

## EXPERIMENTAL EVALUATION OF ABLATIVE PROPERTIES IN COMPOSITES THROUGH BAYESIAN INFERENCE

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***Abstract.** Composite materials are commonly used in thermal shields of space and sub-orbital vehicles. In order to achieve the correct dimensioning of such thermal protection systems, the ablative properties of these materials should be known. In this work, techniques for solution of inverse problems are used for determination of these parameters. A mathematical model is employed to simulate the ablation in a composite used in thermal protection systems. The direct problem is solved via an interface tracking method. The Bayesian technique MCMC (Markov Chain-Monte Carlo) through the Metropolis-Hastings algorithm is proposed for the solution of the inverse problem of determining the ablation properties of the composite. Preliminary results obtained through the use of experimental data are presented for an specific case, demonstrating the viability of this way of solution.*

**Keywords:** Inverse problem, Composite ablation, Bayesian inference, Computational simulation

### 1. INTRODUCTION

Space and sub orbital vehicles reach high temperatures due the hypersonic velocities reached within atmosphere, where the process of aerodynamic warming of the vehicle surface occurs. Diverse types of TPS (Thermal Protection Systems) are employed to protect the structure and the payload. In the region near the stagnation point, where the temperature peak occurs, ablative TPS are commonly used, made with composite materials. The correct dimensioning of these TPS depends not only on the thermal load but also on the ablative properties of the composite. These properties frequently are evaluated in experiments that try to reproduce the flight conditions (Da Costa et al., 1996).

In space vehicles the aerodynamic warming is so intense that the TPS temperature cannot be measured straight by sensors, which must be placed in the internal surface of vehicle structure. Consequently, the external temperature and heat flux have to be compared with the theoretical model, in a process that implies in high uncertainties concerned to the physical phenomena and to the properties of TPS and structure materials. The main difficulties to obtain the properties from tests are the reproduction of the flight environment and the physical modeling of the ablative process (Gregori et al., 2008).

The inverse techniques in heat transfer were initially developed to be applied in problems related to space vehicles, due the previous explained situations. Their development has begun in the 60's, in the American Space Program (Özisik e Orlande, 2000). These techniques allow estimating the temperature field, heating flux or thermophysical properties involved in the heat exchange process from the measurements in a point or region of the domain. With the advent of digital computers such techniques have experienced a fast development and expansion in their utilization. Now a day these techniques are applied not only in the aerospace industry but also in several sectors allowing estimating diverse parameters with accuracy and in a fast way with low cost. In this work to use of an inverse technique is proposed to estimate the thermal parameters and thermophysical properties of ablative composites used in TPS of space and suborbital vehicles.

### 2. DIRECT PROBLEM

#### 2.1 Physical problem and mathematical model

Ablation in composites corresponds to a degradation reaction (oxidation) of the polymer added to the composite of the thermal shield. Theses polymers normally are produced from phenolic or epoxy resins, reinforced with glass, silica or organic spheres made with short fibers. Considering their highly orthotropic properties the composites reinforced with fibers are made through a succession of layers with individual fibers oriented in perpendicular preferential directions, extracted from the TPS design. The pyrolysis temperature varies from 250° C to 600° C, as function of the local pressure and the reaction rate (Torre et al., 2004). As the pyrolysis front goes ahead, a char porous layer is formed, where the gases produced by the reaction flows to outside. In most situations pyrolysis is assumed to be an endothermic

reaction, which the enthalpy of formation can be estimated or evaluated. The physical problem corresponds to the ablation of a flat cylindrical sample of composite and was chosen due the availability of experimental data. A rectangular domain of 5 mm x 12 mm was considered, in the x and y coordinates, respectively – Fig. 1. The domain region of  $0 < y < 10$  mm was filled with composite and the rest with air. The heat flux was imposed in the surface of the composite, at  $y = 10$  mm. The inferior surface in  $y = 0$  was considered thermally insulated. The air was considered as inert media, since its thermal capacity was considered to be null. The composite reproduced was Quartz-Phenolic (Si-Phenolic) resin. The physical properties considered are presented in Tab.1.

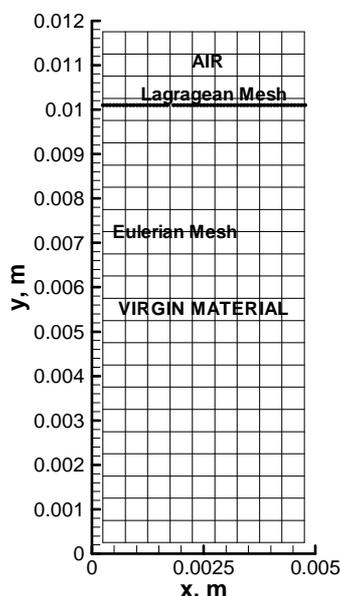


Figure 1. Domain of solution and Lagrangean and Eulerian meshes.

Table 1. Properties of the Si-Phenolic resin used in the solution of direct problem (Willians and Curry, 1992).

Property	Virgin material	Char
K (W/m <sup>o</sup> C)	0,521	0,428
Cp (J/kg.°C)	1256	879,5
$\rho$ (kg/m <sup>3</sup> )	1730	1300
$\epsilon$	0,78	0,78
Heat of Pyrolysis (MJ/kg)	0,214	-
Temperature of Pyrolysis (°C)	325 <sup>o</sup>	-
Heat of melting (MJ/kg)	-	10,5
Temperature of melting (°C)	-	3700 <sup>o</sup>

The ablation model proposed for a composite material will consider the presence of two layers: the virgin material and the char layer that appears after the pyrolysis front. Two moving fronts will be accounted: the pyrolysis and the ablation front of the char layer. Both will appear at constant and specific temperatures. The hypotheses considered for the mathematical model are:

- Solid materials are isotropic with constant properties.
- The pyrolysis front is considered to have zero thickness, and the pyrolysis reaction happens at constant temperature and enthalpy.
- Char layer recession is supposed to occur due oxidation or sublimation at constant temperature.
- Absence of melting layer.
- The resulting gases fully react and perfectly mix with the external air layer, without influence over its properties.
- Air is considered a perfect gas.
- Radiation is absorbed or emitted by the external surface, but not transmitted.

When a heat flux is imposed to the external surface, the TPS warms as in a pure transient heat conduction problem until the ablation temperature is reached. Once the TPS surface reaches the ablation temperature, its thickness is reduced; therefore, a transient, coupled problem of heat conduction and moving boundary appears.

The TPS and the air around it are represented as parts of a continuous domain of calculation. The application of the energy conservation principle to an infinitesimal volume element of the mathematical domain leads to a partial differential equation for the temperature, namely:

$$\frac{\partial(\rho.C_p.T)}{\partial t} = \nabla.K\nabla T + Q \quad (1)$$

where  $K$  is the thermal conductivity and  $Q$  is a source term that takes into account the net heat exchange at the boundary:

$$Q = \int_A q \delta(\mathbf{x} - \mathbf{x}_F) dA \quad (2)$$

where  $\mathbf{x}$  is the position in the coordinate system,  $\delta(\mathbf{x} - \mathbf{x}_F)$  is a Dirac delta function, that is non-zero only at the interface position  $\mathbf{x}_F$ ,  $dA$  is a surface element of the interface and  $q$  is the source term of energy per unit of surface of the interface. One should note that this term might exist in every moving interface. For the external (char) layer:

$$q = \rho L V + \varepsilon \sigma [T_F^4(t, \mathbf{x}_F) - T_\infty^4] \quad (3.a)$$

where  $V$  is the normal interface velocity,  $T_F$  is the interface temperature,  $T_\infty$  is the external temperature,  $L$  is the heat of ablation and  $q_e$  is the prescribed external heat flux. For the pyrolysis front, it is simplified:

$$q = \rho L_p V \quad (3.b)$$

where  $L_p$  is the heat of pyrolysis. Also the mass flux of resulting gases is neglected, due its low density (when compared to the solid material). Indeed, the density in Eq. (3) is the interface density, obtained from the mean average of the two phases separated by this front.

Although the air is included in the domain, its region is considered adiabatic, and the heat capacity and thermal conductivity are assumed to be null. Once ablation or pyrolysis temperatures are reached, the temperature jump condition becomes:

$$T_F - T_A = 0 \quad (4)$$

where  $T_A$  will be the ablation or the pyrolysis temperature, according to the interface.

## 2.2 Method of solution

The moving boundary problem was solved by the Interface Tracking Method, introduced by Unverdi & Trygvason (1992). In this method, a fixed uniform Eulerian grid is generated, where the conservation laws are applied over the complete domain. The interface acts as a Lagrangean referential, where a moving grid is applied. The instantaneous placement of the interface occurs through the constant remeshing of the moving grid, and each region of the domain is characterized by the Indicator Function, which identifies the properties of the wall and the air around it.

This method allows the representation of any geometry used in the TPS, and also the characterization of every layer separately. It is accomplished without a high increase in the computational cost and does not need any pre-processing (construction of unstructured grid or coordinate transformation). In this work, this method is employed to estimate the ablative performance of the TPS, considering a two-dimensional approach in both, the heat conduction and the moving boundary problem. Details of the method and the solution of direct problem can be found in Machado (2014).

## 3. INVERSE PROBLEM

The Bayesian inference consists in a tentative to use every information available with the objective to reduce the uncertainties present in an inference. As new information appears, it is combined with all the anterior information in order to build a base through the statistical proceedings. The formal way employed to combine the new information with the old ones is known as Bayes Theorem. Indeed, the term Bayesian is frequently used to describe a well-known approach of statistical inversion, which is based in the following principles (Cotta, 2009):

1. All variables included in the model are modeled as random.
2. The likelihood describes the degree of information about their realizations.

3. The degree of information relative of these values is codified in terms of probability distributions.
  4. The solution of the inverse problems is the posteriori probability distribution.
- The Bayes theorem can be written as:

$$\pi_{\text{posterior}}(\mathbf{P}) = \pi(\mathbf{P}|\mathbf{Y}) = \frac{\pi_{\text{prior}}(\mathbf{P})\pi(\mathbf{Y}|\mathbf{P})}{\pi(\mathbf{Y})} \quad (5)$$

where  $\pi_{\text{posterior}}(\mathbf{P})$  is the posteriori probability distribution;  $\pi_{\text{prior}}(\mathbf{P})$  is the is the priori probability distribution;  $\pi(\mathbf{Y}|\mathbf{P})$  is the likelihood function, which express the probability to obtain the measurements once given the parameters;  $\pi(\mathbf{Y})$  is the marginal probability density of the measurements, which plays the role of a normalizing constant. Assuming that the measurement errors have a Gaussian distribution, with known averages and covariances and the measurement errors are additive, the likelihood may be written as:

$$\pi(\mathbf{P}|\mathbf{Y}) = (2\pi)^{-I/2} |\mathbf{W}^{-1}| \exp\left[-\frac{1}{2}(\mathbf{Y} - \Theta_s(\mathbf{P}))^T \mathbf{W}(\mathbf{Y} - \Theta_s(\mathbf{P}))\right] \quad (6)$$

where  $I$  is the number of measurements,  $\mathbf{W}$  is the covariance matrix of the measurement errors,  $\mathbf{Y}$  is the vector of measurements and  $\Theta_s(\mathbf{P})$  is the vector of temperatures, extracted from the solution of the direct problem with a parameter estimation. Depending on the priori probability distribution assumed for the parameters, the posteriori probability distribution may not allow an analytical treatment.

In this work, the Monte Carlo Method with Markov Chain (MCMC) is employed to estimate the posteriori values for the parameters to be estimated (Orlande et al., 2011). Samples of every possible parameter are generated, which turns the inference about the posteriori probability into the inference over the samples. In order to implement the Markov chain, a density distribution  $q(\mathbf{P}^*, \mathbf{P}^{(t-1)})$  is necessary to provides the probability to pass from an actual chain state  $\mathbf{P}^{(t-1)}$  to a new one  $\mathbf{P}^*$ . For the case of a uniform distribution:

$$\mathbf{P}_j^* = \mathbf{P}_j^{(t)} + w_j(2r-1) \quad (7)$$

For a Gaussian distribution:

$$\mathbf{P}_j^* = \mathbf{P}_j^{(t)} + w_j \quad (8)$$

The Metropolis-Hastings algorithm is used to implement the MCMC and can be summarized in the following steps (Lamien, 2011):

1. Generate a sample  $\mathbf{P}^*$  from a proposed distribution  $q(\mathbf{P}^*, \mathbf{P}^{(t-1)})$
2. Calculate

$$\alpha = \min\left[1, \frac{\pi(\mathbf{P}^*|\mathbf{Y})q(\mathbf{P}^{(t-1)}, \mathbf{P}^*)}{\pi(\mathbf{P}^{(t-1)}|\mathbf{Y})q(\mathbf{P}^*, \mathbf{P}^{(t-1)})}\right] \quad (9)$$

3. Generate a random number  $U$ , uniformly distributed in  $(0,1)$
4. If  $U \leq \alpha$ , define  $\mathbf{P}^{(t)} = \mathbf{P}^*$ , otherwise define  $\mathbf{P}^{(t)} = \mathbf{P}^{(t-1)}$
5. Return to step 1, in order to generate the sequence  $\{\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \dots, \mathbf{P}^{(n)}\}$

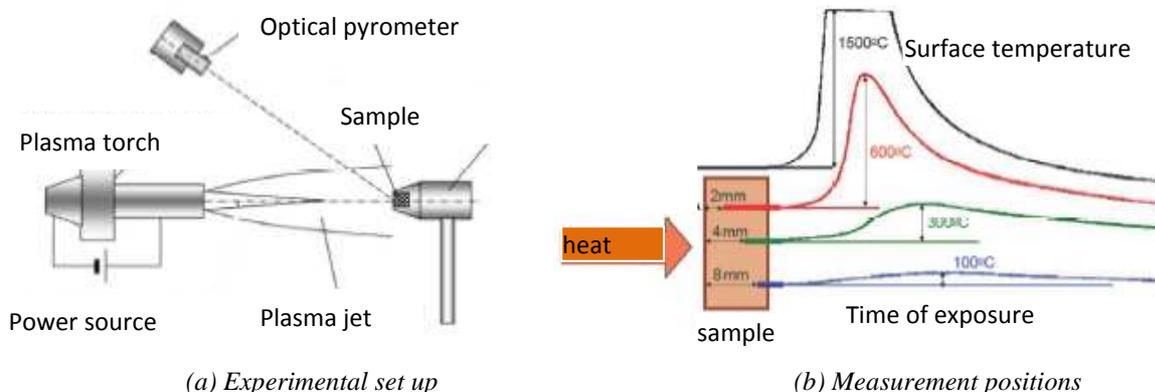
This way, a sequence that represents the posteriori distribution is available and the inference over this distribution is obtained from the inference over the samples  $\{\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \dots, \mathbf{P}^{(n)}\}$ . The values of  $\mathbf{P}^{(i)}$  should be neglected until the convergence of chain reaches the equilibrium.

#### 4. RESULTS AND DISCUSSION

The solution of inverse problem was tested in a one-dimensional ablative process, similar to those performed by Barros (2008). In that work, samples of diverse materials were exposed to a plasma jet and temperatures, heat flux and other parameters were measured during the experiment. A simplified scheme of the experimental set up is shown in Fig. 2.a. Behind the surface temperature, other temperatures were measured, Fig. 2.b. The mass loss rate was evaluated through the weighing before and after the exposure to the plasma torch, through the formula:

$$MLR = -\Delta m / (A \cdot \Delta t) \tag{10}$$

where  $\Delta m$  is the mass loss,  $\Delta t$  is the time of exposure and  $A$  is the area of the sample surface. The samples were flat cylinder of 10 mm height and diameter of 12 mm. The material considered was Quartz-Phenolic resin (Si-Phenolic). Two cases were considered for study:



**Figure 2. Temperature measurements of Barros (2008).**

Case 1: A heat flux of 0.446 MW/m<sup>2</sup> was imposed during 90 seconds. The available measurements for this case are the mass loss rate and the external surface temperature, Tab. 2.

**Table 2. Measurements available for Case 1.**

Time (s)	MLR (kg/m <sup>2</sup> s)	Uncertainty (kg/m <sup>2</sup> s)	T <sub>e</sub> (°C)	Uncertainty (°C)
10	0.057142	0.010101	1.005	102
30	0.048739	0.010101	1.093	29
50	0.040336	0.004040	1.122	15
70	0.031932	0.003232	1.137	13
90	0.026890	0.002828	1.137	13

Case 2: A heat flux of 0.820 MW/m<sup>2</sup> was imposed during 30 seconds. The available measurements for this case are the temperatures, Tab.3, where Ty<sub>1</sub>, Ty<sub>2</sub> and Ty<sub>3</sub> correspond to the temperatures measured at 2 mm, 4 mm and 8 mm from the external surface, respectively.

**Table 3. Measurements available for Case 2.**

Time (s)	T <sub>e</sub>	Ty <sub>1</sub>	Ty <sub>2</sub>	Ty <sub>3</sub>
3	1.170	50	25	25
6	1.380	70	30	25
10	1.430	120	35	30
13	1.440	165	60	40
16	1.460	220	70	45
20	1.460	300	100	50
23	1.460	350	125	65
26	1.460	405	155	70
30	1.460	460	190	80

The solution of the inverse problem was applied to two parameters: the heat of pyrolysis, H<sub>p</sub>, and the temperature of pyrolysis, T<sub>p</sub>. The initial values assumed for the states were the properties in Tab.1. The standard deviations (σ) used were 0.1 MJ/kg and 200° C for H<sub>p</sub> and T<sub>p</sub>, respectively. The searching step was w = 0.05 for both parameters. The number of states was limited to 1000.

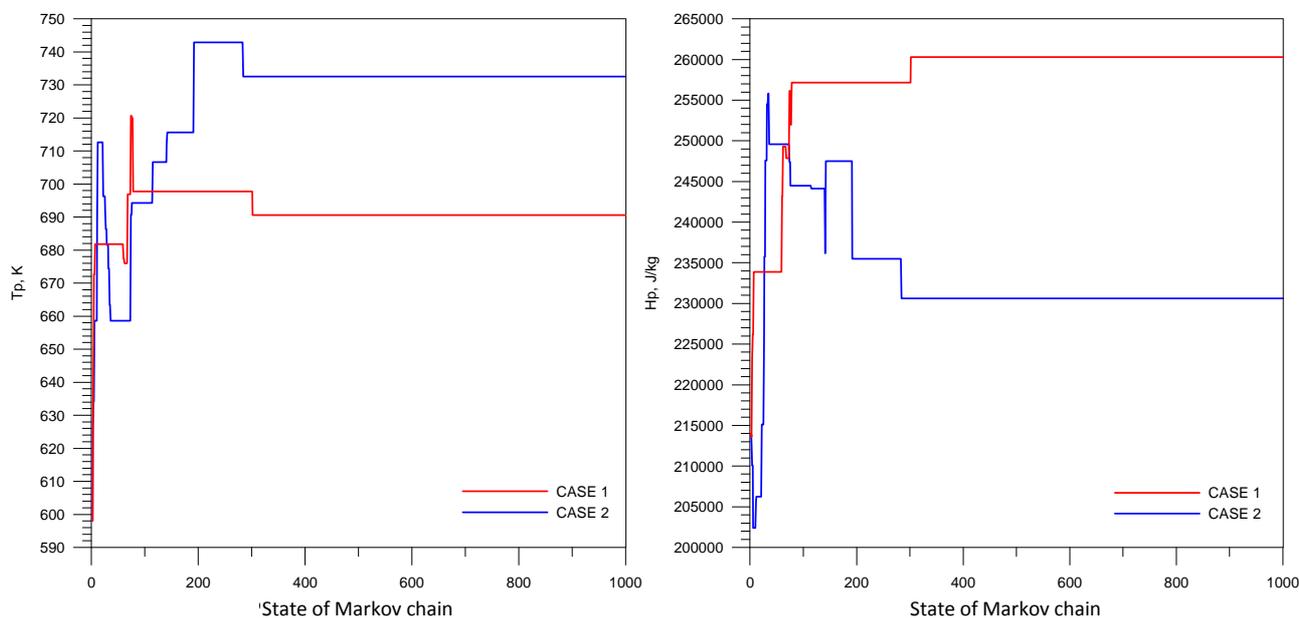
Table 4 shows results for each case. In both cases the acceptance rates were below 2%. The final values and averages were above the initial values, which indicate these values were underestimated. Standard deviations had kept

below 5% in both cases. The dispersion of the pyrolysis temperature in case 2 is quite above the case 1 (19.55 against 5.91). For the heat of pyrolysis, the standard deviations are close (0.00726 and 0.00659).

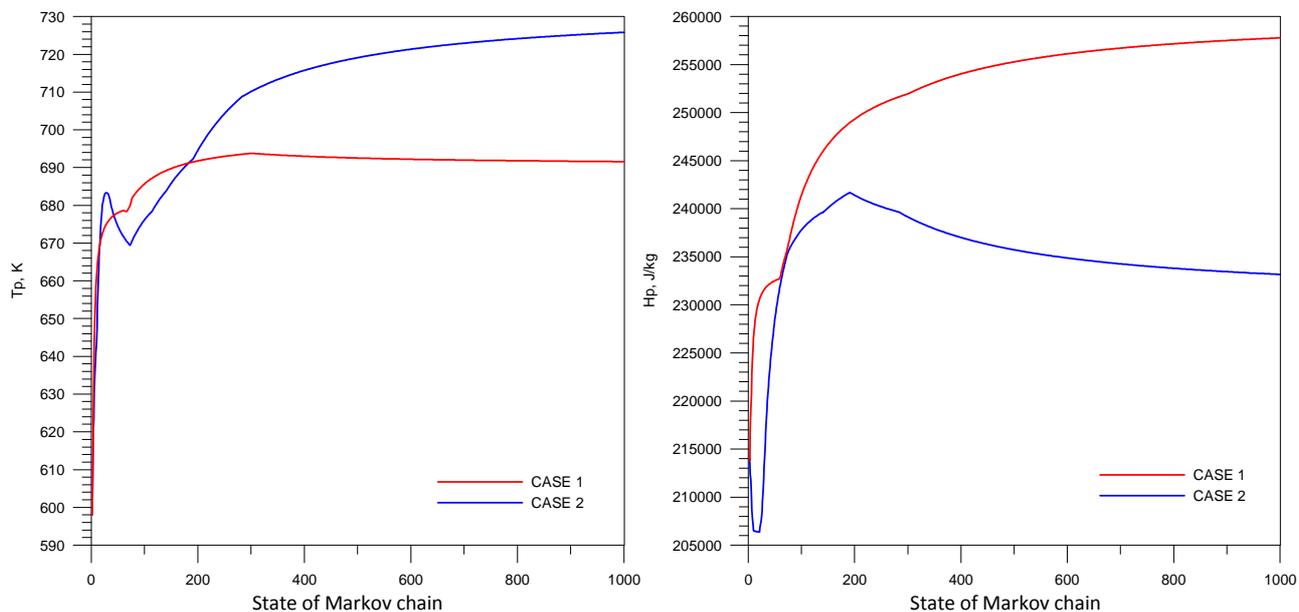
Figs.3, 4 show the evolution for the accepted values and cumulated averages of both parameter in the cases studied. In both cases the rate of acceptance of new values ceases after 300 states. Although different values found for the averages of both parameters, the bias to increasing compared to the initial values was similar. In Fig.5 the acceptance rates fall quickly to values close to the final ones, and stabilize in a bias of slow fall. A reduction of the step of search or elimination of *prioris* as criterions of acceptance would allow an increase in the rates.

**Table 4. Results of parameter estimation after 1000 states.**

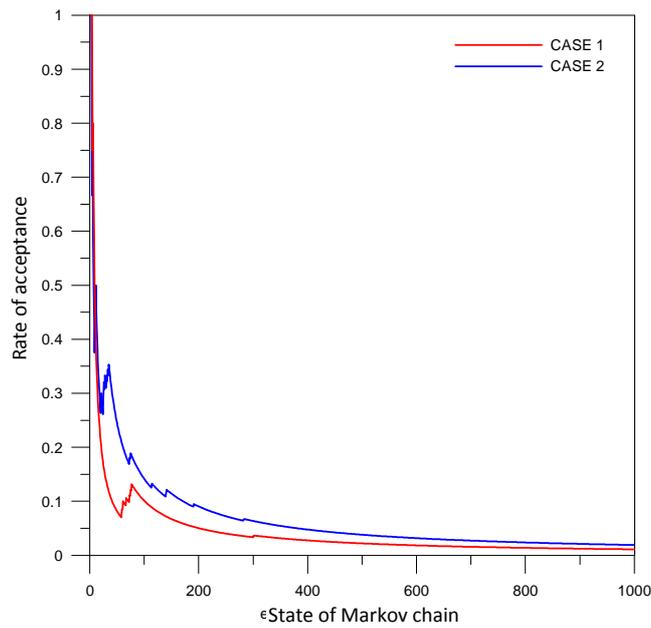
Case	Parameter	Final value	Average	$\sigma$	Acceptance %
1	$T_p$ (K)	690.62	691.56	5.91	1.10
	$H_p$ (MJ/kg)	0.26028	0.25778	0.00659	
2	$T_p$ (K)	732.52	725.82	19.55	1.90
	$H_p$ (MJ/kg)	0.23061	0.23317	0.00726	



**Figure 3. Accepted results according with states for both cases.**

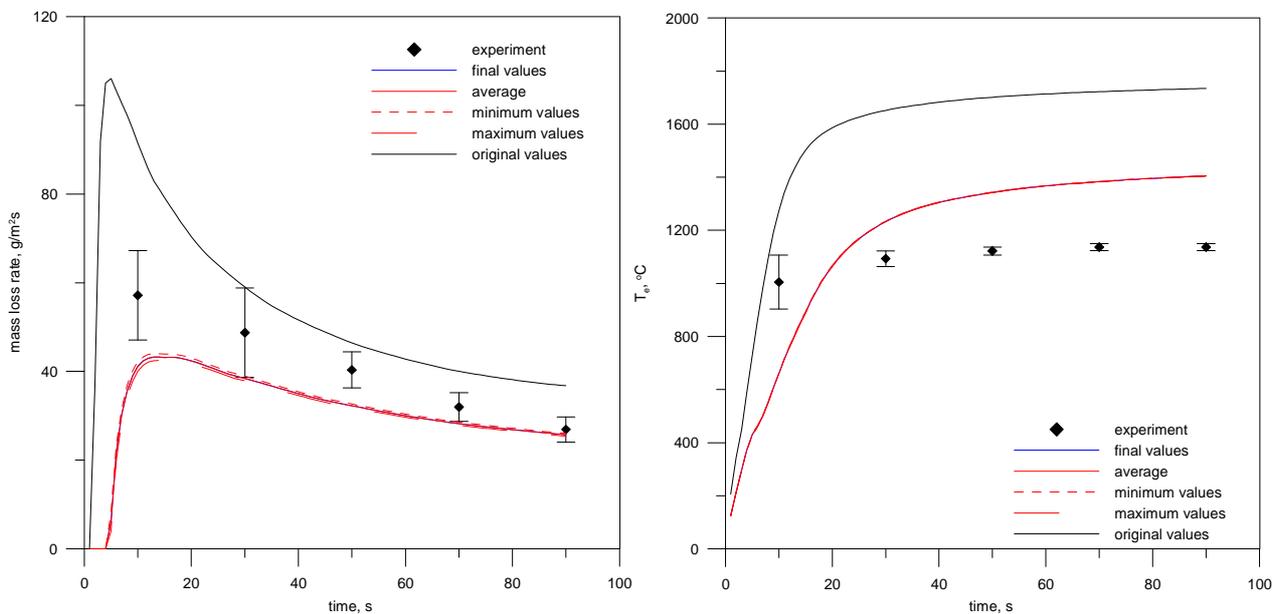


**Figure 4. Cumulative average of accepted results according with states for both cases.**



**Figure 5. Rate of acceptance according with the states of Markov chains.**

The original values presented in Tab.1 were used as initial values in the inverse analysis and the final values, presented in Tab.4, were used to obtain the solution of the direct problem, in order to compare the results with the experimental data. The maximum and minimum values for each case obtained through adding or subtracting the standard deviation from the averages respectively, were also used as inputs. The values obtained in case 1 were also applied to the direct problem for case 2 and vice-versa. Results and the comparison with experimental data are presented in Figs. 6-8. In all cases the results obtained from the inverse analysis are closer to the experimental data than the results from the original values.



**Figure 6. Numerical results for heat flux  $q = 0.44631 \text{ W/m}^2$  (case 1) with values obtained for case 1**

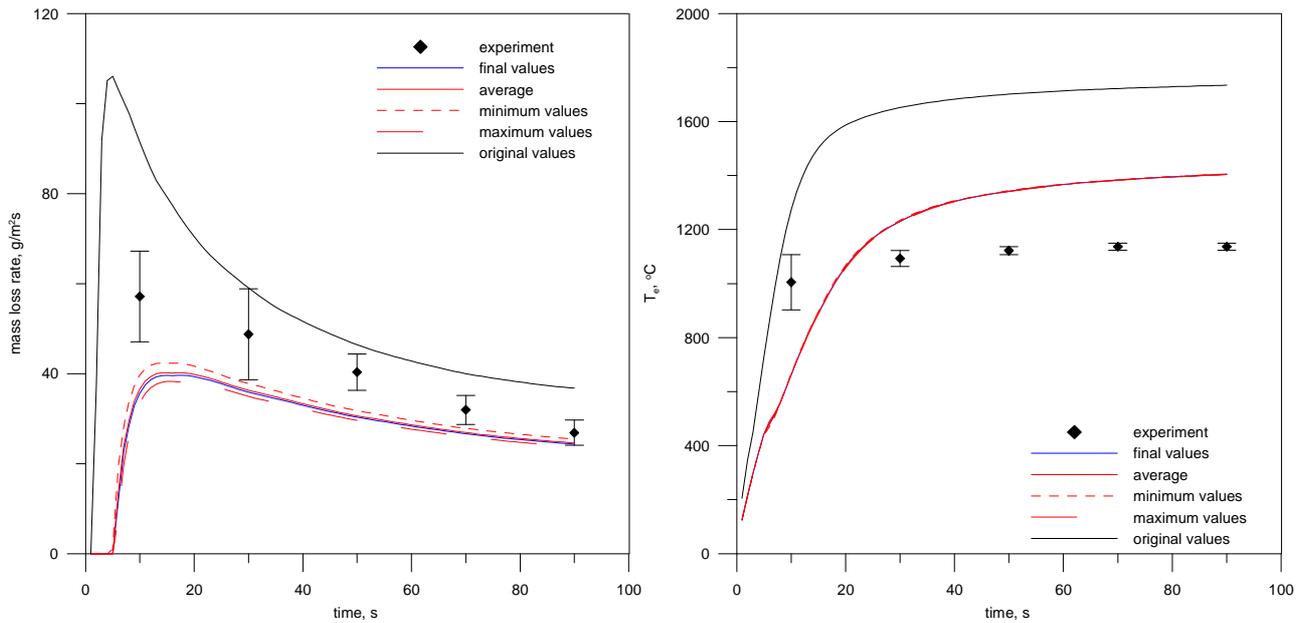


Figure 7. Numerical results for heat flux  $q = 0.44631 \text{ W/m}^2$  (case 1) with values obtained for case 2

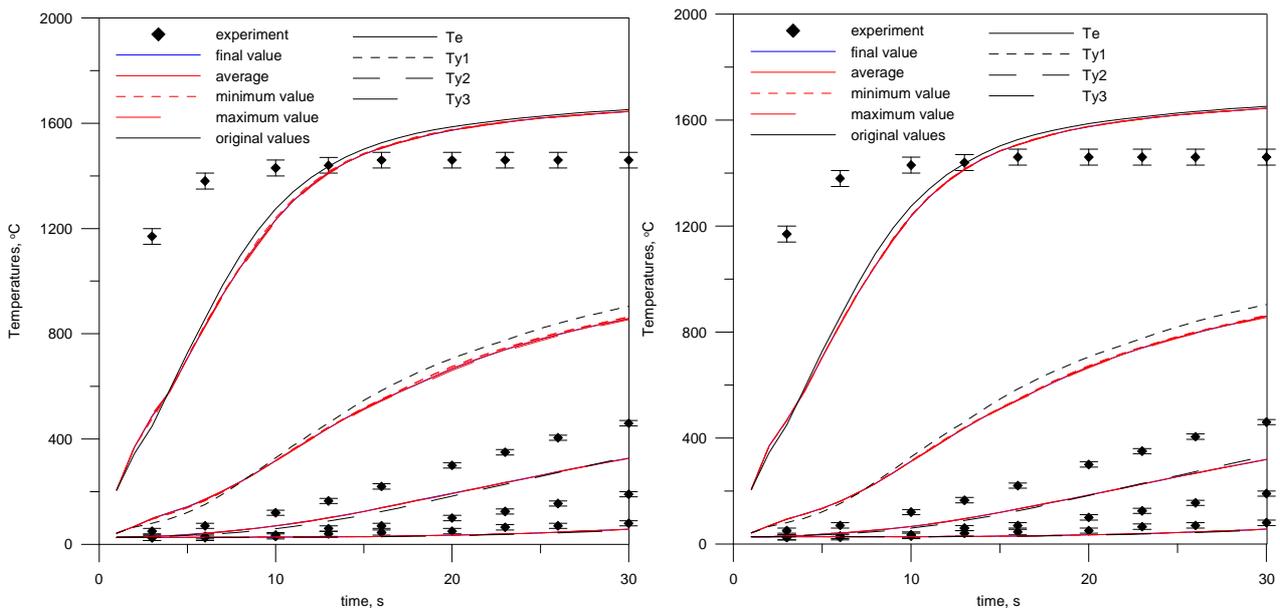


Figure 8. Numerical results for  $q = 0.82 \text{ W/m}^2$  (case 2) with values for case 2 and case 1, respectively.

## 5. CONCLUSIONS

In this work the MCMC Metropolis-Hasting algorithm, based in the Bayesian inference, was applied as the inverse technique of parameter estimation in ablative composites used as thermal Shields. The direct problem was described by a mathematical model and solved via the interface tracking method.

The inverse technique was applied in two cases with experimental data available with independent results. Two specific parameters were selected for test: the heat of pyrolysis and the pyrolysis temperature. The material properties and the *prioris* of these parameters were evaluated from the literature and previous experiments. The averages values of each case were employed in both cases, in order to compare the numerical results with the experimental data available.

Preliminary results obtained for the values estimated in the two cases were both closer to the experimental results than the values extracted from the literature, which may indicate physical coherence and compatibility with the physical model adopted. Considering such results, the method was considered reliable for the solution of this class of problems and this case in particular. However, some improvements in numerical implementation shall be addressed.

## 6. ACKNOWLEDGEMENTS

The authors would like to acknowledge to CNPq for the financial support, which made this work possible.

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