^i)}{\varepsilon(x^i)}\ \xi(y)\ \mathrm{d}\Gamma(y) = \lambda(x^i). \tag{6.55}$$

Let we expand the approximation with respect to the basis functions of their boundary element spaces: we have

$$\lambda(x) = \sum_{i=1}^{N_u} \lambda^i f_i(x), \quad \eta(x) = \sum_{k=1}^{N_q} \eta_h^i \tilde{f}_k(x), \quad \xi(x) = \sum_{i=1}^{N_u^{in}} \xi^i f_i(x).$$

The matrix form of (6.53), (6.54) and (6.55) is:

$$\begin{cases} \mathbf{A}\boldsymbol{\lambda}\ +\ \mathbf{B}\boldsymbol{\eta} = -\mathbf{B}\mathbf{r}, \\ \boldsymbol{\eta} = \mathbf{E}\boldsymbol{\xi}, \\ \mathbf{F}\boldsymbol{\xi} = \boldsymbol{\lambda}, \end{cases} \tag{6.56}$$

where

$$\begin{aligned} \boldsymbol{\lambda} &= [\lambda^1, \ldots, \lambda^{N_u}]^T, \\ \boldsymbol{\eta} &= [\eta^1, \ldots, \eta^{N_q}]^T, \\ \boldsymbol{\xi} &= [\xi^1, \ldots, \xi^{N_u^{in}}]^T, \end{aligned}$$

and:

$$\mathbf{r} = [r^1, \ldots, r^{N_q}]^T,$$

being $r^k = 2\omega(\tilde{x}^k)(u(\tilde{x}^k) - u_d(\tilde{x}^k))$. In eq. (6.56) clearly we can easily eliminate the auxiliary unknowns $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$; moreover, the algorithm of Nowak[7] for the resolution of the discrete state equation (6.49) can be adapted to provide an efficient solution also for the discrete adjoint equation.

7. Numerical optimization and results

Being able to compute approximate solutions of the state and adjoint equations, we can discretize eq. (1.9) and (4.39) to obtain approximate computation of the cost function J and of its gradient with respect the B-spline basis $\{r_i\}$ of the control space. As an example, if we consider a piecewise constant weight function ω, and if we denote by ω_k the value on the boundary element Γ^k, we have:

$$J = \sum_k \omega_k \int_{\Gamma^k} (u - u_d)^2 \; \mathrm{d}\Gamma, \tag{7.57}$$

and

$$J'_i = J'[r_i] = \sum_k \omega_k q^k_{\rho,i} \int_{\Gamma^k} \lambda(y) \; \mathrm{d}\Gamma(y), \tag{7.58}$$

being $q^k_{\rho,i}$ the k-th component of the vector $\mathbf{q}_{\rho,i} = \mathbf{D}^{-1}\boldsymbol{\delta b}_i$, where $\mathbf{D}$ is the matrix that appears in (6.49).
In this manner, we can use classical first-order optimization algorithms, exploiting the descent direction of the gradient $\boldsymbol{\nabla} J = [J'_1, \ldots, J'_{N_\rho}]$. We have some constraints on the control parameters, and we chosen for our numerical software a *projected control* approach. The general structure of this algorithm is the following one (see *picture*):

1. Given the control $\boldsymbol{\rho}^n = [\rho^n_1, \ldots, \rho^n_{N_\rho}]$, compute $\mathbf{u}^n$ solving the discrete state equation (6.49);
2. Compute $\boldsymbol{\lambda}^n$ solving the discrete adjoint equation (6.56), which is dependent by the computed discrete state $\mathbf{u}^n$;
3. Compute J by eq. (7.57) and $\boldsymbol{\nabla} J$ by eq. (7.58) and start a *line-search* procedure, that is update the control parameter by
$$\boldsymbol{\rho}^{n+1/2} = \boldsymbol{\rho}^n + t\mathbf{d}^n,$$
for a suitable step size t and descent direction $\mathbf{d}$, for instance $\mathbf{d} = -\boldsymbol{\nabla} J$;
4. Project the updated control parameter onto the set of the admissible parameters, by means of some projection operator Π:
$$\boldsymbol{\rho}^{n+1} = \Pi \boldsymbol{\rho}^{n+1/2}.$$
5. *Stopping criterion*: given a relative tolerance $\epsilon_{tol} > 0$, if
$$\| \; \Pi'(\boldsymbol{\rho}^n)[\mathbf{d}] \; \| < \epsilon_{tol} \; \|\mathbf{d}\|$$
then stop (here $\|\cdot\|$ is the euclidean norm). Otherwise, set $n \leftarrow n+1$ and restart from 1.

The main drawback of the projected control approach is that it assume we are able to compute J and $\boldsymbol{\nabla} J$ also for a non-admissible control $\boldsymbol{\rho}$. Therefore, we used a mixed approach. We applied classical *bounding box* optimization to handle the constraint $\rho_{min} \le \rho \le \rho_{max}$: that is, we consider the control parameters $\boldsymbol{\rho}$ in a hyper-cube and we project the descent direction on it. We exploited the projected control approach for the SCPS constraint on the admissible flames: the projector Π is computed by a fast optimization of a suitable functional $p(\boldsymbol{\rho})$ which penalizes the non-SCPS shapes.

Now let us show some numerical 3D results, obtained by our Fortran90 BEM code. We consider a simple geometry (see picture 3), and the physical values of table 3. In this case, we observe the temperature distribution on the bottom of the inner surface of the furnace. As the optimization goes on, the flame shape become sharper, to offer a larger radiant surface to far wall's points. The economy for the cost functional J is 30%.

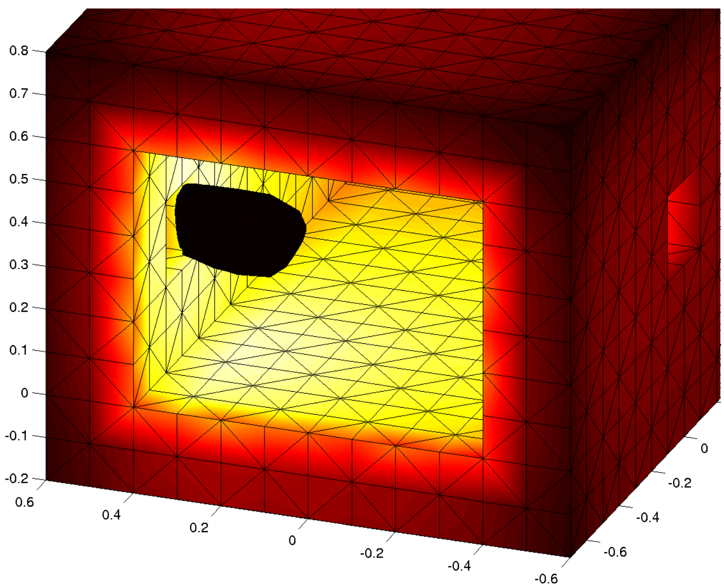

Fig. 3. Temperature distribution on the furnace surfaces for the optimal flame shape.

Table 2.

Quantity	Symbol	Value
Internal convection coeff.	h_{in}	25 $Wm^{-2}K^{-1}$
External convection coeff.	h_{ex}	20 $Wm^{-2}K^{-1}$
Combustion gas temperature	T_{gas}	1000 K
Environment temperature	T_{en}	300 K
Flame temperature	T_f	1500 K
Desired temperature	T_d	910 K
Conduction coeff. in walls	k	1 $Wm^{-1}K^{-1}$
Wall emissivity	ε	0.5

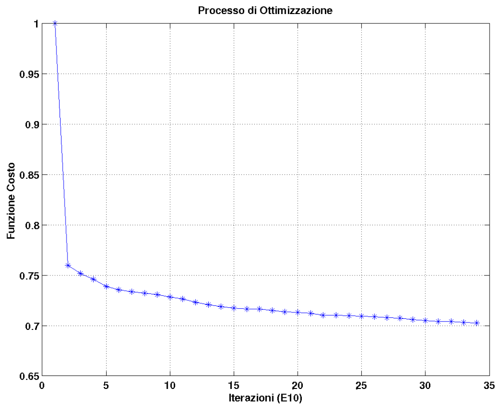

Fig. 4. J values at each iteration number: single flame optimization.

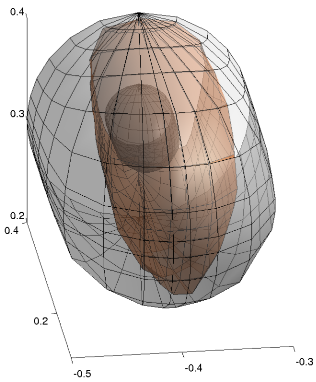

Fig. 5. Minimum, maximum and optimal flame profiles

Similar results can be obtained for multi-flame surfaces. In this case we have several control functions, being each surface $\Gamma_{f,i}$ parametrized by a function $\rho_i \in R_{ad}$, and by linear superposition of the overall flame radiation it is trivial to extend our approach and to consider multi-surface optimization. The picture 7 shows the temperature distribution for a initial small-surfaces configuration, while in the picture 8 we have the final optimized one. The iterations of the gradient-based optimization algorithm are shown in picture 9. A detail of the optimal flame surfaces is shown in picture 10, together with the minimum and maximum admissible shapes.

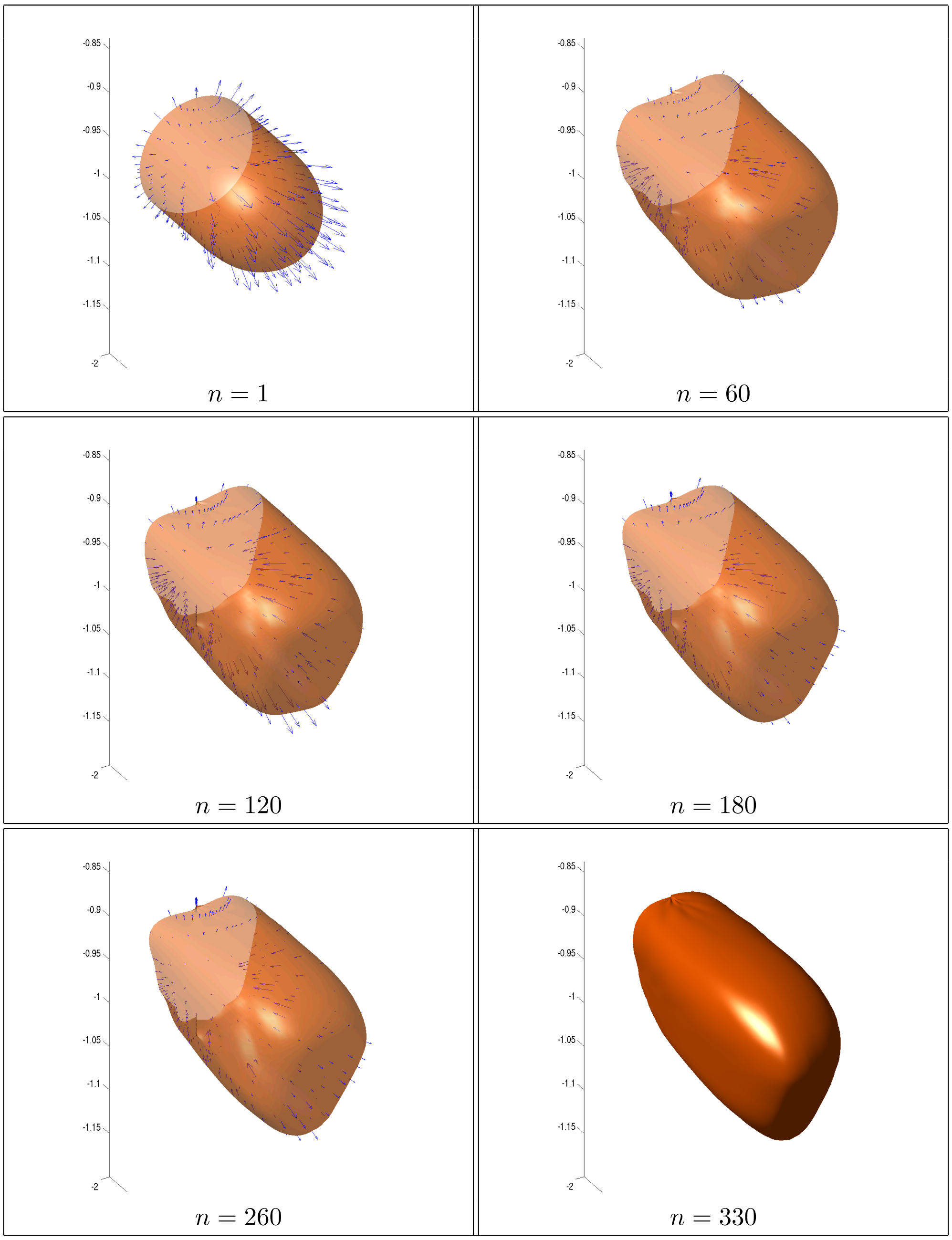

Fig. 6. Some flame shape during the optimization algorithm.

8. Conclusions

In this paper, an optimal control problem for the flame shape in an enclosure has been considered, modeling heat transfer by conduction, convection and radiation.

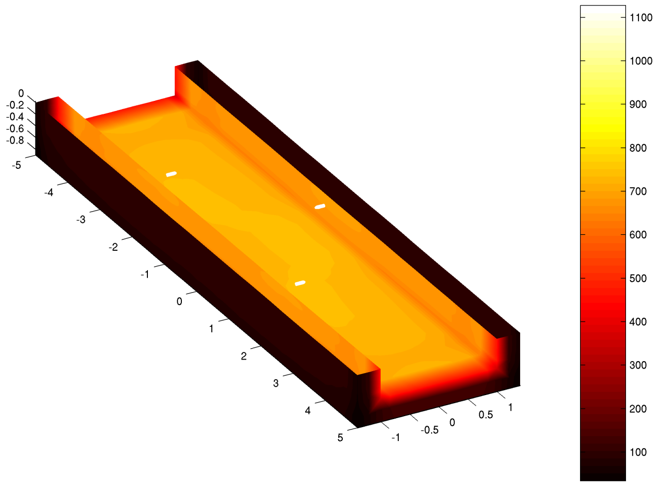

Fig. 7. Half furnace temperature distribution for the initial flame shapes.

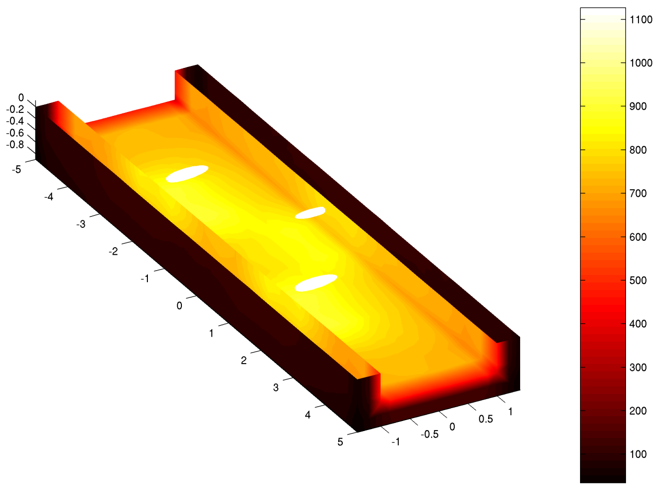

Fig. 8. Half furnace temperature distribution for the optimal flame shapes.

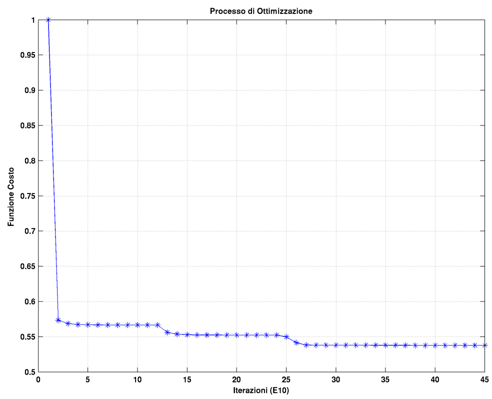

Fig. 9. J values at each iteration number: three flames optimization.

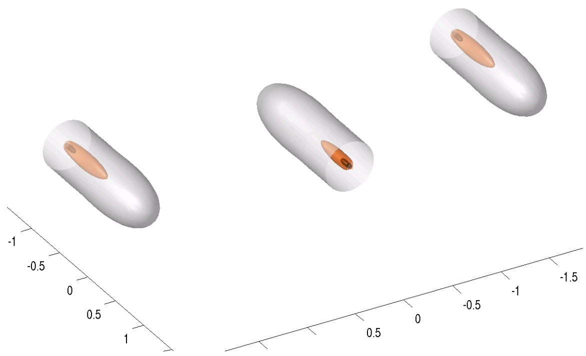

Fig. 10. Minimum, maximum and optimal flame profiles

This problem deals with temperature control in industrial furnaces related to ceramic material processing. We have proved the smoothness of the control-to-state mapping, the existence of an optimum in a suitable admissible class, and we have computed the gradient of the cost functional whit respect to the shape parametrization via a dual approach. Moreover, a BEM numerical scheme for solving the direct and adjoint equations has been implemented in a 3D Fortran90 code, and some optimization results have been obtained by the gradient method. We point out that BEM is very suitable in our case, being both the cost functional and the radiation equations defined by boundary integral expressions.

Aknowledgments

This work has been supported by the company FINCUOGHI, by the research granty "Heat transfer modeling and flame shape optimization in tunnel furnaces for ceramic material". The authors are very grateful to Prof. Sandro Salsa for his precious help and experience.

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