

# INVERSE METHOD FOR PYROLYSABLE AND ABLATIVE MATERIALS

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In the framework of aerospace vehicles design, the thermal protection system is one of the most critical parts of the spacecraft. Atmospheric re-entry missions often rely on its robustness. For such missions, the mass balance is also a challenge and an optimal sizing of the heat shield is of great interest. Therefore, the high level of aerothermal heat fluxes encountered during the descent has to be well known but is in flight only available by indirect methods based on temperature measurements.

ASTRIUM Space Transportation has developed for many years a transient one-dimensional thermal model with one moving boundary (ablative surface). This "direct" simulation tool has been used to model complex chemical processes such as pyrolysis or ablation on thermal protection materials.

The present work deals with inverse analyses used to evaluate highly evolutive heat fluxes. This restitution is based on temperature measurements on thermal protection along a flight trajectory or during ground tests. An inverse problem has been formulated, developed and applied to estimate transient surface heat fluxes (convection coefficient), which are input data parameters for the direct code.

The inverse problem is formulated as a minimization problem involving an objective functional, through an optimization loop. An optimal control formulation (Lagrangian, adjoint and gradient steepest descent method combined with quasi-Newton method computations) has been used, resulting in MONOPYRO inverse code, derived from the already existing and operational direct thermal solver.

To compute numerically the adjoint and gradient quantities, both an analytical manual differentiation and an Automatic Differentiation (AD) engine tool (TAPENADE, developed at INRIA Sophia-Antipolis by the TROPICS team) have been used. Automatic differentiation is a family of techniques for computing the derivatives of a function defined instruction by instruction in a computer program, for sensitivity and gradient analysis applications. Several validation test cases, using synthetic temperatures measurements are carried out, by applying the results of the inverse method with minimization algorithm.

Accurate results of identification on high fluxes test cases and good agreement for temperatures restitutions are obtained, without and with ablation and pyrolysis, using bad values of fluxes as initial guesses. First encouraging results with an automatic differentiation procedure are also presented.

**KEYWORDS:** Inverse Problem, Ablation, Pyrolysis, Thermal Protection, Re-Entry, Optimal Control, Adjoint, Gradients, Optimization, Automatic Differentiation

## Introduction

The success of atmospheric re-entry missions is bound to the design of the Thermal Protection System (TPS) of the aerospace vehicles involved. The high level of heat fluxes encountered in such missions has a direct effect on mass balance of the heat shield. Consequently, the identification of heat fluxes is of great industrial interest but is in flight only available by indirect methods based on temperature measurements. A more detailed description of the problem can be found for instance in some publications on the Atmospheric Reentry Demonstrator (ARD) [1], [2]. The difficulty with flight data is that the uncertainty on the heat flux is coupled with an uncertainty coming also from the material (thermal properties for instance). In this contribution, we restrict ourselves to a supposed well known complex degradable material (with ablation and pyrolysis) and study in details the modeling and identification of thermal fluxes. A lot of studies on degradable materials can be found for pyrolysis and ablation processes and the corresponding applications, like on-ground validations with arc plasma torch, or various work on Thermal Protection Systems and reentry vehicles design. Many authors have already addressed the so-called Inverse Heat Conduction problem, and the estimation of fluxes from temperature measurements [3], [4], [5].

The inverse problem in this paper is concerned with the estimation of time domain surface heat fluxes convection coefficient, for thermally degradable material (ablation and pyrolysis processes), on a one-dimensional slab of thickness  $e$ , by using time domain temperature measurements on thermal protection, taken below the boundary surface, at thermocouple position  $x_0$ , during the time interval  $0 \leq t \leq t_f$ , where  $t_f$  denotes the final time. This inverse problem is formulated as a minimization problem involving a least square problem through an optimization loop. An optimal control formulation (Lagrangian, adjoint and gradient computations, [6]) is then applied and implemented for the optimal control theory on some industrial applications of inverse problems at EADS (European Aeronautics Defense and Space Company) [7].

## Direct problem

For the direct problem, the Monopyro direct and inverse code, which was developed at EADS Astrium-ST Les Mureaux, is used. It is a transient one-dimensional thermal software with one moving boundary (ablative surface) to model complex chemical processes of simultaneous heating, ablation, pyrolysis, thermal degradation of materials [8], [9], [10]. The internal energy balance is a transient conduction equation with additional pyrolysis terms:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) + \left[ F_v + h_g - \int_{T_0}^T A_1 dT \right] \frac{\partial \rho}{\partial t} + \frac{\partial(\dot{m}_g h_g)}{\partial x} \quad (1)$$

with  $x$  the abscissa,  $t$  the time,  $T(x,t)$  the temperature,  $\rho(x,t)$  the specific mass,  $C_p$  the heat capacity,  $\lambda$  the thermal conductivity,  $F_v$  the pyrolysis gas formation heat,  $\dot{m}_g$  the pyrolysis gas mass flow rate,  $h_g$  the pyrolysis gas enthalpy,  $A_1$  a function of temperature  $T$ . The rate of storage of sensible energy is balanced by the net rate of thermal conductive heat flux, the pyrolysis energy-consumption rate and the net rate of energy convected by pyrolysis gas. The evolution of specific mass is given by a first-order rate process based on the Arrhenius equation :

$$\frac{1}{\rho_v} \cdot \frac{\partial \rho}{\partial t} = - \left( \frac{\rho - \rho_c}{\rho_v} \right)^{np} \cdot A \cdot e^{-\frac{B}{T}} \quad (2)$$

$\rho_c$  and  $\rho_v$  are the charred and virgin material densities,  $A$  the frequency factor in pyrolysis,  $B$  the fictitious temperature in pyrolysis,  $np$  the order of the reaction. The pyrolysis gas mass flow rate is related to the decomposition by the simple mass balance:

$$\frac{\partial \rho}{\partial t} = \frac{\partial \dot{m}_g}{\partial x} \quad (3)$$

Let  $s$  be the abscissa of the moving interface (ablation value), then  $\dot{s}$  is the recession rate. The physical process can be splitted in three kinds of ablation:  $\dot{s}_{meca}$  the mechanical recession rate,  $\dot{s}_{chem}$  the chemical recession rate (most of the time a tabulated function), and  $\dot{s}_{hy}$  the hydroerosion recession rate. The surface energy balance on the moving boundary takes the following form:

$$\alpha_0(h_r - h_w) - \varepsilon\sigma(T_w^4 - T_r^4) + \dot{m}_g[H_c - \eta_1(h_r - h_w)] + \dot{m}_c[H_v - \eta_2(h_r - h_w)] = \lambda \frac{\partial T}{\partial x} \quad (4)$$

with  $\alpha_0(t)$  the convection coefficient (unknown for the inverse problem),  $h_r$  the athermanous enthalpy,  $h_w$  the surface enthalpy,  $\varepsilon$  the total emissivity,  $\sigma$  the Stefan-Boltzmann constant,  $T_w$  the surface temperature,  $T_r$  the equivalent temperature,  $\eta_1$  the pyrolysis gas blocking factor,  $H_c$  the pyrolysis gas heat combustion,  $\dot{m}_c$  the ablation mass flow rate,  $\eta_2$  the ablation gas blocking factor,  $H_v$  the ablation heat. The first term of equation (4) is the convective heat flux, the second one represents the heat loss by re-radiation of the surface. The third and fourth terms are the contributions of pyrolysis and ablation gas respectively. The right hand of (4) represents the rate of conduction into the TPS. Let  $U = \begin{pmatrix} T \\ s \end{pmatrix}$  be the vector of temperatures  $T$  and ablation  $s$ , functions of time  $t$  and position  $x$ . The direct problem can be represented in condensed vector form by the following system of coupled nonlinear time domain evolution differential equations:

$$\frac{dU}{dt} = F(U) \quad T(x,0) = T_0 \quad s(x,0) = 0 \quad t \in [0, t_f] \quad x \in [s(t), e] \quad (5)$$

where  $F(U)$  is a non linear operator and  $T_0$  the reference initial temperature. The other physical quantities and variables described above are hidden in the formulation of  $F$ . Space partial derivatives are computed with a centered finite difference type scheme. The abscissa  $x$  belongs to the interval  $[s(t), e]$ . It is parameterized by a reduced scaled space variable  $\xi \in [0,1]$   $x = (1-\xi)s(t) + \xi e$

The system (5) is rewritten relatively to the variables  $(t, \xi)$  with implicit Euler scheme and a constant time step  $\Delta t$ . Let  $K$  denote the number of one-dimensional grid points,  $k$  the space index,  $N$  the number of time iterations,  $n$  the time index in the numerical scheme,  $u = (u^1, \dots, u^K)$  the discrete direct state variables with the discrete vector  $u^n = (T_1^n, T_2^n, \dots, T_K^n, s^n)$  of dimension  $(K+1)$ ,  $T_m^n$  the discrete computed temperature at time  $n$ , at grid point  $m$ ,  $s^n$  the discrete computed ablation, at time  $n$ . The equation (5) is written at time  $(n+1)$  :

$$\frac{u^{n+1} - u^n}{\Delta t} = f(u^{n+1}) \quad u^0 = 0 \quad 0 \leq n \leq N \quad (6)$$

We make a linearization of the equation (6) at time  $n$  and after some calculations, we finally obtain a forward time discrete linearized Euler scheme, with initial vanishing condition. To solve the discrete matrix problem, we use an adapted sparse solver.

## Inverse problem

The aim of the inverse problem in this paper is to estimate time domain surface heat fluxes (convection coefficient), for degradable material (ablation and pyrolysis), on a one-dimensional slab of thickness  $e$ , by using time domain temperature measurements  $\theta(t)$  on thermal protection, taken below the boundary surface, at thermocouple position  $x_0$ , during the time interval  $0 \leq t \leq t_f$ , with  $t_f$  the final time. The inverse problem is formulated as a minimization problem involving a cost objective functional, through an optimization loop, requiring the computation of derivatives or gradients quantities and adjoint variables (optimal control formulation).

For a good accurate approximation of the gradient, the key strategy is to compute the exact gradient of the discretized problem, instead of applying a discretization scheme to the above systems of PDE-s. Let us consider that the time domain heat flux convection coefficient is represented by a vector  $p = (p^1, \dots, p^N)$ , where the subscripts refer to the sampled time. These sampled values are the *control parameter variables* for the optimization process. The quadratic error or cost function  $J(p)$ , which measures the difference between model predictions  $T_m^n$  of temperature, given a heat flux parameter  $p$  value, and measurements temperatures  $\theta_m^n$ , depending on the source parameters ( $p$ ), is defined by :

$$J(p) = J(\underbrace{u^1(p), \dots, u^N(p)}_{\text{variables } U}) = \frac{1}{2} \sum_{n=1}^N (T_m^n - \theta_m^n)^2 \Delta t \quad (7)$$

To minimize this quantity, by optimization algorithm, we need to compute the derivatives of this least squares objective function  $J(p)$ , with respect to the parameters  $p$ .

We introduce the adjoint state matrix  $u^* = (u^{*1/2} \dots; u^{*N+1/2})$  adjoint of the direct state  $u$ ,  $u^{*n+1/2}$  being a vector  $(K+1) \times 1$ , for all  $n=0, N$ . A Lagrangian formalism is used in the minimization of the functional  $J(p)$  because the estimated dependent variable  $u(p)$  appearing in such functional  $J(p)$  needs to satisfy a constraint, which is the solution of the discrete direct problem. The governing equation of the direct problem, is therefore multiplied by the Lagrange multiplier, integrated in the space and time domains and added to the original cost functional  $J(p)$ . The Lagrangian  $L$  is :

$$L(p, u, u^*) = L \left( \underbrace{p^1, \dots, p^N}_{\text{parameter } p}, \underbrace{u^1, \dots, u^N}_{\text{variables } u}, \underbrace{u^{*1/2}, \dots, u^{*N+1/2}}_{\text{adjoint variables } u^*} \right) \quad (8)$$

$$= \sum_{n=1}^N (T_m^n - \theta_m^n)^2 \Delta t + \sum_{n=0}^{N-1} \left\langle u^{*n+1/2}, \frac{u^{n+1} - u^n}{\Delta t} - f(u^n) - (df)(u^n)(u^{n+1} - u^n) \right\rangle$$

Differentiating the Lagrangian  $L$  with first order variations  $\delta p, \delta u, \delta u^*$ , the variations of  $\delta L$  with respect to  $\delta u$  are cancelled with an adequate choice of the adjoint state  $u^*$  (saddle point condition). It leads to the discrete adjoint system in  $u^{*n-1/2}$  unknown,  $n$  going backward from  $N$  to  $0$ ,

$$\frac{u^{*n-1/2} - u^{*n+1/2}}{\Delta t} = df^t(u^{n-1})u^{*n-1/2} + [(d^2 f)(u^n)(u^{n+1} - u^n)]u^{*n+1/2} + (T_m^n - \theta_m^n) \Delta t \quad (9)$$

$$u^{*N+1/2} = 0 \quad N \geq n \geq 0$$

With this particular choice of  $u^*$ , the gradient of the cost function is simply obtained by :

$$\nabla J = \frac{\partial J}{\partial p} = \frac{\partial L}{\partial p} = \sum_{n=0}^{N-1} \left\langle u^{*n+1/2}, -\frac{\partial f}{\partial p}(u^n) - \frac{\partial df}{\partial p}(u^n)(u^{n+1} - u^n) \right\rangle \quad (10)$$

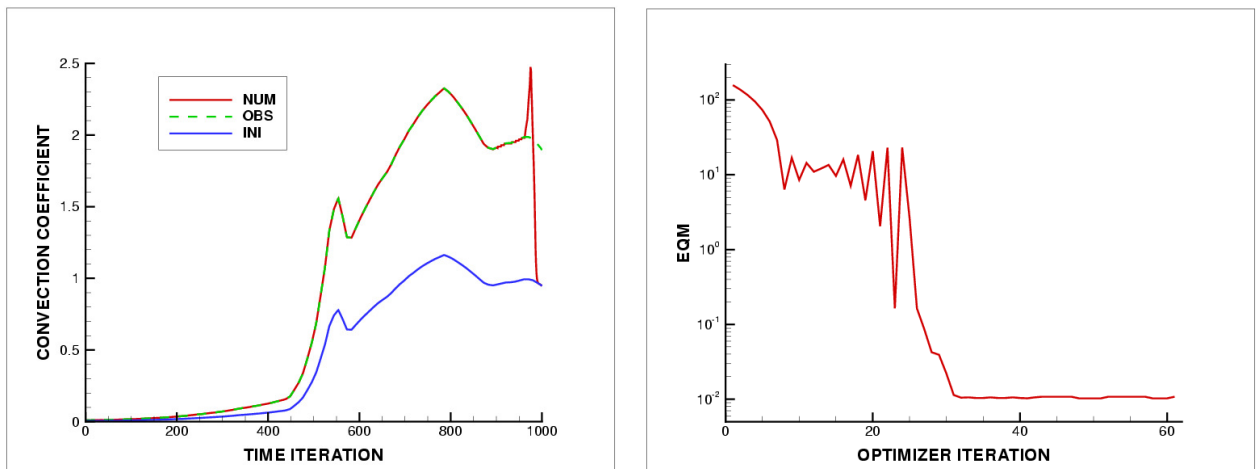
Gradient expression is a combination of direct and adjoint discrete quantities. Once the gradient of cost function is computed, we can apply an iterative inverse minimizing procedure to  $J(p)$  to obtain an estimation of the optimal parameter  $p_{opt}$ . We use a combination of a gradient steepest descent method at the beginning of minimization and a Quasi Newton method [11] at the end.

## Numerical results

We now present some applications of this inverse problem of estimation of time domain surface heat convection coefficient for a thermally degradable material, on a one-dimensional slab of thickness  $e$ , by using time domain temperature measurements taken below the boundary surface, at a given thermocouple position, during a time interval  $[0, t_f]$ . The final time is denoted by  $t_f$ . These tests have been carried out for the problem of fluxes identification on a carbon/resin material. We first tried to examine the effects of pyrolysis (test 1), ablation (test 2) separately, then we applied the new method to operational cases, such as the ARD (Atmospheric Reentry Demonstrator, test 3 with a different material: alestrasil) or plasma torch (test 4). For test 1 and test 2, we used synthetic data (errorless measurements).

### **Test 1 : Identification of Virgin material flux : without ablation , pyrolysis., $x_0=1.3$ mm**

We start (INI) with a bad initial guess, half the value of the convection coefficient used to generate the synthetic data, with sharp discontinuity. Figure 1 shows a good agreement for the reconstruction (NUM) of the convection coefficient, compared to the reference convection coefficient (OBS). To compute numerically the adjoint and gradient discrete quantities for the inverse problem in heat convection coefficient, we have both used manual differentiation and the Automatic Differentiation (AD) engine tool, Tapenade, developed at INRIA Sophia-Antipolis by the Tropics team [12]. Automatic differentiation is a family of techniques for computing the derivatives of a function defined by a computer program, for sensitivity and gradient analysis applications [13]. The good result below (except near the final time) is obtained with the inverse code using Tapenade (Automatic Differentiation tool was used). The RMS error on the flux is 0.04. Near final time, the value of the estimated flux has very little influence on the temperature in the material, at  $x_0$  and is all the more difficult to compute accurately.

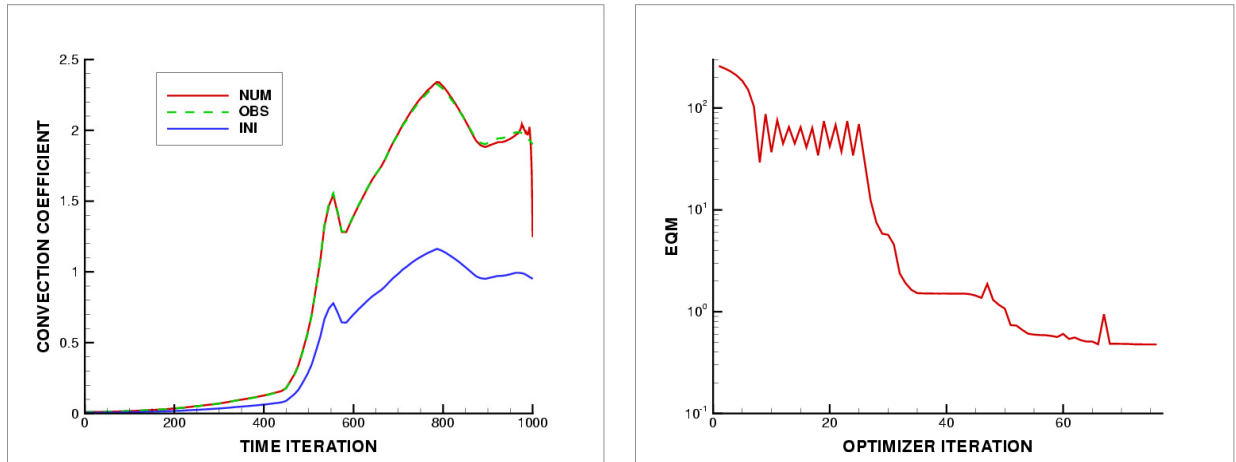


**Figure 1. Flux Identification; Temperature RMS error Automatic Differentiation tool  
Test1: Virgin material: without ablation, pyrolysis,  $x_0=1.3$  mm**

Figure 1 shows also that the RMS error on temperature obtained at the end of optimization process is very low (0.01), and we can observe the change in optimizer (iteration 25), switching from gradient steepest descent at the beginning, to Quasi Newton after. The gain in convergence is promising, after 60 optimizer iterations.

### **Test 2 : Identification of High Flux with ablation, Carbon/Resin material , $x_0=2.6$ mm**

It is a quite difficult test case, with high fluxes. On Figure 2, a good agreement in the reconstructed convection coefficient value is observed, except at final time, with an initial guess of half the expected value and using synthetic data (errorless measurements). The RMS error on the flux is 0.06 and RMS error on measured temperature obtained at the end of optimization process is very low (0.7), after 70 optimizer iterations.



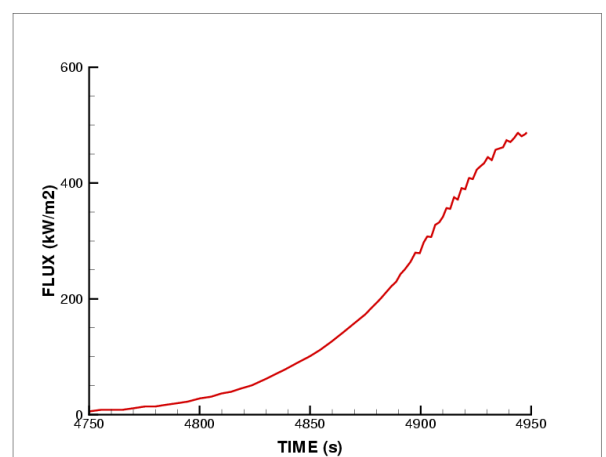
**Figure 2. Flux Identification; Temperature RMS error  
Test 2: Identification of High Flux with ablation,  $x_0=2.6$  mm**

### **Test 3 : ARD Test case**

We investigate the inverse analysis approach for the ARD flight test case. The Atmospheric Reentry Demonstrator (ARD) was a suborbital reentry test flown on the third Ariane 5 flight. ARD was launched in October 1998 from Kourou, French Guyana, by an Ariane 5. It was recovered and transported in EADS Astrium Aquitaine plant for expertise (Figure 3). More than 200 different parameters were recorded during flight. After ARD recovery, a preliminary analysis of recorded data was performed. Successful results are obtained in the reconstructed flux (Figure 4), which are very similar to those obtained before (during post-flight analysis).



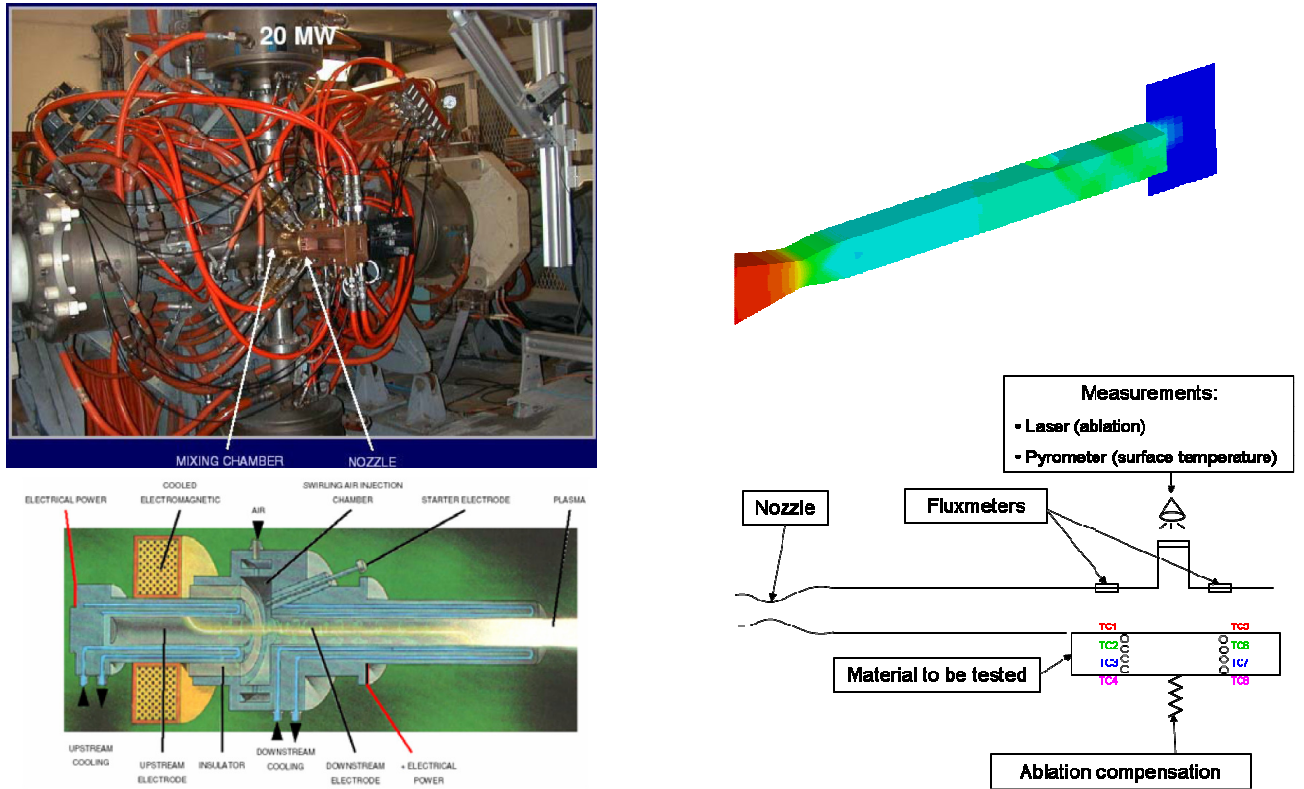
**Figure 3. ARD heat shield**



**Figure 4. ARD heat flux restitution**

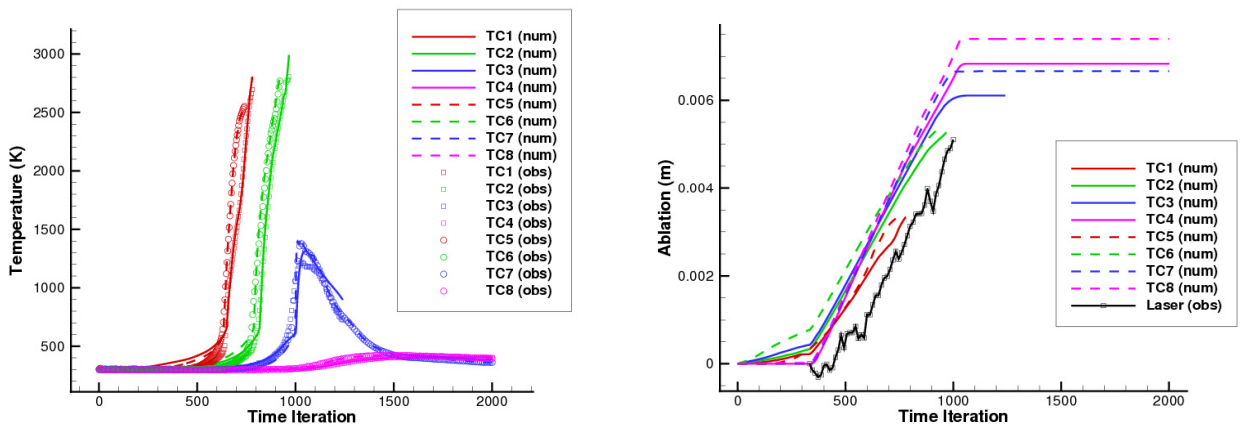
**Test 4 : Operational test case (Plasma Jet case)**

This case has been investigated to improve the robustness on an industrial problem where many experimental data were available. The industrial applications are straight forward. The plasma jet facility of the Astrium's Aquitaine plant is shown on Figure 15, with the schema of a plasma torch. The experimental test facility uses four coupled plasma torchs. The tested material is equipped with eight thermocouples at two stations in the duct. A Navier Stokes numerical rebuilding of the flow is also illustrated Figure 15



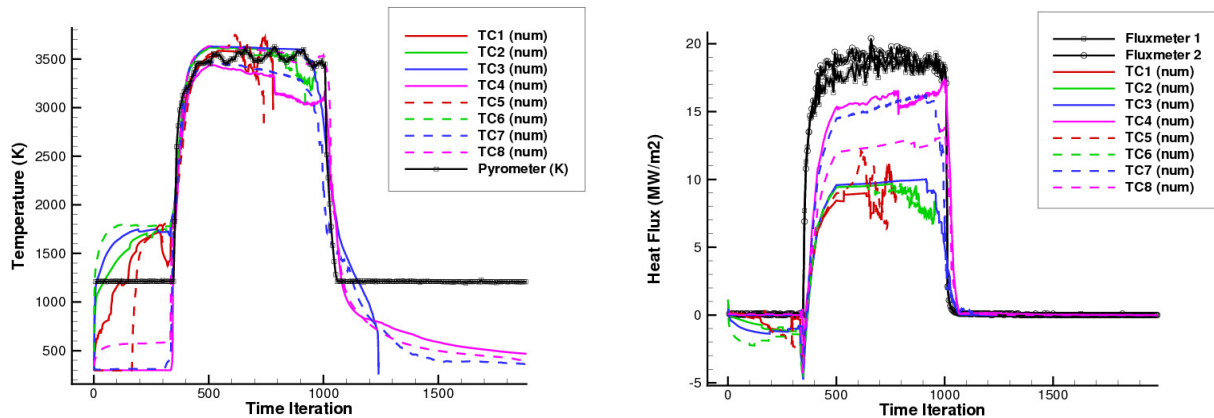
**Figure 15. Plasma jet facility**

We show Figure 16 the comparisons between the measurements of temperature and the simulated temperatures obtained after the optimisation process. The ablation measurements are also compared to the computed ones. As could be foreseen, the measurement thermocouples which are located the nearest to the surface exposed to fluxes give the best temperature reconstruction results.



**Figure 16. simulated (num) and measured (obs) levels of temperatures and ablation  
Test 4: Plasma torch case**

Figure 17(a) compares the restitution of surface temperature and the measurements of the pyrometer, and Figure 17(b) compares heat fluxes and the fluxmeters measurements located in front of the material. The results are quite good for the surface temperatures, but heat fluxes are found lower than the measured values (far from surface, the behaviour of the method becomes subject to questions. The Navier Stokes numerical rebuilding also indicates lower fluxes than those measured. A good explanation is that radiative effects are seen by the fluxmeters and could explain the remaining differences between measurements and simulation. The technology of the fluxmeters is being improved too.



**Figure 17. simulated (num) and measured (obs) levels of surface temperatures (a) and heat fluxes (b)  
Test 4: Plasma torch operational case**

## Conclusion

Motivated by atmospheric re-entry of aerospace vehicles and Thermal Protection System dimensioning problems, this article is concerned with inverse analyses of highly dynamical heat fluxes. It addresses the inverse problem of using temperature measurements to estimate the heat flux (convection coefficient), at the surface of ablating materials. Several validation test cases, using synthetic, noisy on-ground and in-flight data temperature measurements are carried out, by applying the results of the minimization algorithm. Main results are:

- Validity of the inverse formulation for the temperature and ablation variables evolution
- Improvement by using a combined gradient steepest descent method at the beginning of minimization process and Quasi Newton method to finish the minimization,
- Convection coefficient restitution has been improved for hard cases (with great ablation) for fluxes functions containing sharp corners and discontinuities,
- Successful test case on carbon/resin material with high heat fluxes and large magnitudes, ablation and pyrolysis effects, and on operational data,
- Encouraging results with an automatic differentiation tool are also obtained, without ablation

Future works have to be done on:

- Robustness to initial guess, sensitivity to measurements, number and position of sensors, and application of regularization methods to stabilize noise errors on measurements,
- Validation of the automatic differentiation tool used to generate the inverse code, especially for ablation test cases,
- Thermal model uncertainties influences on the accuracy of identified flight heat flux, athermanous enthalpy identification,
- Validations on aerothermal flight measurements.



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