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On nonlinear inverse problems of dehydration of gypsum plasterboards exposed to fire via the heat conduction problem with radiation boundary conditions

A. Belmiloudi¹ and F. Mahé²

Abstract

The paper investigates boundary optimal controls and parameter estimates to the well-posedness nonlinear model of dehydration of gypsum plasterboard exposed to fire. We develop the general formulations for the boundary control for initial-boundary value problem for nonlinear partial differential equations modeling the heat transfer during a fire exposure and derive necessary optimality conditions, including the adjoint equation, for the optimal set of parameters minimizing objective functions J . Numerical simulations illustrate several numerical optimization methods and several examples and realistic cases, in which several interesting phenomena are observed. A large amount of computational effort is required to solve the coupled state equation and the adjoint equation (which is backwards in time), and the algebraic gradient equation (which implements the coupling between the adjoint and control variables). The state and adjoint equations are solved using the finite element method.

Key words: Optimal control, model calibration, numerical approximation, control constraint, adjoint model, dehydration of gypsum, Comsol, Matlab.

1 Introduction and mathematical setting of the problem

1.1 Motivation

Since several years, a considerable effort has been made to develop materials having a good fire resistance. Such materials must provide a sufficient mechanical resistance to avoid the premature collapse of a building structure undergoing a fire. Consequently this type of material must withstand significant heating without burning and keep its mechanical resistance sufficient. Criteria which permit to appreciate the fire resistance of materials are given by several norms which define the minimum fire exposure duration that must support the building structure.

One of the building materials presenting the best fire resistance is gypsum plasterboard, which in turn is due to the hydration phenomenon. This material presents the particularity to undergoing two chemical reactions of dehydration during its heating. These two endothermic reactions considerably slow down the heating of the material (since the dehydration process consumes large amount of heat), and provides to the plasterboard an excellent fire resistance.

The main particularity of gypsum plasterboard is that it contains 21% of chemically combined water by weight. When the temperature reaches $100^{\circ}C$ in a point of the plasterboard, a reaction of dehydration occurs in the material. This chemical reaction dissociates a certain quantity of water which is combined to the crystal lattice. In terms of fire safety, the reaction of dehydration and the vaporization of free water absorb a certain amount of energy which significantly slows down the heating of the material and in particular the temperature rise on the unexposed side of plasterboard.

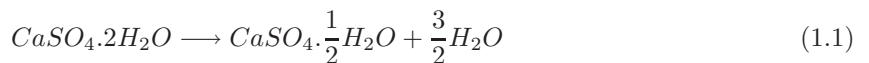
Although necessary, experimental testing is not a convenient way to estimate the fire resistance of a material. Indeed, full-scale testing poses the problem of the high cost of the experimental setup and the difficulty to implementing the experiment. In addition pilot-scale testing does not allow to accurately reproducing the real conditions of a fire exposure. Consequently, the development of a mathematical model, and the numerical simulation of the heating of gypsum plasterboard exposed to fire appears as a suitable means to study the thermal behaviour of the material during a fire exposure.

¹IRMAR-INSA de Rennes, 20 avenue des Buttes de Coësmes, CS70839, 35708 Rennes Cédex7, France. (e-mail: Aziz.Belmiloudi@insa-rennes.fr)

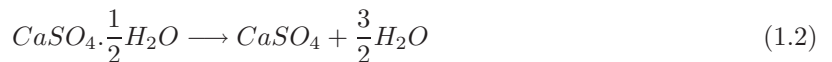
²IRMAR-Université Rennes 1, Campus de Beaulieu, 35042, Rennes Cedex France. (e-mail: Fabrice.Mahe@univ-rennes1.fr)

1.2 Thermo-chemistry of gypsum

Gypsum plasterboard is commonly used as construction material to improve fire resistance of building structures. The pure Gypsum, existing at the natural state as a more or less compact rock, is composed of calcium sulphate with free water at equilibrium moisture (approximately 3%) and approximately 20% per weight of chemically combined water of crystallization (see e.g. [8, 13, 15]). Its chemical formula is $CaSO_4 \cdot 2H_2O$ (calcium sulphate di-hydrate). The industrials add various chemical elements (in small quantities) in order to increase their performance when exposed to elevated temperatures. The chemical reaction which consists in removing chemically combined water of crystallization is called calcination. During heating, gypsum plaster undergoes two endothermic decomposition reactions. The first dehydration reaction occurs at approximately $100 - 120$ °C when the calcium sulphate di-hydrate is converted to calcium sulphate hemihydrate (the reaction is always complete by 160 °C) as shown by the following reaction



The amount of energy required by this first dehydration is about 500 kJ per kg of gypsum (see [21]). The second dehydration reaction occurs when calcium sulphate hemihydrate is converted to calcium sulphate anhydrite as shown by the following reaction



The amount of energy corresponding to this second reaction is about 169 kJ per kg (see [3]).

Remark 1.1 *several other analysis of the energy can be found in the literature see e.g. [20, 23, 24] and the references therein.*

Both reactions are endothermic, produce liquid water and absorb a large amount of energy. The effect of the endothermic reactions on the heating of the wall of plasterboard is taken into account by including the latent heats of reactions (1.1) and (1.2) in the specific heat evolution. The first dehydration reaction occurs at approximately $100 - 160$ °C, on the other hand there is some discrepancy to when the second dehydration reaction occurs. Andersson et al. [2] (for example) estimate that the second reaction occurs between 210 °C and 300 °C. That consists in introducing two peaks in the evolution of the specific heat according to the temperature, corresponding to the temperatures to which the reactions occur. The areas under the two peaks are equal to the latent heats of the two chemical reactions. Other experiences show that this second reaction occurs immediately after the first one. In the numerical examples, we will choose this model with only one peak between 100 and 170 °C in the evolution of the the specific heat. The information on the thermophysical properties of gypsum plasterboard, at high temperatures, are difficult to measure and then are limited, because the derived results are always complicated by the dynamic nature of the (fire resistive) materials, and vary considerably with the used method of measurement (a wide variety of experimental techniques exists for measuring these properties), and the rate of temperature change (for more details see e.g. [2, 9, 22, 23]).

1.3 Outline of the paper

The paper is organized as follows. In the next subsection, we give a sketch of the modeling leading to problem and we establish the governing equations. In Section 2 we give a description of the parameter estimates (identification problems) as nonlinear optimal control problems with boundary control. This includes results concerning the existence of the optimal solutions, necessary optimality conditions

(necessary to develop numerical optimization methods), the optimization problem and adjoint model. Section 3 contains details of the computational algorithm and numerical simulation-optimizations of the optimal control problems. Numerical results for several examples are presented and a realistic model is analyzed. Section 4 contains a summary and a discussion of future work.

1.4 Modeling of the wall of plasterboard heating and the direct forward model

This section is devoted to an introduction of the derivation of dehydration of gypsum plasterboards (exposed to fire) model we study. It is well known that the problem of heat and mass transfer in plasterboard exposed to fire is essentially one-dimensional, so the model is derived in one-dimensional formulation.

Let us consider a wall of plasterboard exposed to fire, which is located vertically on a retaining structural frame. The left hand side is exposed to a heat source, as may occur in furnace in which fire tests are conducted. We suppose that the depth (h) and the width (w) of the wall are much bigger than the thickness (L). Therefore heat fluxes in lateral (y) direction and vertical (z) direction can be neglected in front of the heat flux in direction x . On the other hand, the heat source is distributed uniformly on the heated side of the plasterboard. Applying these physical considerations, the heat transfer can be treated as 1-dimensional process in x -direction. The one-way heat transfer through a plane wall is described by the heat equation in its one-dimensional form

$$\begin{aligned} \lambda(u) \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} (\kappa(u) \frac{\partial u}{\partial x}) &= 0, \text{ in } \mathcal{Q} = \Omega \times (0, T), \\ u(x, 0) &= u_0(x), \quad x \in \Omega, \end{aligned} \quad (1.3)$$

where Ω is the boundary subset $(0, L)$, u is the temperature, $\lambda = \rho c$, ρ is the density of body material, c is the specific heat and κ is the thermal conductivity. The functions λ and κ are variables, positives and bounded.

The external surface of the wall of plasterboard exposed to fire receives a heat flux which consists of convective and radiative components. Consequently, the boundary condition on this side is written as:

$$-\kappa(u(0)) \frac{\partial u}{\partial x}(0) = h_0(u_f - u(0)) + \varphi_0(|u_f|^3 u_f - |u(0)|^3 u(0)), \text{ in } (0, T), \quad (1.4)$$

where, for all $t \in [0, T]$, $h_0(t) > 0$ is the convective heat transfer coefficient between the furnace and the plasterboard surface, $u_f(t) > 0$ is the furnace temperature, $\varphi_0(t) = \sigma \epsilon_0(t) > 0$, $\sigma = 5.67 \cdot 10^{-8} \text{W/m}^2 \text{K}^4$ is Stefan-Boltzmann's constant and ϵ_0 is effective emissivity of the surface.

The external surface of the plasterboard, which is not exposed to fire, transfers heat to the surroundings by means of convection and radiation. As the previous case, the boundary condition on this side is written as:

$$\kappa(u(L)) \frac{\partial u}{\partial x}(L) = h_1(u_a - u(L)) + \varphi_1(|u_a|^3 u_a - |u(L)|^3 u(L)), \text{ in } (0, T), \quad (1.5)$$

where, for all $t \in [0, T]$, $h_1(t) > 0$ is convective heat transfer coefficient between the surroundings and the plasterboard surface, $u_a(t) > 0$ is the surroundings temperature, $\varphi_1(t) = \sigma \epsilon_1(t) > 0$ and ϵ_1 is effective emissivity of the surface.

We assume that :

(H1) functions $f = (h_0, h_1)$ and $\phi = (\varphi_0, \varphi_1)$ are in $(L^2(0, T))^2$ and satisfy the following pointwise constraint

$$\begin{aligned} 0 \leq a_i \leq \varphi_i \leq b_i & \quad a.e. \ t \in (0, T), \text{ for } i = 0, 1 \\ 0 \leq c_i \leq h_i \leq d_i & \quad a.e. \ t \in (0, T), \text{ for } i = 0, 1, \end{aligned} \quad (1.6)$$

for some positive constants $a_i, b_i, c_i, d_i, i = 0, 1$,

(H2) operators $\kappa(v), \lambda(v) \in C^1(0, \infty)$ with $0 < K_0 \leq \kappa(v) \leq K_1$ and with $0 < C_0 \leq \lambda(v) \leq C_1$ for any $v > 0$.

Remark 1.2 1. *Emissivity of a material is defined as the ratio of energy radiated by a particular material to energy radiated by a black body at the same temperature. It is a dimensionless quantity (i.e. a quantity without a physical unit).*

2. *In the physical case there is not absolute values under the boundary conditions (since the temperature is non negative). For real physical data and operators λ and κ , we can prove by using the maximum principle that the temperature is positive and then we can remove the absolute values.*

3. *It is clear that we can derived easily in the same way the model in N -dimensional for $N \leq 3$ as follows*

$$\begin{aligned} \lambda(u) \frac{\partial u}{\partial t} - \operatorname{div}(\kappa(u) \nabla u) &= 0, \text{ in } \mathcal{Q}, \\ \text{under the initial condition} \\ u(., 0) &= u_0, \text{ in } \Omega, \\ \text{and boundary conditions} \\ \kappa(u) \nabla u \cdot \mathbf{n} &= h_0(u_f - u) + \varphi_0(|u_f|^3 u_f - |u|^3 u), \text{ in } \Sigma_f = \Gamma_f \times (0, T), \\ \kappa(u) \nabla u \cdot \mathbf{n} &= h_1(u_a - u) + \varphi_1(|u_a|^3 u_a - |u|^3 u), \text{ in } \Sigma_c = \Gamma_c \times (0, T), \\ \text{(and for example) } u &= u_a, \text{ in } \Sigma_s = \Gamma_s \times (0, T), \end{aligned} \quad (1.7)$$

where $\Omega \subset \mathbb{R}^N$ is an open bounded domain with boundary $\Gamma = \partial\Omega$, $\Gamma = \Gamma_c \cup \Gamma_f \cup \Gamma_s$ such that $\Gamma_c \cap \Gamma_f \cap \Gamma_s = \emptyset$, and \mathbf{n} is the outward unit normal vector on Γ . Boundaries Γ_c and Γ_f denote the cold side and the fire side, respectively, and Γ_s denotes the other surface of the plasterboard.

3. *The well-posedness of problem (1.7) in 3-dimensional, can be obtained in similar way as in [5].*

A priori, most researchers who have worked on the modeling of the behavior of gypsum board (literature in the public domain in this field is sparse, see e.g. [1, 14, 21, 3, 15, 22]), have assumed the convective heat transfer coefficients h_0 and h_1 and the relative emissivity ϵ_0 as constants or/and neglected the relative emissivity ϵ_1 on cold surface. The choice of a constant for these coefficients is not a good physical representation of plasterboard exposed to fire. Moreover, the convective heat transfer coefficients and emissivities depend, among other things, on the surface states of the external surfaces. During the exposition to fire, mechanical resistance of the external surfaces decreases and that causes appearance and growing of crazes (degradation). These modifications of surface states of the external surfaces modify convective and radiative heat transfers. Consequently, the resultant emissivities and convective heat transfer coefficients depends on temperature and large uncertainties exist in regard to the quality of the data reported. Moreover the work of [4] shows very clearly that the radiative heat transfer between the unexposed surface and the surrounding can not be neglected. Then it is necessary to estimate the convective heat transfers and the emissivity coefficients.

To satisfy this requirement, we estimate this parameters, by using inverse problem techniques as optimal control methods. It is clear that the accuracy of the parameter estimate from furnace, fire test data and target observations (or measurement results) depend significantly on the thermal characteristics

of a furnace, on the geometry of the studied element and on the input thermal properties of the material. So, it is important to have a consistent set of values for these data.

2 Inverse problem and model calibration

2.1 Problem formulation

We assume that there exists a unique solution u of problem (1.3), (1.6) with boundary conditions (1.4), (1.5), under some hypotheses for the data and some regularity of the operators λ and κ , satisfying the following regularity (by using e.g. [4] and [18]):

$$\begin{aligned} u \in L^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; L^2(\Omega)), \quad \frac{\partial u}{\partial t} \in L^2(0, T; (H^1(\Omega))'), \\ |u(0)|^3 u(0) \in L^{\frac{5}{4}}(0, T) \text{ and } |u(L)|^3 u(L) \in L^{\frac{5}{4}}(0, T). \end{aligned} \quad (2.1)$$

Introduce now the mapping \mathcal{F} which maps the source term (f, ϕ) of (1.3)-(1.5) into the corresponding solution $u = \mathcal{F}(f, \phi)$, where $f = (h_0, h_1)$ and $\phi = (\varphi_0, \varphi_1)$. In this section we formulate the inverse problem as an optimal control problem. The control procedure consists of finding the optimal controls $f^{opt} = (h_0^{opt}, h_1^{opt})$ and $\phi^{opt} = (\varphi_0^{opt}, \varphi_1^{opt})$ and the corresponding optimal temperature $u^{opt} = \mathcal{F}(f^{opt}, \phi^{opt})$ which minimize a cost criterion $J(f, \phi)$. The cost functional J measure the distance between a measured temperature (the observation u_{obs} and v_{obs}) and the corresponding predicted temperature obtained from the primal (or direct) model (1.3)-(1.5). Precisely we will study the following optimal control problem (\mathcal{P}_c):

$$\begin{aligned} \text{find } (u, f, \phi) \text{ such that the following objective function} \\ J(f, \phi) = \frac{1}{2} \int_{\mathcal{Q}} |C(u - u_{obs})|^2 dxdt + \frac{1}{2} \int_{\Omega} |D(u(T) - v_{obs})|^2 dx \\ + \frac{1}{2} \int_0^T |Mf|^2 dt + \frac{1}{2} \int_0^T |N\phi|^2 dt \\ \text{is minimized with respect to } (f, \phi) \in \mathcal{Y}_{ad} = V_{ad} \times W_{ad} \text{ subject to (1.3)-(1.5),} \end{aligned} \quad (2.2)$$

where \mathcal{Y}_{ad} is the set of admissible controls, $u = \mathcal{F}(f, \phi)$ and $M = \text{diag}(\sqrt{\alpha_0}, \sqrt{\alpha_1})$, $N = \text{diag}(\sqrt{\beta_0}, \sqrt{\beta_1})$ are predefined nonnegative weights such that $\sum_{i=0,1} (\alpha_i + \beta_i) \neq 0$. The operators C and D are unbounded operators on $L^2(\Omega)$ satisfying $(\forall v \in H^1(\Omega))$

$$\|Cv\|_{L^2(\Omega)}^2 \leq \delta_1 \|v\|_{L^2(\Omega)}^2 + \delta_2 \|v\|_{H^1(\Omega)}^2 \quad \text{and} \quad \|Dv\|_{L^2(\Omega)}^2 \leq \delta_1 \|v\|_{L^2(\Omega)}^2 + \delta_2 \|v\|_{H^1(\Omega)}^2,$$

with $\delta_1 + \delta_2 > 0$ and $\delta_i \geq 0$, for $i = 1, 2$; for example : ($C = dI$ and $D = 0$) or ($C = 0$ and $D = dI$, terminal control)

According to (1.6) the set of admissible controls describing the constraint is

$$\begin{aligned} W_{ad} = \{\phi = (\varphi_0, \varphi_1) \in (L^2(0, T))^2 \text{ such that } 0 \leq a_i \leq \varphi_i \leq b_i \quad \text{a.e. in } (0, T), \text{ for } i = 0, 1\}, \\ V_{ad} = \{f = (h_0, h_1) \in (L^2(0, T))^2 \text{ such that } 0 \leq c_i \leq h_i \leq d_i \quad \text{a.e. in } (0, T), \text{ for } i = 0, 1\}. \end{aligned}$$

2.2 First-order necessary conditions

Assume that the nonlinear control problem (2.2) admits an optimal solution (for similar result see e.g. [6] and [19]), the necessary conditions for this optimum is given by the following theorems (see e.g. [6])

Theorem 2.1 *If J attains a (local) minimum at a point $(f^*, \phi^*) \in \mathcal{Y}_{ad} = V_{ad} \times W_{ad}$, then the following first optimality conditions hold.*

$$J'(f^*, \phi^*). (f - f^*, \phi - \phi^*) \geq 0 \quad \forall (f, \phi) \in \mathcal{Y}_{ad},$$

and

$$J'(f^*, \phi^*). (g, \psi) \geq 0 \quad \forall (g, \psi) \in (L^\infty(0, T))^4 \text{ such that } \phi + \epsilon\psi \in W_{ad}, \quad f + \epsilon g \in V_{ad}, \text{ for } \epsilon \text{ small,}$$

where

$$J'(f, \phi). (g, \psi) = \frac{\partial J}{\partial f}(f, \phi). g + \frac{\partial J}{\partial \phi}(f, \phi). \psi = \lim_{\epsilon \rightarrow 0} \frac{J(f + \epsilon g, \phi + \epsilon \psi) - J(f, \phi)}{\epsilon}$$

is the directional G -derivative of J at point $(f, \phi) \in \mathcal{Y}_{ad}$ along the direction $(g, \psi) \in (L^\infty(0, T))^4$ such that $\phi + \epsilon\psi \in W_{ad}$ and $f + \epsilon g \in V_{ad}$.

In order to solve numerically the optimal control problem it is necessary to derive the gradient of the cost functional J with respect to the control (f, ϕ) . For this we suppose that the operator solution \mathcal{F} is continuously differentiable on \mathcal{Y}_{ad} and its derivative

$$w = \mathcal{F}'(f, \phi). (g, \psi) = \lim_{\epsilon \rightarrow 0} \frac{\mathcal{F}(f + \epsilon g, \phi + \epsilon \psi) - \mathcal{F}(f, \phi)}{\epsilon}$$

is the unique solution of the following system (for $f = (h_0, h_1)$, $\phi = (\varphi_0, \varphi_1)$, $g = (\eta_0, \eta_1)$ and $\psi = (\theta_0, \theta_1)$)

$$\begin{aligned} \lambda(u) \frac{\partial w}{\partial t} - \frac{\partial}{\partial x} (\kappa(u) \frac{\partial w}{\partial x}) + F(u, w) &= 0, \text{ in } \mathcal{Q}, \\ -\kappa(u(0)) \frac{\partial w}{\partial x}(0) &= -(h_0 - G(u)(0) + 4\varphi_0 |u(0)|^3)w(0) \\ &\quad + \eta_0(u_f - u(0)) + \theta_0(|u_f|^3 u_f - |u(0)|^3 u(0)), \text{ in } (0, T), \\ \kappa(u(L)) \frac{\partial w}{\partial x}(L) &= -(h_1 + G(u)(L) + 4\varphi_1 |u(L)|^3)w(L) \\ &\quad + \eta_1(u_a - u(L)) + \theta_1(|u_a|^3 u_a - |u(L)|^3 u(L)), \text{ in } (0, T), \\ w(x, 0) &= 0, \quad x \in \Omega, \end{aligned} \tag{2.3}$$

where operators F and G are defined as follows,

$$F(u, w) = \frac{\partial}{\partial t} (\lambda(u)w) - \frac{\partial}{\partial x} (w \frac{\partial}{\partial x} (\kappa(u))), \quad G(u) = \frac{\partial}{\partial x} (\kappa(u)).$$

In order to derive (2.3), we write the two systems satisfied by $u_\epsilon = \mathcal{F}(f + \epsilon g, \phi + \epsilon \psi)$ and $u = \mathcal{F}(f, \phi)$ as

$$\begin{aligned} \lambda(u_\epsilon) \frac{\partial u_\epsilon}{\partial t} - \frac{\partial}{\partial x} (\kappa(u_\epsilon) \frac{\partial u_\epsilon}{\partial x}) &= 0, \text{ in } \mathcal{Q}, \\ -\kappa(u_\epsilon(0)) \frac{\partial u_\epsilon}{\partial x}(0) &= (h_0 + \epsilon \eta_0)(u_f - u_\epsilon(0)) \\ &\quad + (\varphi_0 + \epsilon \theta_0)(|u_f|^3 u_f - |u_\epsilon(0)|^3 u_\epsilon(0)), \text{ in } (0, T), \\ \kappa(u_\epsilon(L)) \frac{\partial u_\epsilon}{\partial x}(L) &= (h_1 + \epsilon \eta_1)(u_a - u_\epsilon(L)) \\ &\quad + (\varphi_1 + \epsilon \theta_1)(|u_a|^3 u_a - |u_\epsilon(L)|^3 u_\epsilon(L)), \text{ in } (0, T), \\ u_\epsilon(x, 0) &= u_0(x), \quad x \in \Omega \end{aligned} \tag{2.4}$$

and

$$\begin{aligned} \lambda(u) \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} (\kappa(u) \frac{\partial u}{\partial x}) &= 0, \text{ in } \mathcal{Q}, \\ -\kappa(u(0)) \frac{\partial u}{\partial x}(0) &= h_0(u_f - u(0)) + \varphi_0(|u_f|^3 u_f - |u(0)|^3 u(0)), \text{ in } (0, T), \\ \kappa(u(L)) \frac{\partial u}{\partial x}(L) &= h_1(u_a - u(L)) + \varphi_1(|u_a|^3 u_a - |u(L)|^3 u(L)), \text{ in } (0, T), \\ u(x, 0) &= u_0(x), \quad x \in \Omega. \end{aligned} \tag{2.5}$$

By subtracting (2.4) from (2.5), dividing the obtained system by ϵ and letting ϵ tend to zero, the system satisfied by w , called the tangent linear model (TLM) is given by the system (2.3).

We can now show the first-order necessary conditions (optimality conditions), by using TLM and by introducing an intermediate co-state model. We introduce the following projection:

$$\Pi_{[a,b]}(\Psi) = \max(a, \min(b, \Psi))$$

where Ψ is an arbitrary function and a, b are given real constants.

Theorem 2.2 *If J attains a (local) minimum at a point $(f^*, \phi^*) \in \mathcal{Y}_{ad}$, then*

$$\begin{aligned} h_0^* &= \Pi_{[c_0, d_0]} \left(\frac{(-u_f + u^*(0))\tilde{u}^*(0)}{\alpha_0} \right), \\ h_1^* &= \Pi_{[c_1, d_1]} \left(\frac{(u_a - u^*(L))\tilde{u}^*(L)}{\alpha_1} \right), \\ \varphi_0^* &= \Pi_{[a_0, b_0]} \left(\frac{(-|u_f|^3 u_f + |u^*(0)|^3 u^*(0))\tilde{u}^*(0)}{\beta_0} \right), \\ \varphi_1^* &= \Pi_{[a_1, b_1]} \left(\frac{(|u_a|^3 u_a - |u^*(L)|^3 u^*(L))\tilde{u}^*(L)}{\beta_1} \right), \end{aligned}$$

or in the variational inequality formulation (for all $(f, \phi) \in \mathcal{Y}_{ad}$)

$$\begin{aligned} & - \int_0^T (h_1 - h_1^*) ((u_a - u^*(L))\tilde{u}^*(L) - \alpha_1 h_1^*) dt \\ & - \int_0^T (\varphi_1 - \varphi_1^*) ((|u_a|^3 u_a - |u^*(L)|^3 u^*(L))\tilde{u}^*(L) - \beta_1 \varphi_1^*) dt \\ & + \int_0^T ((h_0 - h_0^*) ((u_f - u^*(0))\tilde{u}^*(0) + \alpha_0 h_0^*)) dt \\ & + \int_0^T (\varphi_0 - \varphi_0^*) ((|u_f|^3 u_f - |u^*(0)|^3 u^*(0))\tilde{u}^*(0) + \beta_0 \varphi_0^*) dt \geq 0, \end{aligned}$$

where $u^* = \mathcal{F}(f^*, \phi^*)$, the function $\tilde{u} = \mathcal{F}^*(f, \phi)$ is the unique solution of the adjoint (co-state) problem (2.8) given below and $\tilde{u}^* = \mathcal{F}^*(f^*, \phi^*)$.

Moreover, the gradient of J at any element (f, ϕ) of \mathcal{Y}_{ad} can be given by

$$\begin{aligned} \frac{\partial J}{\partial f}(f, \phi) &= ((u_f - u(0))\tilde{u}(0) + \alpha_0 h_0, (u_a - u(L))\tilde{u}(L) + \alpha_1 h_1) \\ \frac{\partial J}{\partial \phi}(f, \phi) &= ((|u_f|^3 u_f - |u(0)|^3 u(0))\tilde{u}(0) + \beta_0 \varphi_0, (|u_a|^3 u_a - |u(L)|^3 u(L))\tilde{u}(L) + \beta_1 \varphi_1). \end{aligned}$$

Proof: By using the same technique as in e.g. [6], we start by calculating the variation of J .

According to the regularity of the operator solution \mathcal{F} and the nature of the cost function J (J is composition of differentiable mappings), we have that J is differentiable and the directional G-derivative of J at point (f, ϕ) along the direction (g, ψ) can be given by

$$\begin{aligned} J'(f, \phi).(g, \psi) &= \iint_{\mathcal{Q}} \mathcal{C}^* \mathcal{C}(u - u_{obs}) w dx dt + \int_{\Omega} \mathcal{D}^* \mathcal{D}(u(T) - v_{obs}) w(T) dx \\ &+ \int_0^T \mathcal{M}^2 f g dt + \int_0^T \mathcal{N}^2 \phi \psi dt. \end{aligned}$$

Remark 2.1 *We verify easily that*

$$\begin{aligned} \lambda(u) \frac{\partial w}{\partial t} - \frac{\partial}{\partial x} (\kappa(u) \frac{\partial w}{\partial x}) + F(u, w) &= \frac{\partial(\lambda(u)w)}{\partial t} - \frac{\partial^2}{\partial x^2} (\kappa(u)w), \\ \kappa(u(0)) \frac{\partial w}{\partial x}(0) + G(u(0))w(0) &= \frac{\partial(\kappa(u)w)}{\partial x}(0), \\ \kappa(u(L)) \frac{\partial w}{\partial x}(L) + G(u(L))w(L) &= \frac{\partial(\kappa(u)w)}{\partial x}(L). \end{aligned}$$

Now, we simplify the directional derivative of J . For this we multiply the first part of (2.3) by some regular function \tilde{u} , using Green's formula and integrating by parts in times, we obtain (since $w(., 0) = 0$)

$$\begin{aligned}
& \int_0^T \left\langle -\lambda(u) \frac{\partial \tilde{u}}{\partial t}, w \right\rangle dt - \int_0^T \left\langle \frac{\partial}{\partial x} (\kappa(u) \frac{\partial \tilde{u}}{\partial x}), w \right\rangle + \left\langle G(u) \frac{\partial \tilde{u}}{\partial x}, w \right\rangle dt \\
& \quad - \int_0^T (\kappa(u(L)) \frac{\partial w}{\partial x}(L) + G(u(L)) w(L)) \tilde{u}(L) dt \\
& \quad + \int_0^T (\kappa(u(0)) \frac{\partial w}{\partial x}(0) + G(u(0)) w(L)) \tilde{u}(0) dt \\
& \quad + \int_0^T \kappa(u(L)) \frac{\partial \tilde{u}}{\partial x}(L) w(L) dt - \int_0^T \kappa(u(0)) \frac{\partial \tilde{u}}{\partial x}(0) w(0) dt \\
& \quad + \left\langle \lambda(u(T)) \tilde{u}(T), w(T) \right\rangle = 0, \text{ in } \mathcal{Q}, \\
& -\kappa(u(0)) \frac{\partial w}{\partial x}(0) = -(h_0 - G(u(0)) + 4\varphi_0 |u(0)|^3) w(0) \\
& \quad + \eta_0(u_f - u(0)) + \theta_0(|u_f|^3 u_f - |u(0)|^3 u(0)), \\
& -\kappa(u(L)) \frac{\partial w}{\partial x}(L) = (h_1 + G(u(L)) + 4\varphi_1 |u(L)|^3) w(L) \\
& \quad - \eta_1(u_a - u(L)) - \theta_1(|u_a|^3 u_a - |u(L)|^3 u(L)), \\
& w(., 0) = 0, \text{ in } \Omega.
\end{aligned} \tag{2.6}$$

According to the second and third parts of (2.3) (boundary conditions), we can deduce that

$$\begin{aligned}
& \int_0^T \left\langle -\lambda(u) \frac{\partial \tilde{u}}{\partial t}, w \right\rangle dt - \int_0^T \left\langle \frac{\partial}{\partial x} (\kappa(u) \frac{\partial \tilde{u}}{\partial x}), w \right\rangle + \left\langle G(u) \frac{\partial \tilde{u}}{\partial x}, w \right\rangle dt \\
& \quad + \int_0^T (h_1 + 4\varphi_1 |u(L)|^3 + \kappa(u(L)) \frac{\partial \tilde{u}}{\partial x}(L)) w(L) dt \\
& \quad - \int_0^T (\eta_1(u_a - u(L)) + \theta_1(|u_a|^3 u_a - |u(L)|^3 u(L))) \tilde{u}(L) dt \\
& \quad + \int_0^T ((h_0 + 4\varphi_0 |u(0)|^3 - \kappa(u(0)) \frac{\partial \tilde{u}}{\partial x}(0)) w(0) \\
& \quad - \int_0^T (\eta_0(u_f - u(0)) + \theta_0(|u_f|^3 u_f - |u(0)|^3 u(0))) \tilde{u}(0) dt \\
& \quad + \left\langle \lambda(u(T)) \tilde{u}(T), w(T) \right\rangle = 0.
\end{aligned} \tag{2.7}$$

In order to simplify the problem (2.7), we assume that \tilde{u} satisfies the following "adjoint" (or dual) problem (with initial value given at final time T)

$$\begin{aligned}
& -\lambda(u) \frac{\partial \tilde{u}}{\partial t} - \frac{\partial}{\partial x} (\kappa(u) \frac{\partial \tilde{u}}{\partial x}) + G(u) \frac{\partial \tilde{u}}{\partial x} = \mathcal{C}^* \mathcal{C}(u - u_{obs}), \text{ in } \mathcal{Q}, \\
& -\kappa(u(0)) \frac{\partial \tilde{u}}{\partial x}(0) = -(h_0 + 4\varphi_0 |u(0)|^3) \tilde{u}, \text{ in } (0, T), \\
& \kappa(u(L)) \frac{\partial \tilde{u}}{\partial x}(L) = -(h_1 + 4\varphi_1 |u(L)|^3) \tilde{u}, \text{ in } (0, T), \\
& \lambda(u(., T)) \tilde{u}(., T) = \mathcal{D}^* \mathcal{D}(u(., T) - v_{obs}), \text{ in } \Omega.
\end{aligned} \tag{2.8}$$

Then the problem (2.7) becomes

$$\begin{aligned}
& \int_0^T \left\langle \mathcal{C}^* \mathcal{C}(u - u_{obs}), w \right\rangle dt + \left\langle \mathcal{D}^* \mathcal{D}(u(., T) - v_{obs}), w(., T) \right\rangle \\
& \quad + \int_0^T (\eta_1(u_a - u(L)) + \theta_1(|u_a|^3 u_a - |u(L)|^3 u(L))) \tilde{u}(L) dt \\
& \quad - \int_0^T (\eta_0(u_f - u(0)) + \theta_0(|u_f|^3 u_f - |u(0)|^3 u(0))) \tilde{u}(0) dt = 0.
\end{aligned} \tag{2.9}$$

According to the previous result, we can deduce that

$$\begin{aligned} J'(f, \phi).(g, \psi) &= - \int_0^T (\eta_1(u_a - u(L)) + \theta_1(|u_a|^3 u_a - |u(L)|^3 u(L))) \tilde{u}(L) dt \\ &+ \int_0^T (\eta_0(u_f - u(0)) + \theta_0(|u_f|^3 u_f - |u(0)|^3 u(0))) \tilde{u}(0) dt + \int_0^T \mathcal{M}^2 f g dt + \int_0^T \mathcal{N}^2 \phi \psi dt \end{aligned}$$

and then

$$\begin{aligned} J'(f, \phi).(g, \psi) &= \int_0^T \eta_1((u_a - u(L)) \tilde{u}(L) + \alpha_1 h_1) dt + \int_0^T \theta_1((|u_a|^3 u_a - |u(L)|^3 u(L)) \tilde{u}(L) + \beta_1 \varphi_1) dt \\ &+ \int_0^T \eta_0((u_f - u(0)) \tilde{u}(0) + \alpha_0 h_0) + \int_0^T \theta_0((|u_f|^3 u_f - |u(0)|^3 u(0)) \tilde{u}(0) + \beta_0 \varphi_0) dt. \end{aligned}$$

Consequently the gradient of J can be given by

$$\begin{aligned} \frac{\partial J}{\partial f}(f, \phi) &= ((u_f - u(0)) \tilde{u}(0) + \alpha_0 h_0, (u_a - u(L)) \tilde{u}(L) + \alpha_1 h_1), \\ \frac{\partial J}{\partial \phi}(f, \phi) &= ((|u_f|^3 u_f - |u(0)|^3 u(0)) \tilde{u}(0) + \beta_0 \varphi_0, (|u_a|^3 u_a - |u(L)|^3 u(L)) \tilde{u}(L) + \beta_1 \varphi_1). \end{aligned}$$

Since (f^*, ϕ^*) is an optimal solution of J , then according to Theorem 2.1, we have that

$$\begin{aligned} 0 &\leq J'(f^*, \phi^*).(g, \psi) \\ &= - \int_0^T \eta_1((u_a - u^*(L)) \tilde{u}^*(L) - \alpha_1 h_1^*) dt \\ &\quad - \int_0^T \theta_1((|u_a|^3 u_a - |u^*(L)|^3 u^*(L)) \tilde{u}^*(L) - \beta_1 \varphi_1^*) dt \\ &\quad + \int_0^T \eta_0((u_f - u^*(0)) \tilde{u}^*(0) + \alpha_0 h_0^*) dt \\ &\quad + \int_0^T \theta_0((|u_f|^3 u_f - |u^*(0)|^3 u^*(0)) \tilde{u}^*(0) + \beta_0 \varphi_0^*) dt. \end{aligned}$$

By using a standard control argument concerning the sign of the variations $(\eta_0, \eta_1, \theta_0, \theta_1)$ (depending, respectively, on the size of $(h_0, h_1, \varphi_0, \varphi_1)$), we obtain that

$$\begin{aligned} h_0^* &= \Pi_{[c_0, d_0]} \left(\frac{(-u_f + u^*(0)) \tilde{u}^*(0)}{\alpha_0} \right), \\ h_1^* &= \Pi_{[c_1, d_1]} \left(\frac{(u_a - u^*(L)) \tilde{u}^*(L)}{\alpha_1} \right), \\ \varphi_0^* &= \Pi_{[a_0, b_0]} \left(\frac{(-|u_f|^3 u_f + |u^*(0)|^3 u^*(0)) \tilde{u}^*(0)}{\beta_0} \right), \\ \varphi_1^* &= \Pi_{[a_1, b_1]} \left(\frac{(|u_a|^3 u_a - |u^*(L)|^3 u^*(L)) \tilde{u}^*(L)}{\beta_1} \right). \end{aligned}$$

This completes the proof.

We point out that the adjoint problem (2.8), which is backward in time, can be transformed into an initial-boundary value problem by the time transformation $t := T - t$, which allows to employ [4] for the existence of a unique solution of (2.8) for a sufficiently regular data.

2.3 Optimization procedure

By using the successive resolutions of both the direct problem and the adjoint problem, we can therefore calculate the gradient of the objective function relative to the control parameters $f = (h_0, h_1)$ and $\phi = (\varphi_0, \varphi_1)$. Once the gradient of the objective function J , ∇J , is known, we can seek a minimum of J . For a given observation (u_{obs}, v_{obs}) , the optimization algorithm is summarized in Table.1.

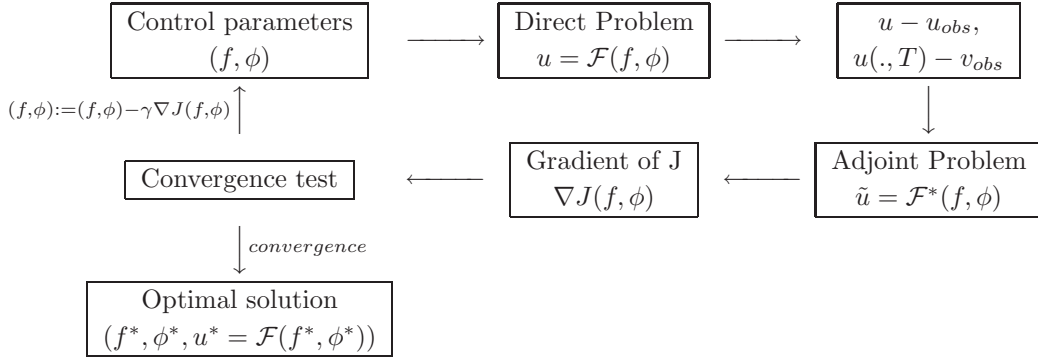


Table 1: Optimization algorithm : J is minimized until some convergence criteria are attained.

3 Numerical analysis and simulations

In this section, we assume that the functions φ_0 and φ_1 are fixed (unless otherwise) and we seek to estimate only the parameters h_0 and h_1 . In order to facilitate the presentation we denote by η the control function which plays the role of h_i , for $i = 0$ or 1 , according to the considered application example. Moreover, we assume that the operator \mathcal{C} is the identity function and the operator $\mathcal{D} = 0$. So, the cost function J becomes

$$J(\eta) = \frac{1}{2} \|u - u_{obs}\|_{L^2(\mathcal{Q})}^2 + \frac{\alpha_i}{2} \|\eta\|_{L^2(0,T)}^2, \quad \text{for } i = 0 \text{ or } 1 \quad (3.1)$$

where u is the solution of the direct problem corresponding to the control function η which will be denoted in the sequel by $\mathcal{F}(\eta)$. Then, the expression of the corresponding gradient can be given by

$$\begin{aligned} g = \nabla J(\eta) &= [u_f - u(0, \cdot)] \tilde{u}(0, \cdot) + \alpha_0 \eta & \text{if } i = 0, \\ g = \nabla J(\eta) &= [u_a - u(L, \cdot)] \tilde{u}(L, \cdot) + \alpha_1 \eta & \text{if } i = 1, \end{aligned} \quad (3.2)$$

where \tilde{u} is the solution of adjoint problem (2.8), corresponding to the direct model.

3.1 Numerical implementation and outline

As noted in the previous subsection, the resolution of the nonlinear boundary control problem (2.2) by a gradient method requires, at each iteration of the optimization algorithm, the resolution of the direct problem and its corresponding adjoint problem. In order to solve numerically these two problems, we use first the discretization in space with Lagrange finite elements of order 2 and the derived differential systems are integrated by using variable-order, variable-step-size backward differentiation formulas [7]. Finally the obtained non linear algebraic systems are solved with a Newton's Method [12] and at each iteration, a direct method is used to solve the considered linear system. In order to solve the optimization problems, we have used the Gradient Method (GM) and the Conjugate Gradient Method (GCM). For the GCM method we have considered the following well-known descent direction methods : Fletcher-Reeves, Polak-Ribière, Hestenes-Stiefel and the recent method of Dai and Yuan [11]. More precisely, for $k=1, \dots$ (the iteration index), we denote by $g^{(k)}$ the numerical approximation of the gradient function g (given by (3.2)), $d^{(k)}$ the descent direction, ρ_k the descent step and η_k the numerical approximation of the control function η , at the k th iteration of the algorithm, the considered gradient schemes are as follows:

1. Initialization: η_0 (given)

- (a) Resolution of the direct problem gives $u_0 = \mathcal{F}(\eta_0)$.
 - (b) Resolution of the adjoint problem gives \tilde{u}_0 .
 - (c) Gradient of J at η_0 , $g^{(0)}$ is given by (3.2).
 - (d) Determine the direction : $d^{(0)} = -g^{(0)}$.
 - (e) Determine $\eta_1 = \eta_0 + \rho_0 d^{(0)}$ and initialization $k = 1$.
2. Resolution of the direct problem, where the source term is η_k , gives $u_k = \mathcal{F}(\eta_k)$.
 3. Resolution of the adjoint problem gives \tilde{u}_k .
 4. Gradient of J at η_k , $g^{(k)}$ is given by (3.2).
 5. Determine the direction $d^{(k)}$ by one of the following expressions (where $(\cdot; \cdot)$ and $\| \cdot \|$ are the scalar product and its associated norm) :

Method	Notation	Descent direction	Parameter
Gradient	$Grad$	$d^{(k)} = -g^{(k)}$	-----
Fletcher-Reeves	$GCFR$	$d^{(k)} = -g^{(k)} + \beta_{k-1} d^{(k-1)}$	$\beta_{k-1} = \frac{\ g^{(k)}\ ^2}{\ g^{(k-1)}\ ^2}$
Polak-Ribieres	$GCPR$	$d^{(k)} = -g^{(k)} + \beta_{k-1} d^{(k-1)}$	$\beta_{k-1} = \frac{(g^{(k)} - g^{(k-1)}; g^{(k)})}{\ g^{(k-1)}\ ^2}$
Hestenes-Stiefel	$GCHS$	$d^{(k)} = -g^{(k)} + \beta_{k-1} d^{(k-1)}$	$\beta_{k-1} = \frac{(g^{(k)}; g^{(k)} - g^{(k-1)})}{(d^{(k-1)}; g^{(k)} - g^{(k-1)})}$
Dai-Yuan	$GCDY$	$d^{(k)} = -g^{(k)} + \beta_{k-1} d^{(k-1)}$	$\beta_{k-1} = \frac{\ g^{(k)}\ ^2}{(d^{(k-1)}; g^{(k)} - g^{(k-1)})}$

6. Determine the descent step ρ_k by the following methods :

Method	Notation	Description
Constant step	$cst\rho$	$\rho_k = \rho$
Decreasing step	$dim\rho$	$\rho_0 = \rho$, $\rho_k = \frac{\rho_{k-1}}{2}$ if $J(\eta_k) > J(\eta^{(k-1)})$ (not changed else)
Minimum step	min	$\rho_k = \min(1, \frac{1}{\ g^{(k)}\ _\infty})$
Optimal step	opt	ρ_k is an approximate solution of $\min_{\rho \geq 0} J(\eta_k + \rho d^{(k)})$

7. Determine $\eta_{k+1} = \eta_k + \rho_k d^{(k)}$
8. IF the gradient is sufficiently small THEN end; ELSE set $k:=k+1$ and GOTO 2. The approximation of the optimal solution η^* is η_k .

Remark 3.1 If the exact control function η_{ex} is known, we can measure the efficiency of the method with the following relative error on η_k :

$$errel(\eta_k) = \frac{\|\eta_{ex} - \eta_k\|_{L^2(\mathcal{Q})}}{\|\eta_{ex}\|_{L^2(\mathcal{Q})}}. \quad (3.3)$$

Then, to solve the optimal control problem (2.2), we have developed a specific software, based on Comsol and Matlab tools and their bi-directional link, taking into account on : first, the nature of the nonlinearity in the operators λ and κ , and the nonlinear radiative term on the boundary of the domain,

second, the nature of the adjoint problem which is backward in time and coupled with the direct problem. In order to validate our approach, we have studied several examples in different situations and by using different descent direction methods for the optimization algorithm. In this paper we present only two application examples and a realistic simulation model. For the first application, we consider the model without the radiative boundary conditions and we assume that the observation u_{obs} is a given function. In the second one, the observation is deduced from the resolution of the model with the radiative boundary conditions, corresponding to given convective heat transfer parameters. For the realistic situation, we consider the real parameters and data given in [4, 21] and we construct the observation model as in the second application.

The numerical simulations are performed on a computer with a processor 2.8 GHz Core 2 Duo and 4 Go memory and take between 1400 and 2200s for 50 optimization iterations (depending on the descent direction method and on the treated example).

3.2 Numerical examples and validation

In this section, we denote by η_{ex} the exact value of the control function η that we want approximate by η_k , at the k th iteration of the gradient algorithm. Moreover, we assume $T = L = 1$ and we fix the time step δt and space step δx to 10^{-3} .

3.2.1 Examples without radiation conditions

Example 3.2.1.1 : Control on the convective heat transfer coefficient h_1

In this example, the control function η plays the role of h_1 , the observation is the given function $u_{obs} = e^{t+L-x}$ and $\eta_{ex}(= h_1) = 1 + \cos(t)$. The other operators and data of the model are given by: $h_0 = 1$, $\varphi_0 = \varphi_1 = 0$, $\lambda(u) = 1 + u$, $\kappa(u) = 1 + u^2$, $u_0(x) = e^{L-x}$, $u_f(t) = [2 + e^{2(t+L)}] e^{t+L}$, $u_a(t) = \left[1 - \frac{1 + e^{2t}}{1 + \cos t}\right] e^t$ and the source term $F = e^{2(t+L-x)}(1 - 3e^{t+L-x})$ added to the equation (1.3) as

$$\lambda(u) \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} (\kappa(u) \frac{\partial u}{\partial x}) = F$$

to ensure that u_{obs} is a solution of the direct problem (corresponding to η_{ex}).

Remark 3.2 *We want to emphasize on the fact that the addition of the source term F does not change the definition of the adjoint problem, the expression of the gradient of the objective function, nor the optimization algorithm.*

To validate our approach, we have tested all the gradient methods described above. With all these gradient methods we get computed values η_k which converge towards the exact value η_{ex} : the relative error (3.3) decreases when k increases (see Figures 1, 2, 3). But the convergence speed depends on the method and on the initial value. So, we are going to discuss these two points.

First, to use the optimization algorithm we have chosen an initial value η_0 for the control function η . We present on Figure 1 the convergence curves, $\log_{10}(errel(\eta_k))$ versus k , for different initializations and on Figure 2 the function $\eta_k(t)$ for some k (computed with the GCDYOPT method : Dai-Yuan Conjugate Gradient with optimal step) and for the following initializations: (a) $\eta_0 = 2.2$, (b) $\eta_0 = \eta_{ex}(0)$, (c) $\eta_0 = 1.7$, (d) $\eta_0 = \eta_{ex}(T)$, (e) $\eta_0 = 1$, (f) $\eta_0 = \frac{(\eta_{ex}(T) - \eta_{ex}(0))t}{T} + \eta_{ex}(0)$. As expected, the method converge for each initialization and the convergence speed depends on the proximity of the initial value

η_0 from the exact value η_{ex} but the best accuracy that can be obtained with the method depends on the gap between $\eta_0(T)$ and $\eta_{ex}(T)$.

Indeed, for each graphic on Figure 2, we note that $\eta_k(T) = \eta_0$ for each k : the last value of η_k is never modified. For this kind of optimization problem, there is not final observation and the gradient (like the descent direction) is always zero for $t = T$. Then the parameter can not be well approximated near the final time T . Of course, this has no effect when the initialization $\eta_0 = \eta_{ex}(T)$ is chosen (see figure 2-(d)) or when the initialization is a continuous function with $\eta_0(T) = \eta_{ex}(T)$ (see figure 2-(f)). It is why, on Figure 1, the best accuracy is obtained for $\eta_0 = \eta_{ex}(T)$ and $\eta_0 = \frac{(\eta_{ex}(T) - \eta_{ex}(0))t}{T} + \eta_{ex}(0)$.

From a physical point of view, the good choice for the initial value can be η_0 such that $\eta_0(0) = \eta_{ex}(0)$ because the parameters are assumed known at ambient temperature (corresponding to $t = 0$). In an other way to study the convergence of the method, to avoid the effect to the absence of final observation, it is interesting to use $\eta_0 = \eta_{ex}(T)$. It is why, we use these two possibilities or an intermediate value for the next examples.

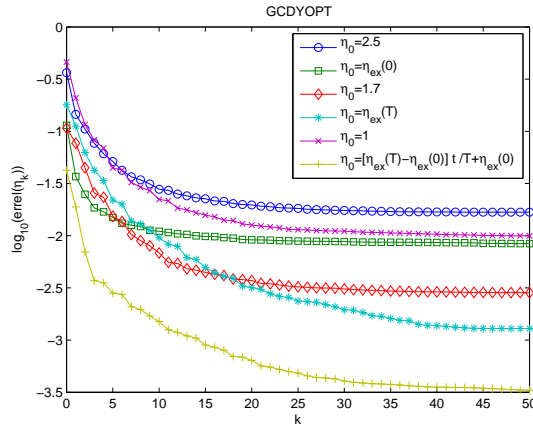


Figure 1: Example 3.2.1.1 - $\log_{10}(\text{errel}(\eta_k))$ versus k for different initializations

To compare the different gradient methods, we fix the initialization to $\eta_0 = \eta_{ex}(T)$ and we present on Figure 3-(a) the convergence curves, $\log_{10}(\text{errel}(\eta_k))$ versus k , for the GCPR Method with different optimization steps, and on Figure 3-(b) the convergence curves for the different gradient methods with optimal step. Numerical values can be found in Table 2. We conclude that the choice of the optimal step gives a significant improvement compared to other possibilities. As expected the Conjugate Gradient Methods have a better convergence speed than the gradient method. Among the Conjugate Gradient Methods, the Dai-Yuan method seems the better choice because it gives the better result for almost all iterations. This is in agreement with the literature results in optimization. It is why we present mainly the results for this method for the next examples.

Example 3.2.1.2 : Control on the convective heat transfer coefficient h_0

To explore the difference between the control on the cold side of the domain ($x = L$) and the control on the hot side of the domain ($x = 0$), the control function η plays now the role of h_0 . We consider the same data as in the previous example except for the values of h_0 and h_1 that are exchanged $\eta_{ex}(= h_0) = 1 + \cos(t)$, $h_1 = 1$ and the related data $u_f(t) = \left[1 + \frac{1 + e^{2(t+L)}}{1 + \cos t}\right] e^{t+L}$, $u_a(t) = -e^{3t}$.

Following the study of the initialization in the previous example, we present here results for only one initialization. The control function η is initialized to an arbitrary value between the minimum and the

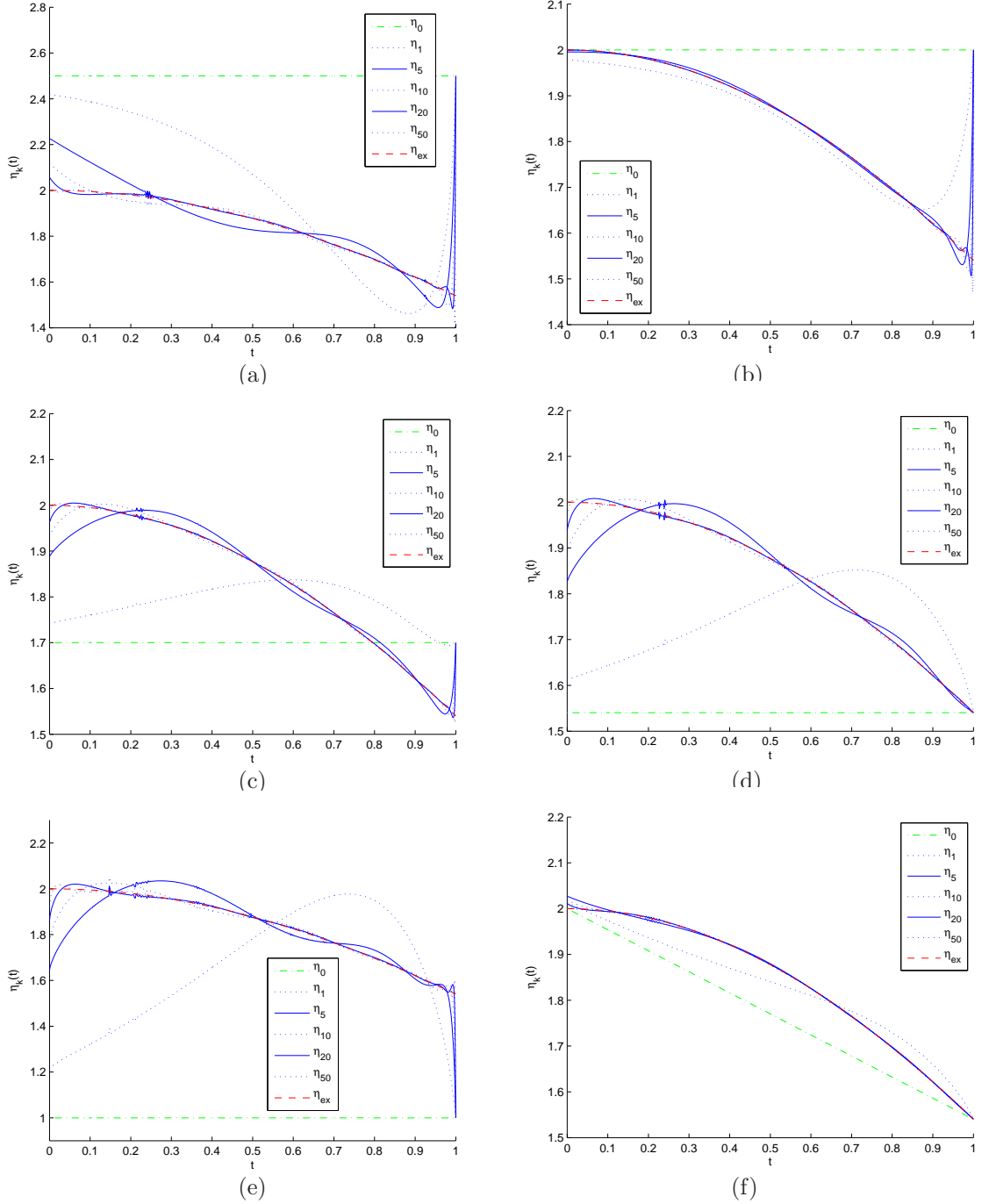


Figure 2: Example 3.2.1.1 - $\eta_k(t)$ for some k with different initializations : (a) $\eta_0 = 2.2$, (b) $\eta_0 = \eta_{ex}(0)$, (c) $\eta_0 = 1.7$, (d) $\eta_0 = \eta_{ex}(T)$, (e) $\eta_0 = 1$, (f) $\eta_0 = \frac{(\eta_{ex}(T) - \eta_{ex}(0))t}{T} + \eta_{ex}(0)$.

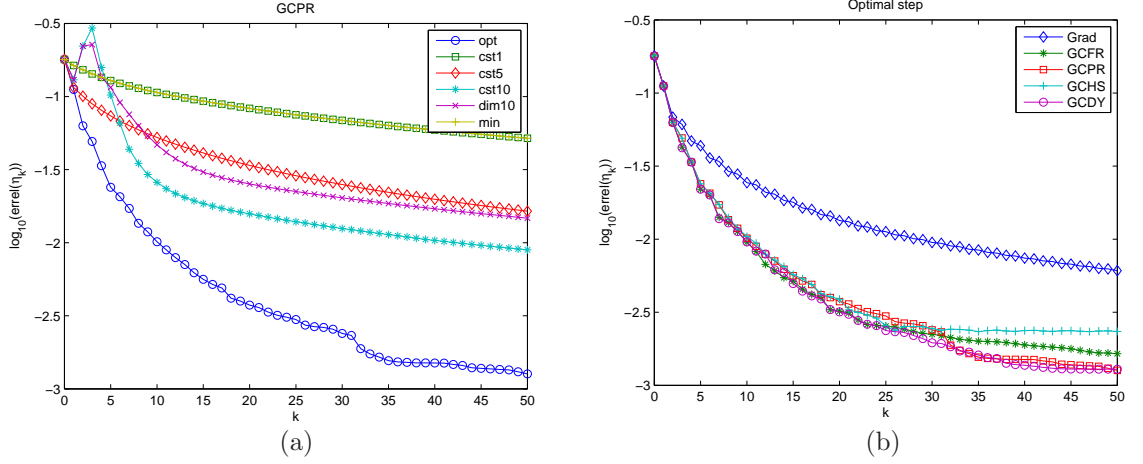


Figure 3: Example 3.2.1.1 - $\log_{10}(errel(\eta_k))$ versus k with (a) GCPR method and different optimization steps, (b) an optimal step and different gradient methods.

maximum of η_{ex} on $[0, T]$: $\eta_0 = 1.7$. On Figure 4-(a) are plotted the convergence curves, $\log_{10}(errel(\eta_k))$ versus k , for three gradient methods with optimal step. We check that the GCDYOPT method is always the best choice. We present on Figure 4-(b) the function $\eta_k(t)$ for some k computed with the GCDYOPT method. These results are similar to those of the previous example. Numerical values can be found in Table 2.

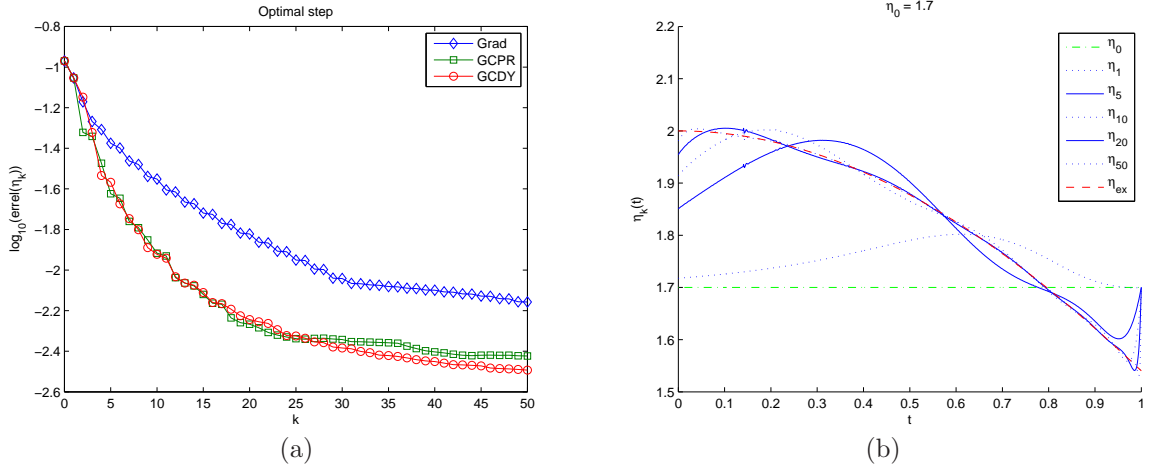


Figure 4: Example 3.2.1.2 - (a) $\log_{10}(errel(\eta_k))$ versus k with an optimal step and different gradient methods, (b) $\eta_k(t)$ for some k with the GCDYOPT method.

3.2.2 Examples with radiation conditions

For this second kind of tests, there is no more analytical expression for the observation u_{obs} which is now computed as the solution of the direct problem (1.3)-(1.4)-(1.5) with the exact value η_{ex} of the control function η . Then, solving the control problem from an initialization η_0 of η , we compute approximations η_k of η_{ex} using the GCDYOPT method.

k	Example 3.2.1.1	Example 3.2.1.2
0	$1.7956e - 01$	$1.0733e - 01$
1	$1.1184e - 01$	$8.8416e - 02$
5	$2.1982e - 02$	$2.7083e - 02$
10	$9.5890e - 03$	$1.1958e - 02$
20	$3.1778e - 03$	$5.7010e - 03$
50	$1.2304e - 03$	$2.4576e - 03$

Table 2: Relative error on η_k for some k with the GCDYOPT method.

Example 3.2.2.1 : Control on the convective heat transfer coefficient h_1

With the data $h_0 = 1$, $h_1 = 1 + \cos(t)$, $\varphi_0 = \varphi_1 = 10^{-4}$, $\lambda(u) = 1 + u$, $\kappa(u) = 1 + u^2$, $u_a = 10$, $u_f(t) = 20 + \ln(t)$, $u_0 = u_a$, we compute the observation u_{obs} , as numerical solution of (1.3)-(1.4)-(1.5). It is a problem with radiation boundary conditions.

The observation being known on the boundary and because of the time dependence of h_0 and h_1 , we can consider an optimization problem without radiation condition on the boundary. Indeed, the boundary conditions of the direct problem become

$$\begin{aligned} -\kappa(u(0)) \frac{\partial u}{\partial x}(0) &= H_0(u_f - u(0)), \text{ in } (0, T), \\ \kappa(u(L)) \frac{\partial u}{\partial x}(L) &= H_1(u_a - u(L)), \text{ in } (0, T), \end{aligned}$$

with

$$\begin{aligned} H_0 &= h_0 + \varphi_0(u_f + u_{obs})(u_f^2 + u_{obs}^2), \\ H_1 &= h_1 + \varphi_1(u_a + u_{obs})(u_a^2 + u_{obs}^2). \end{aligned}$$

The functions h_0 and H_0 , h_1 and H_1 are compared on Figure 5.

In this example, the control function η plays the role of H_1 with $\eta_{ex} = H_1$ and we solve the same optimization problem as in Example 3.2.1.1 with $F = 0$ and (h_0, h_1) replaced by (H_0, H_1) . The functions u_{obs} and u_a being known, we can deduce φ_1 from H_1 and h_1 , or h_1 from H_1 and φ_1 .

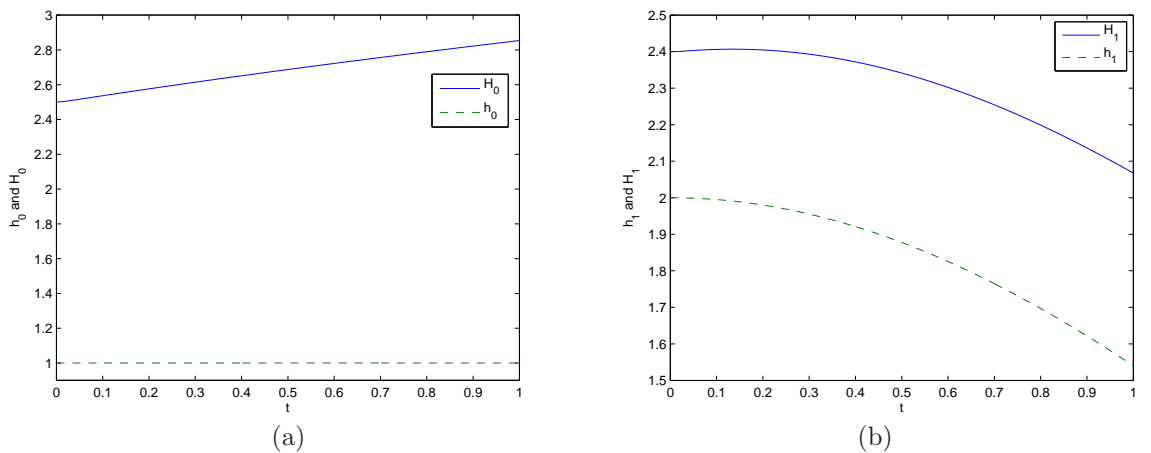


Figure 5: Example 3.2.2.1 - Comparing data (a) h_0 and H_0 , (b) h_1 and H_1 .

For the two different initializations $\eta_0 = \eta_{ex}(0)$ and $\eta_0 = \eta_{ex}(T)$, we present on Figure 6 the convergence curves, $\log_{10}(errel(\eta_k))$ versus k , and on Figure 7 the function $\eta_k(t)$ for some k . We observe that the result is better if we initialize our algorithm with $\eta_0 = \eta_{ex}(0)$ (instead of $\eta_0 = \eta_{ex}(T)$). It can be explained by the fact that for $\eta_0 = \eta_{ex}(T)$ we observe that η_k is not changed for t small because without a source term in the equation (1.3), the value of H_1 , used in the boundary condition at the point $x = L$, has not a significant effect immediately on u . This comes from the fact that the source term u_f is only on the boundary at the point $x = 0$, and there is a delay depending on the parameters of the equation. We check in the next example that there is no more delay when the source term and the control are at the same point $x = 0$. Numerical values can be found in Table 3.

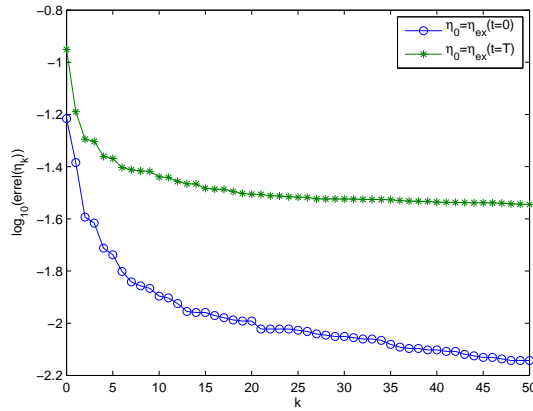


Figure 6: Example 3.2.2.1 - $\log_{10}(errel(\eta_k))$ versus k , with with 2 different initializations.

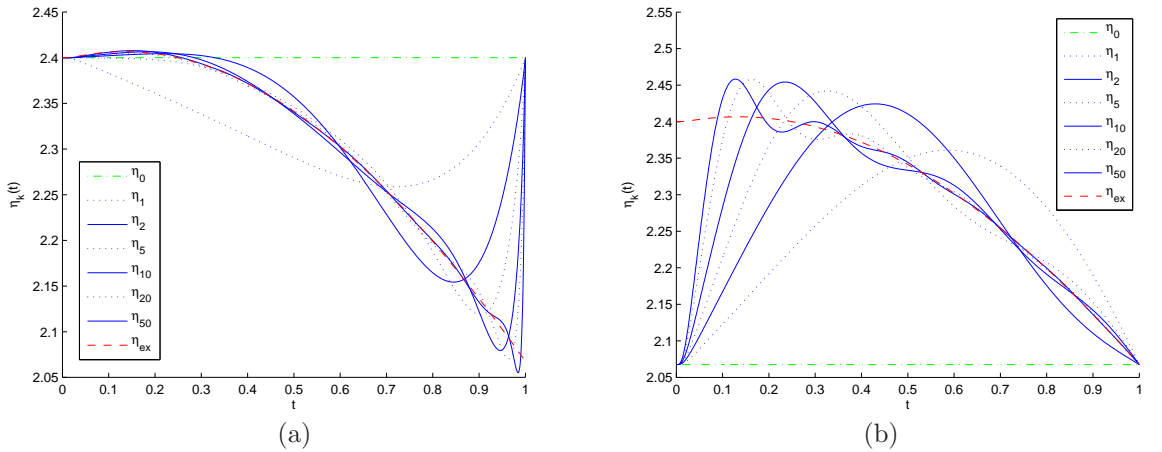


Figure 7: Example 3.2.2.1 - $\eta_k(t)$ for some k with (a) $\eta_0 = \eta_{ex}(0)$ and (b) $\eta_0 = \eta_{ex}(T)$.

Example 3.2.2.2 : Control on the convective heat transfer coefficient h_0

The control function plays now the role of H_0 with $\eta_{ex} = H_0$. The data is the same than for Example 3.2.2.1.

For the two different initializations $\eta_0 = \eta_{ex}(0)$ and $\eta_0 = \eta_{ex}(T)$, we present on Figure 8 the convergence curves, $\log_{10}(errel(\eta_k))$ versus k , and on Figure 9 the function $\eta_k(t)$ for some k . We check

that with the source term and the control at the same point $x = 0$, there is not the delay of the previous example and the result is better for $\eta_0 = \eta_{ex}(T)$, the rapid convergence coming from the big dependance of u from H_0 . Numerical values can be found in Table 3.

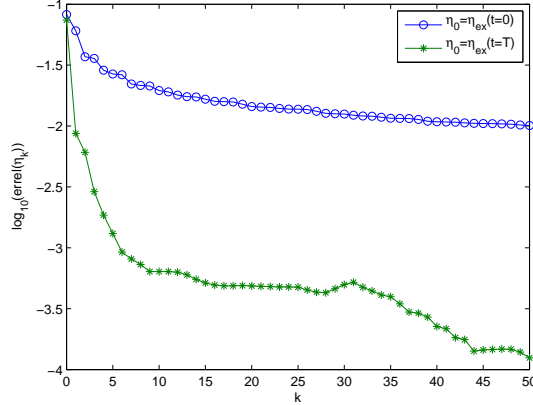


Figure 8: Example 3.2.2.2 - $\log_{10}(\text{errel}(\eta_k))$ versus k , with 2 different initializations.

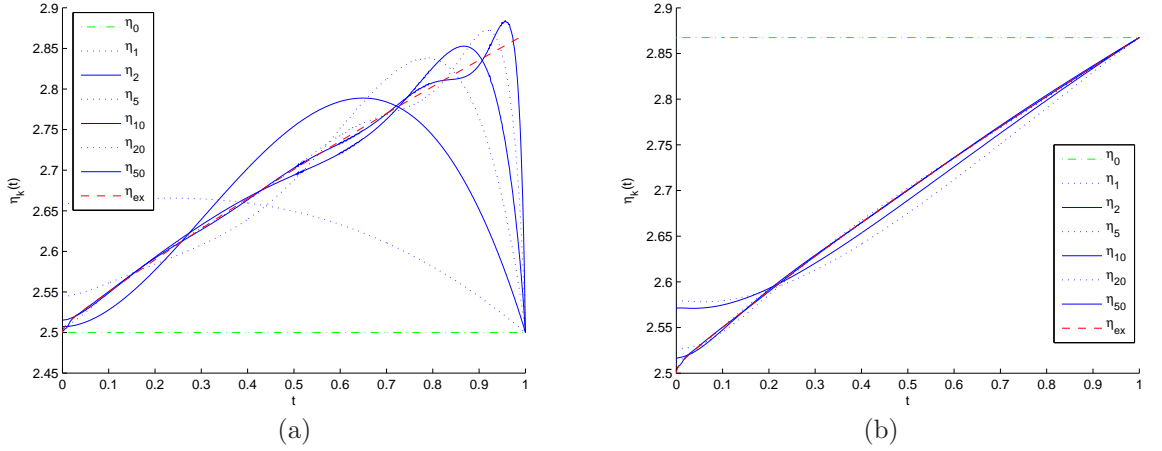


Figure 9: Example 3.2.2.2 - $\eta_k(t)$ for some k with (a) $\eta_0 = \eta_{ex}(0)$ and (b) $\eta_0 = \eta_{ex}(T)$.

3.3 Simulation on real data

We now apply our method to a realistic problem. To that purpose, we take similiary data as in [4, 21]. We consider a gypsum plasterboard, with thickness $L = 4\text{ cm}$, exposed to fire in $x = 0$, during $T = 1200\text{ s}$. The surroundings temperature is $u_a = 20^\circ\text{C}$ and the furnace temperature is $u_f = u_a + 345 \log_{10}(1 + \frac{8t}{60})$ (see Figure 10). The initial temperature is $u_0 = u_a$. The thermal conductivity is given by

$$\kappa(u) = \begin{cases} 0.25 & \text{if } u < 112.5^\circ\text{C}, \\ 0.1116 + 6.578 \cdot 10^{-5}u & \text{if } 112.5^\circ\text{C} \leq u < 393.75^\circ\text{C}, \\ 0.0277 + 2.788 \cdot 10^{-4}u & \text{if } 393.75^\circ\text{C} \leq u < 797.2^\circ\text{C}, \\ -0.91323 + 1.459 \cdot 10^{-3}u & \text{if } 797.2^\circ\text{C} \leq u. \end{cases}$$

k	Example 3.2.2.1 $\eta_0 = \eta_{ex}(t = T)$	Example 3.2.2.1 $\eta_0 = \eta_{ex}(t = 0)$	Example 3.2.2.2 $\eta_0 = \eta_{ex}(t = T)$	Example 3.2.2.2 $\eta_0 = \eta_{ex}(t = T)$
0	$1.1210e - 01$	$6.0811e - 02$	$7.3971e - 02$	$8.2286e - 02$
1	$6.4723e - 02$	$4.1257e - 02$	$8.6915e - 03$	$6.0451e - 02$
5	$4.2787e - 02$	$1.8325e - 02$	$1.3104e - 03$	$2.6765e - 02$
10	$3.6398e - 02$	$1.2723e - 02$	$6.3730e - 04$	$1.9551e - 02$
20	$3.1214e - 02$	$1.0177e - 02$	$4.8591e - 04$	$1.4462e - 02$
50	$2.8538e - 02$	$7.1703e - 03$	$1.1368e - 04$	$1.0078e - 02$

Table 3: Relative error on η_k for some k with the GCDYOPT method.

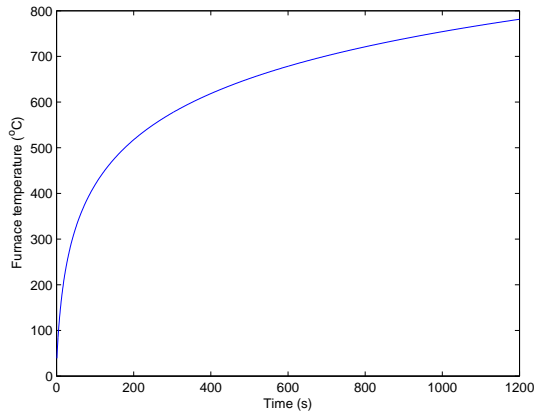


Figure 10: Furnace temperature versus time.

We have $\lambda(u) = \rho(u)C_p(u)$ where the density is defined by

$$\rho(u) = \begin{cases} 648 & \text{if } u < 120^\circ C, \\ 534.6 & \text{if } 120^\circ C \leq u \leq 650^\circ C, \\ 500.6 & \text{if } 650^\circ C < u \end{cases}$$

and the specific heat is defined with a peak between 100 and 170°C, and a value corresponding to the total amount of energy of the two dehydration reactions, 669kJ:

$$C_p(u) = \begin{cases} \frac{6.69 \cdot 10^4}{7} & \text{if } 100^\circ C \leq u \leq 170, \\ 950 & \text{else .} \end{cases}$$

We supposed that the convective heat transfer coefficient $h_1 = 5$ and the effective emissivity $\epsilon_1 = 0.82$ are known in $x = L$. We deduce $\varphi_1 = \sigma\epsilon_1$ with $\sigma = 5.6697 \cdot 10^{-8} W/m^2 K^4$ the Stefan-Boltzmann's constant.

We want to estimate h_0 , supposing $\epsilon_0 = 0$ on the furnace side. The control function η plays here the role of h_0 . We choose the following exact expression for h_0 : $\eta_{ex}(= h_0) = 25 + \cos(t/T)$. Then we can compute the observation u_{obs} as the solution of the direct problem (1.3), solve the control problem (2.2) (with the cost function and its gradient given by (3.1) and (3.2)) by the optimization algorithm (using the GCDYOPT method) and compute error estimations on the control function η at each optimization iteration.

Following [4], we choose discretization steps respecting the CFL condition : $\delta x = 0.02 \text{ cm}$ as space step and $\delta t = 1 \text{ s}$ as time step.

First, we study the dependance of the problem with the regularization parameter α_0 and present in Figure 11 the value $\log_{10}(\text{errel}(\eta_k))$ for $k = 10$ and for different values of α_0 . The best choice is here around 10^{-7} and we present for this value on Figure 12-(a) the convergence curve, $\log_{10}(\text{errel}(\eta_k))$ versus k , and on Figure 12-(b) the function $\eta_k(t)$ for some k . Numerical values can be found in Table 4.

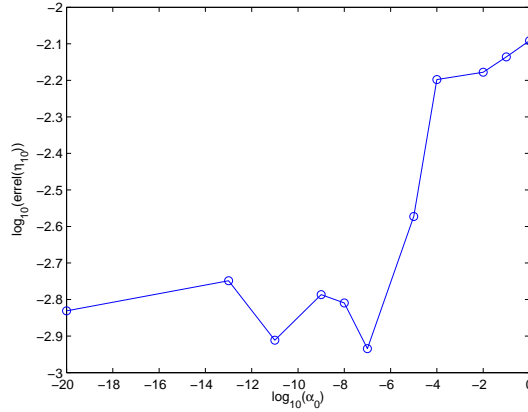


Figure 11: Variations of the regularization parameter - $\log_{10}(\text{errel}(\eta_{10}))$ versus α_0 .

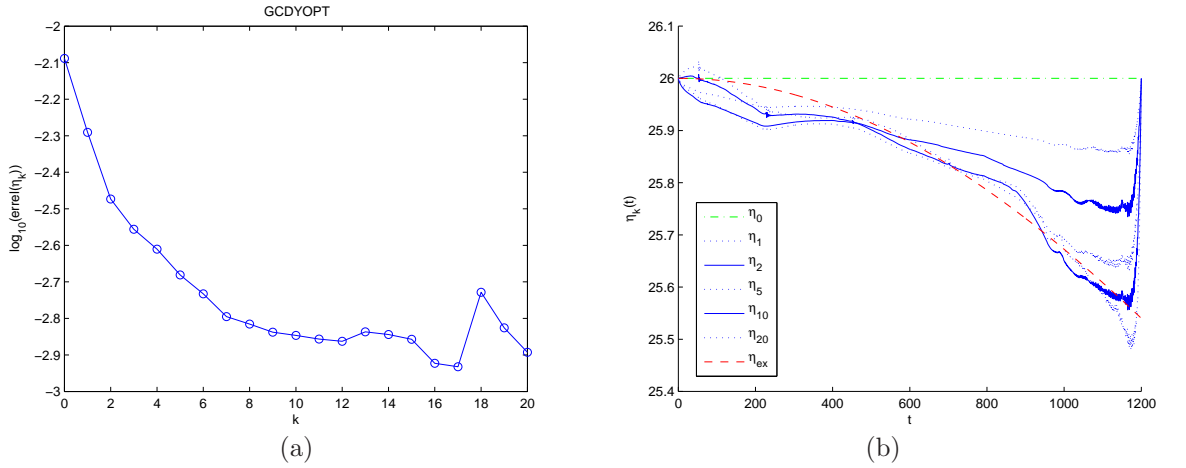


Figure 12: Simulation on real data with $\alpha_0 = 10^{-7}$: (a) $\log_{10}(\text{errel}(\eta_k))$ versus k , (b) $\eta_k(t)$ for some k .

k	Real data (for $\eta_0 = \eta_{ex}(t = 0)$)
0	$8.1570e - 03$
1	$5.1219e - 03$
5	$2.0838e - 03$
10	$1.4236e - 03$
20	$1.2511e - 03$

Table 4: Relative error on η_k for some k with the GCDYOPT method.

4 Conclusion

Optimal boundary heating control strategies for time-dependent thermal problems in spatially 1-dimensional domains, related to dehydration of gypsum plasterboards exposed to fire, are developed. Optimal heating strategies and calibration of process models (parameter identification) are obtained as solutions of certain minimization problems and are computed from conjugate gradient method by considering the following well-known descent direction methods : Fletcher-Reeves, Polak-Ribière, Hestenes-Stiefel and Dai and Yuan. Other choices of control variables can be envisaged. The numerical results show the efficiency of the developed method. It would be interesting in a next study to use this method with observations coming from experimental data.

In order to take into account the influence of noises and fluctuations, we can also study robust control problems by using the approach developed in Belmiloudi's Book [6].

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