Implementation of a conjugate gradient algorithm for thermal diffusivity identification in a moving boundaries system

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Abstract. The aim of this paper is to investigate the thermal diffusivity identification of a multilayered material dedicated to fire protection. In a military framework, fire protection needs to meet specific requirements, and operational protective systems must be constantly improved in order to keep up with the development of new weapons. In the specific domain of passive fire protections, intumescent coatings can be an effective solution on the battlefield. Intumescent materials have the ability to swell up when they are heated, building a thick multilayered coating which provides efficient thermal insulation to the underlying material. Due to the heat aggressions (fire or explosion) leading to the intumescent phenomena, high temperatures are considered and prevent from linearization of the mathematical model describing the system state evolution. Previous sensitivity analysis has shown that the thermal diffusivity of the multilayered intumescent coating is a key parameter in order to validate the predictive numerical tool and therefore for thermal protection optimisation. A conjugate gradient method is implemented in order to minimise the quadratic cost function related to the error between predicted temperature and measured temperature. This regularisation algorithm is well adapted for a large number of unknown parameters.

1. Introduction

Fire protection technologies mainly consist in two kinds of approaches:

- active fire protections, such as alarm systems, water sprinklers or automatic extinguishers, which are triggered in a specific area when fire is detected, due to smoke emission or temperature elevation,
- passive fire protections, which are designed to minimise the impact of fire. They can consist in architectural dispositions in buildings (fire doors, stairways pressurisation, …). Insulating coatings and radiation reflectors are also considered as passive fire protections.

Complete fire safety systems generally involve a combination of active and passive fire protection devices. During the intumescing process, the paint’s chemical structure undergoes strong modifications, similar to phase change transformations, leading to successive apparition of a viscous layer and a carbonised layer [1]. In order to assess the relevance of their use in military applications, intumescent paints were tested experimentally using a 45 kW solar furnace, capable of reproducing
thermal effects of several typical aggressions in combat conditions (strong fires, explosions, ...).
Simultaneously, a mathematical model describing the mechanical and thermal behavior of an in
turescent coating under high thermal fluxes was developed [2]. Temperature evolution and
protection predictions based upon such a numerical tool depend on model parameters inaccuracies. It
has been previously shown that the thermal diffusivity of the moving layers is a key parameter [3].
Thus, an identification process is investigated. Many well-known identification methodologies are
based on the observation of a material’s thermal behavior exposed to a calibrated excitation (heat
pulse, periodic flux, etc.) [4]. The material’s geometry is usually assumed not to be time dependent. In
the studied configuration, the thermal diffusivity has to be identified in a swelling material and the
complexity induced by moving boundaries has to be taken into account. Thermal diffusivity has to be
carefully discretized ; in fact, inturescent phenomenon is irreversible and strongly connected to the
amount of thermal energy brought to the material. For situations where this parameter depends on
temperature (and can also be spatial or time dependent) the discretization leads to a large number of
unknown coefficients. The context of inverse problems for partial differential equations [5] is widely
investigated in thermal sciences. Even for non linear system and large number of unknown
coefficients, the conjugate gradient algorithm [6] is efficient to achieve convergence in a reasonable
time (a complete illustration is given for example in [7]). It is important to notice that the system’s
input (heat flux delivered on the inturescent layer’s front face) has to be well known, but any spatial
distribution and time dependent flux can be considered.

The following paragraph is focused on inturescent paint and mathematical model for temperature
evolution prediction. Then, implementation of the conjugate gradient algorithm is exposed: resolution
of direct problem (thermal, mechanical and chemical processes are described by coupled partial
differential equations), the adjoint problem and the sensitivity problem.

2. Direct problem

2.1. About inturescent paints

Inaturescent coatings can be adapted to a wide range of materials, such as buildings, vehicles or
missiles. Inaturescent paints react when exposed to thermal aggressions, and develop a thick
multilayered coating, which structure evolves through the reactive process from one to three stratified
layers (figure 1). The first original layer, made of ablative paint, melts into a viscous reactive layer
which releases gases and swells up because of gas pressure. This reaction ends when the heat flux
stops or when the ablative layer is depleted. If the aggression heats the exposed face of the reactive
layer to a sufficient temperature, it turns into a solidified carbonaceous layer. Chemical composition
and reactive process are detailed in [1]. An example of temporal evolution of the system structure is
described in figure 2.

![Figure 1. Cross section view of a fully developed inaturescent paint on a steel plate](image)

![Figure 2. Steps of the intumescenting process under heat aggression.](image)
2.2. Thermal model

Temperature at point of depth $x$ at time $t \in T = [0, t_f]$ is denoted by $\theta (x, t)$. In order to evaluate protection provided by intumescent paint, temperature evolution of the coated structure (steel plate $x \in [0, p]$) has to be described. The active coating is a multilayered system, consisting of a regressing layer (original ablative paint layer $x \in ]p, f(t)[$) and an expanding layer (combining the viscous swelling layer and the carbonaceous layer $x \in ]f(t), g(t)[$).

Let us consider the notations given in table 1 and the partial differential equations system (1-9) detailed in [8].

| Notation Parameter                          | Unit                        |
|-------------------------------------------|-----------------------------|
| $\theta_v$ vaporisation temperature       | (K)                         |
| $\dot{\rho}$ local losses                 | (kg.m$^{-3}$.s$^{-1}$)      |
| $\rho_a$ ablative material density        | (kg.m$^{-3}$)               |
| $A$ pre-exponential factor                 | (s$^{-1}$)                  |
| $E$ activation energy of the pyrolysis reaction | (J.mol$^{-1}$)           |
| $\rho_s C_s, \rho_a C_a, \rho_v C_v, \rho_c C_c$ volumic heat | (J.m$^{-3}$.K$^{-1}$)          |
| $\lambda_s, \lambda_a, \lambda_v, \lambda_c$ thermal conductivity | (W.m$^{-1}$.K$^{-1}$) |
| $L_v$ vaporisation enthalpy                | (J.kg$^{-1}$)               |
| $\theta_c$ swelling layer carbonisation temperature | (K)                      |
| $h_h, h_f$ heat exchange coefficient       | (W.m$^{-2}$.K$^{-1}$)       |
| $\Phi$ time dependent heating flux.       | W.m$^2$                     |
| $\alpha_f$ front face absorptivity        |                            |
| $k_f, k_g$ moving boundaries coefficients |                            |
Both interfaces (steel / ablative coating and ablative coating / growing layer) are assumed to be perfect contacts. Therefore, hypothesis of gradients and temperature continuity is considered. The previous coupled equations systems (ordinary differential equations for the free boundaries evolution (1-3) ; conduction equations (4-6) for the thermal evolution within \( \partial \); boundaries conditions (7-8) ; initial condition (9)) are numerically implemented using a finite element method (Comsol® software). An example of numerical results is given in figure 4 for a set of realistic parameters. Presented configuration is steel plate 2mm thick, initial intumescent coating 1mm thick. One can observe the swelling layer (after 8 s) and the thermal insulating effect of the expanding foam.

In the following paragraph, parametric identification is investigated in order to improve model adequacy.

3. Inverse problem
A previous preliminary sensitivity analysis based on numerical design of experiment [9] has been performed in order to list input parameters whose uncertainties are crucial for results predicted by mathematical model (1-9). Let us focused on some parameters which are not accurately defined in literature.

- \( \theta_s \), \( \theta \), A, E and \( L_o \) can be measured for a given intumescent paint by thermal and chemical approaches,
- \( k_f \) can be investigated by measuring mass losses evolution \( \rho \) during material ablation,
- \( k_g \) can be obtained by measuring the free boundary position,
- \( \rho_x C_a \) and \( \lambda_g \) are the thermal properties of the virgin intumescent paint and can be measured by several methods until the vaporisation temperature \( \theta \geq \theta_v \) is not reached.
\( \rho, C, \lambda \) and \( \lambda \) are the thermal properties of the carbonaceous foam which can be obtained at the end of a sufficient thermal aggression \( \theta \geq \theta \). Since such a porous material is stable (but fragile), studied parameters can be measured by specific techniques dedicated to porous media.

The main difficulty is the identification of \( \rho, C, \lambda \) and \( \lambda \), thermal properties of the viscous layer which is quite difficult to obtain without ablative or carbonaceous layers and whose both boundaries can move (ablative/viscous and viscous/carbonaceous). Let us denote by \( \frac{\lambda(\theta)}{\rho C_v} \) in m².s⁻¹, the thermal diffusivity which is the key parameter under interest in the following. Unknown parameter \( a(\theta) \) is regularly discretized on \( \theta \in [\theta_1, \theta_2] \) (in configuration presented in figure 4, \( \theta_1 = 453 \text{K} \) and \( \theta_2 = 600 \text{K} \)). Thus, the unknown parameter is denoted by \( \bar{a} = (a_i)_{i=1,\ldots,N} \). In order to identify \( \bar{a} \), the following methodology is proposed. A steel plate coated by an intumescent coating is exposed to a calibrated heat flux so as to maintain the viscous layer as long as possible and to deplete the ablative layer and form the carbonaceous foam as late as possible. Temperature is measured on the steel plate rear face \((x=0)\) : \( \hat{\theta}(t) \) is the measured temperature at instant \( t \). If all the parameters are known (excepted \( a \)), the inverse problem \( P_{in} \) can be defined as follows

\[
\text{Problem } P_{in} = \min_{\bar{a} \in \mathbb{R}^N} J(\bar{a}) \quad \text{where} \quad J(\bar{a}) = \frac{1}{2} \int \left( \theta(0,t;\bar{a}) - \hat{\theta}(t) \right)^2 dt \quad \text{with} \quad \theta(0,t;\bar{a}) \quad \text{solution of (1)-9}
\]

For a large number \( N \) of unknown parameters \( a \), for non linear direct problem (1-9) and for ill-posed problem defined as \( P_{in} \), the conjugate gradient method (CGM) can be efficient for identification purposes :

CGM Algorithm :
(a) initialization \( n = 0 \) ; let us denote by \( \bar{a}^0 \) the given initial approximation of \( \bar{a} \) and 
\[
\bar{d}^0 = -\nabla J(\bar{a}^0) = - \left( \frac{\partial J}{\partial a_i} \right) \quad \text{the initial descent direction,}
\]
(b) at iteration \( n \), from point \( \bar{a}^n \), the next point is obtained : 
\[
\bar{a}^{n+1} = \bar{a}^n + \gamma_n \bar{d}^n 
\]
where \( \gamma_n = \arg \min_{\gamma \in \mathbb{R}} J(\bar{a}^n + \gamma \bar{d}^n) \). The next direction is defined by : 
\[
\bar{d}^{n+1} = -\nabla J(\bar{a}^{n+1}) + \beta_n \bar{d}^n 
\]
with :
\[
\beta_n = \frac{\|\nabla J(\bar{a}^{n+1})\|^2}{\|\nabla J(\bar{a}^n)\|^2} .
\]
(c) stopping of the iterative process if \( J(\bar{a}^{n+1}) \leq J_{adm} \) or : \( n \leftarrow n + 1 \) and go to (b).

where \( J_{adm} \) is the admissible threshold for the minimization of the quadratic cost function \( J(\bar{a}) \).

For the calculation of descent direction (also called conjugate direction), gradient \( \nabla J(\bar{a}^n) \) is obtained from the resolution of the adjoint problem and the descent depth \( \gamma_n \) is obtained by solving the sensitivity problem. In the following, sensitivity, adjoint and adjoint problems are briefly defined.
### 3.1. Sensitivity problem

At each iteration of the minimization algorithm, descent depth $\gamma_n$ is:

$$
\gamma_n = \arg\min_{\gamma \in \mathbb{R}} \left( \frac{1}{2} \int_t \left( \theta(0,t;\bar{a}^n + \gamma \bar{d}^n) - \hat{\theta}(t) \right)^2 \, dt \right)
$$

(10)

Solution of (10) is $\gamma_n = \frac{\int_t (\delta \theta(0,t;\bar{a}^n) \left( \theta(0,t;\bar{a}^n) - \hat{\theta}(t) \right) \, dt}{\int_t (\delta \theta(0,t;\bar{a}^n))^2 \, dt}$ where the sensitivity function is defined as follows: $\delta \theta(0,t;\bar{a}^n) = \lim_{\mu \to 0} \frac{\delta \theta_{\mu^2}(0,t)}{\mu} = \lim_{\mu \to 0} \frac{\theta(0,t;\bar{a}^n + \mu \bar{d}^n) - \theta(0,t;\bar{a}^n)}{\mu}$. In this formula, $(\delta \theta)_{\mu^2}$ is the temperature variation resulting from the variation $\mu \bar{d}^n$.

Equations (1-9) for the solution: $\theta^* = \theta(x,t;\bar{a}^n + \mu \bar{d}^n)$ are written as:

- $\forall (x,t) \in p, f^+(t)[\times T] \quad \rho^+(\theta^*(x,t)) = \begin{cases} 
0 & \text{if } \theta^*(x,t) < \theta_i \\
-\rho A \exp\left(\frac{-E}{8.31 \theta^*(x,t)}\right) & \text{if } \theta^*(x,t) \geq \theta_i
\end{cases}$

(11)

- $\forall t \in T \quad \hat{f}^+ = -k f \frac{\rho^+(\theta^*(x,t))}{\rho_a} \, dx$

(12)

- $\forall t \in T \quad \hat{g}^+ = k_j \hat{f}^+$

(13)

- $\forall (x,t) \in ]0,p[\times T \quad \rho_c \frac{\partial \theta^*(x,t)}{\partial t} - \text{div} \left( \frac{\lambda_c}{\partial \theta^*(x,t) \text{grad} \theta^*(x,t)} \right) = 0$

(14)

- $\forall (x,t) \in ]p,f^+(t)[\times T \quad \rho_c \frac{\partial \theta^*(x,t)}{\partial t} - \text{div} \left( \frac{\lambda_c}{\partial \theta^*(x,t) \text{grad} \theta^*(x,t)} \right) = -\lambda^+ \rho^+(\theta^*(x,t))$

(15)

- $\forall (x,t) \in ]f^+(t),g^+(t)[\times T \quad \frac{\partial \theta^*(x,t)}{\partial t} - \text{div} \left( \frac{\lambda^+(\theta^*) + \mu \delta \theta^*}{\partial \theta^*(x,t) \text{grad} \theta^*(x,t)} \right) = 0$ if $\theta^*(x,t) < \theta_i$

(16)

- $\lambda^+(\theta^*) \frac{\partial \theta^*(x,t)}{\partial x} = h_c (\theta^*) (\theta^*(x,t) - \theta_{es}) - \alpha \Phi(t)$

(17)

- $\forall t \in T \quad \lambda_c (\theta^*) \frac{\partial \theta^*(x,t)}{\partial x} = h_c (\theta^*) (\theta^*(x,t) - \theta_{es})$

(18)

- $\forall x \in [0,e], \quad t = 0 \quad \theta^*(x,0) = \theta_{es}, f(0) = e, g(0) = e$

(19)

For more academic situations, it is usual to subtract both systems and considering while $\mu \to 0$, a set of sensitivity equations which is easily obtained. In the studied configuration, moving boundaries are different for each system: $\left[p,f(t)\right] \neq \left[p,f^+(t)\right], \left[f(t),g(t)\right] \neq \left[f^+(t),g^+(t)\right]$ and boundary
conditions (7), (17) are not considered on the same point. This inherent characteristic avoid an easy formulation of a classical sensitivity problem as in [10]. Then, a numerical way is chosen : for a given value of parameter $\mu$ (close to zero) solution of the previous system (11-19) is calculated with the same finite element method implemented for direct problem resolution (Comsol® software). An approximation of the sensitivity function at iteration $n$ is

$$\delta \theta(0,t;\bar{a}^n) = \frac{\theta^\star(0,t; \bar{a}^n + \mu \bar{a}^n) - \theta(0,t;\bar{a}^n)}{\mu}.$$  

Parameter $\mu$ is fixed such as $\delta \theta(0,t;\bar{a}^n)$ estimation does not depend on numerical error. In the following paragraph, adjoint problem for the cost-function gradient $\nabla J(\bar{a}^n)$ estimation is briefly presented in order to determine the conjugate direction $\bar{d}^n$.

3.2. Adjoint problem

The gradient is obtained by solving the Lagrange equation associated to the cost function minimization problem:

$$\ell(\theta,a,\psi) = \frac{1}{2} \int_0^T \left( \left( \theta(x,t) - \hat{\theta}(t) \right)^2 \delta_\theta(x) dt \right) + \int_0^T \left( \frac{\partial \theta}{\partial t} \right)_t - \nabla \theta \cdot \nabla \theta + B(\theta) \right) \psi dt dx \quad (20)$$

where $\delta_\theta(x)$ the sensor Dirac distribution and

$$\forall x \in [0,p[, \quad A(\theta) = \frac{\lambda_\theta(\theta)}{\rho a C_a}, \quad B(\theta) = 0$$

$$\forall x \in [p,f(t)], \quad A(\theta) = \frac{\lambda_\theta(\theta)}{\rho a C_a}, \quad B(\theta) = \frac{L, \dot{\rho}(\theta(x,t))}{\rho a C_a}$$

$$\forall x \in [f(t),g(t)], \quad A(\theta) = \begin{cases} \alpha(\theta) = \frac{\lambda_\theta(\theta)}{\rho a C_a} & \text{if } \theta(x,t) < \theta_c, \\
\frac{\lambda_\theta(\theta)}{\rho a C_a} & \text{else} \end{cases} \quad B(\theta) = 0$$

$\psi(x,t)$ is a Lagrange multiplier. When $\psi$ is fixed then : $\delta \ell = \frac{\partial \ell}{\partial \theta} \delta \theta + \frac{\partial \ell}{\partial a} \delta a$. Moreover, the Lagrange multiplier $\psi(x,t)$ is fixed such that $\frac{\partial \ell}{\partial \theta} \delta \theta = 0 \quad , \quad \forall \delta \theta$. Then the following adjoint problem has to be solved (once the temperature $\theta$ and geometry ($f(t)$ and $g(t)$) evolutions are computed thanks to the direct problem resolution):

$$\forall (x,t) \in [0,g(t)] \times T, \quad \frac{\partial \psi}{\partial t} - A(\theta) \Delta \psi + \psi \frac{\partial B(\theta)}{\partial \theta} = \hat{\theta} - \theta \delta \theta(x) \quad (21)$$

$$x = \{0, g(t)\}, \quad \forall t \in T, \quad \psi(0,t) = \frac{\partial \psi(0,t)}{\partial x} = 0 \quad ; \quad \psi(g(t),t) = \frac{\partial \psi(g(t),t)}{\partial x} = 0 \quad (22)$$

$$\forall x \in [0, g(t)], \quad \psi(x,t_f) = 0 \quad (23)$$

Considering $\theta(x,t)$ the computed solution of the direct problem, then $\ell(\theta,\psi,a) = J(a)$, it becomes : $\delta J = \delta L$ and
\[
\frac{\partial J}{\partial a} = -\int \int \frac{\partial \theta}{\tau(t)} \frac{\partial \psi}{\partial x} \xi(\theta) dt dx
\]  

(24)

where \( \xi(\theta) = \begin{cases} 1 & \text{if } \theta(x,t) < \theta_i \\ 0 & \text{else} \end{cases} \). Numerical resolution of system (21-23) leads to the Lagrange multiplier \( \psi(x,t) \) estimation (the same finite element method implemented for direct problem and sensitivity problem resolution is implemented). Then, (24) is considered for the gradient calculation and both descent direction and descent depth is computed as required for CGM algorithm previously presented.

4. Concluding remarks
In this communication, a conjugate gradient method has been proposed for the resolution of an inverse problem in a moving geometry.

The main difficulty is encountered for the sensitivity problem formulation. This is due to the moving geometry which depends on the unknown thermal diffusivity. A way to overcome this specificity could be to estimate temperature evolution in the moving layers through a Landau transformation in order to convert the variable volume to a constant volume. Thus, the sensitivity function could be calculated \( \forall (x,t) \in ]0,g(t)\times ]0,t_f[ \) and formulation of boundaries condition (22) is simplified for the adjoint problem.

Experimentations are actually in progress using a 45 kW solar furnace in order to measure temperature evolution on the non irradiated face of the coated steel plate.

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