Automatic Differentiation for thermal inverse problems

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Abstract

Thermal Protection System is a key element for atmospheric re-entry missions of aerospace vehicles. Consequently, the identification of heat fluxes is of great industrial interest and is usually based on temperature measurements. This contribution is concerned with inverse analyses of highly evolutive heat fluxes. An inverse problem is used to estimate transient surface heat fluxes (or convection coefficient), for thermally degradable material (with ablation and pyrolysis phenomena), by using time domain temperature measurements on thermal protection. 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) is then developed and applied. Accurate results of identification on high fluxes test cases, and good agreement for temperatures restitutions, are obtained using synthetic, noisy, on-ground and in-flight data measurements, without and with ablation and pyrolysis. First encouraging results with an automatic differentiation procedure are also presented in this paper.

1. 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. For a more detailed description of the problem, we refer to some publications on the Atmospheric Reentry Demonstrator (ARD) suborbital reentry test flown[1-2]. 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, Inverse Heat Conduction problem, and the estimation of fluxes from temperature measurements.
The inverse problem in this paper deals about the identification of time domain surface heat fluxes (or convection coefficient $\alpha_0(t)$), for thermally degradable material (ablation and pyrolysis processes), 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 $0 \leq t \leq t_f$, where t_f denotes the final time.
This inverse problem is solved as a minimization problem involving a least square problem and an optimization loop. An optimal control formulation (Lagrangian, adjoint and gradient computations) is then applied and developed with the help of optimal control theory[3] and experience on some industrial applications of inverse problems at EADS [4] (European Aeronautics Defense and Space Company).

2. Direct problem

Continuous equations

EADS ASTRIUM-ST has developed[5] a transient one-dimensional thermal problem with one moving boundary (ablative surface) that is used at to model complex chemical processes of simultaneous heating, pyrolysis, ablation and thermal degradation behaviour of ablative materials. We briefly present the direct model used.

Internal energy balance (for pyrolysable ablative material) :

The internal energy balance is a transient thermal conduction equation with additional pyrolysis terms

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) + \left[F_V + h_g - \int_{T0}^{T} A_1 dT\right]\frac{\partial \rho}{\partial t} + \frac{\partial(\dot{m}_g h_g)}{\partial x} \quad (1)$$

with x the abscissa, t the time, T (x,t) the temperature, ρ (x,t) the specific mass, C_p the heat capacity, λ the thermal conductivity, $\dot{m}_g$ the pyrolysis gas mass flow rate, h_g the pyrolysis gas enthalpy, A_1 a constant, F_v the pyrolysis gas formation heat.

Pyrolysis with internal decomposition modelled via a first-order rate process based on the Arrhenius equation

The time domain evolution of specific mass is given by :

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

ρ_c and ρ_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. Internal decomposition converts some of the solid into pyrolysis gas.
The pyrolysis gas mass flux is related to the decomposition by the simple mass balance:

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

The surface recession : we denote by s the abscissa of the moving interface (ablation value), then $\dot{s}$ is the recession rate. This physical process can be splitted in three kinds of ablation: mechanical recession rate, chemical recession rate and hydroerosion recession rate :

$$\dot{s} = \dot{s}_{meca} + \dot{s}_{chem} + \dot{s}_{hy} \quad (4)$$

Surface energy balance on the moving boundary:

The physical conditions at the hot surface are determined by convective heating and by thermochemical interactions of the surface with the boundary-layer gas. The surface energy balance takes the following form:

$$\begin{aligned} &\alpha_0(h_r - h_w) - \varepsilon\sigma(T_w^4 - T_r^4) + \dot{m}_g\left[H_c - \eta_1(h_r - h_w)\right] \\ &+ \dot{m}_c\left[H_v - \eta_2(h_r - h_w)\right] = \lambda \frac{\partial T}{\partial x} \end{aligned} \quad (5)$$

with η_1 the pyrolysis gas blocking factor, H_c the pyrolysis gas heat combustion, $\dot{m}_c$ the ablation mass flow rate, h_r the athermanous enthalpy, h_w the surface enthalpy, η_2 the ablation gas blocking factor, H_v the ablation heat, ε the total emissivity, σ the Stefan-Boltzmann constant, T_w the surface temperature, T_r the equivalent temperature.

Denote by $W = \begin{pmatrix} T \\ s \end{pmatrix}$, the vector of temperature and ablation, functions of time t and position x. Therefore, the direct problem can be represented in condensed vector form by the following system of coupled nonlinear time domain evolution differential equations:

$$\begin{aligned} &\frac{dW}{dt} = F(W) \\ &T(x,0) = T_0 \qquad s(x,0) = 0 \\ &t \in \left[0, t_f\right], \; x \in \left[s(t), e\right] \end{aligned} \tag{6}$$

with $F(W)$ a non linear operator and T_0 the reference initial temperature.

Space partial derivatives are computed with a centered finite difference type scheme. The abscissa x belongs to the interval $\left[s(t), e\right]$. It is parameterized by a reduced scaled space variable $\xi \in [0,1]$:

$$x = (1-\xi)s(t) + \xi e \tag{7}$$

Then the system (6) is rewritten relatively to the variables (t, ξ) . The variable ξ is discretized with the help of K grid points.
For simplicity, we explain our method on the implicit Euler scheme with a constant time step Δt . We define K the number of one-dimensional grid points, N the number of time iterations, k the space index, n the time index in the numerical scheme, $w = (w^1, \ldots, w^N)$ the discrete direct state variables matrix of dimension (K+1)*N, with the discrete vector $w^n = (T_1^n, T_2^n, \cdots, T_K^n, s^n)$ of dimension (K+1), T_m^n the discrete computed temperature at time n, at grid point m, for the K different points on the grid, s^n the discrete computed ablation, at time n. The equation (6) is written at time *(n+1) :*

$$\begin{aligned} &\frac{w^{n+1} - w^n}{\Delta t} = f\left(w^{n+1}\right) \\ &w^0 = 0 \qquad 0 \le n \le N \end{aligned} \tag{8}$$

A linearization of the equation (8) is made at time *n* and after some calculations, we finally obtain a forward time discrete linearized Euler scheme, with initial condition vanishing:

$$\begin{aligned} &\frac{w^{n+1} - w^n}{\Delta t} = f\left(w^n\right) + (df)\left(w^n\right)\left(w^{n+1} - w^n\right) \\ &w^0 = 0 \qquad 0 \le n \le N \end{aligned} \tag{9}$$

2. Inverse problem

Parameter, cost function, Lagrangian

Inverse problems deals with the identification of unknowns and the improvement of the understanding of physical processes quantities which appear in the mathematical formulation of physical problems, by using measurements of the system response.
The inverse problem concerns the identification of the 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 $0 \le t \le t_f$, where t_f denotes the final time. The inverse problem is reformulated 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).
The key strategy to obtain an accurate numerical approximation of the gradient, 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 content of the unknown heat flux convection coefficient is represented by a vector $p = \left(p^1,\ldots,p^N\right)$ which is sampled over time, where the subscripts refer to the sampled time. N is the number of unknowns and time iterations. These sampled values will be the *control parameter variables*.
To simplify our presentation, we present the inverse problem with measurements data with only one thermocouple sensor, point m in the grid. Therefore, the first step in establishing a procedure for the solution of either inverse is thus the definition of an objective (cost) function: it is in our case a least squares performance index *J(p)* that measures the difference between model predictions T_m^n of temperature, given a heat flux parameter *p* value, and measurements temperatures θ_m^n, at point m on the grid, time (n). The quadratic error or cost function j(p), depending on the source parameters p, is defined by :

$$J(p) = J\Big(\underbrace{w^1(p),\ldots,w^N(p)}_{\text{variables } W}\Big) = \sum_{n=1}^{N}\left(T_m^n - \theta_m^n\right)^2 \Delta t \qquad (10)$$

with θ_m^n the discrete measured temperature, at time n, point m, and T_m^n the discrete computed temperature vector, at time n, point m. To minimize this quantity, by optimization algorithm, we need the derivatives of this least squares objective function J(p), with respect to the parameters p.

<u>Adjoint and gradients computations</u>

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

$$\begin{aligned}
L(p,w,\varphi) &= L\Bigg(\underbrace{p^1,\ldots,p^N}_{parameter\ p},\underbrace{w^1,\ldots,w^N}_{\text{variables } w},\underbrace{\varphi^{1/2},\ldots,\varphi^{N+1/2}}_{\text{adjoint variables } \varphi}\Bigg) \\
&= \sum_{n=1}^{N}\left(T_m^n - \theta^n\right)^2 \Delta t \qquad (11)\\
&+ \sum_{n=0}^{N-1}\left\langle \varphi^{n+1/2}, \frac{w^{n+1}-w^n}{\Delta t} - f\left(w^n\right) - (df)\left(w^n\right)\left(w^{n+1}-w^n\right)\right\rangle
\end{aligned}$$

Differentiating the Lagrangian *L* with first order sensitivity variations, computing δL as function of $\delta p, \delta w, \delta\varphi$, the variations of δL with respect to δw are cancelled with an adequate choice of the adjoint state φ. It leads to the discrete adjoint system[31] in $\varphi^{n-1/2}$ unknown, *n* going backward from N to 0,

$$\begin{aligned}
&\frac{\varphi^{n-1/2} - \varphi^{n+1/2}}{\Delta t} = df^{\,t}\left(w^{n-1}\right)\varphi^{n-1/2} \\
&+ \left[\left(d^2 f\right)\left(w^n\right)\left(w^{n+1} - w^n\right)\right]\varphi^{n+1/2} + 2\left(T_m^n - \theta_m^n\right)^2 \Delta t \qquad (12)\\
&w^{N+1/2} = 0 \qquad N \geq n \geq 0
\end{aligned}$$

With this particular choice of φ, the gradient of the cost function is simply obtained by :

$$\nabla J = \frac{\partial J}{\partial p} = \frac{\partial L}{\partial p} \qquad (13)$$

<u>Optimization</u>

After computation of the gradient of cost function, we can now apply an iterative inverse procedure minimizing *J(p)* to obtain an estimation of the unknown parameter optimal function p_{opt} . We will use the combination of a gradient steepest descent method at the beginning of minimization and a Quasi Newton method to finish the minimization.

2. Automatic Differentiation

To compute numerically the adjoint and gradient discrete quantities for the inverse problem in heat convection coefficient, we have also used the Automatic Differentiation (AD) engine tool, Tapenade, developed at INRIA Sophia-Antipolis by the Tropics team[6]**.** Automatic differentiation is a family of techniques for computing the derivatives of a function defined by a computer program (interpreted as computing a mathematical function, including arbitrarily complex simulation codes), for sensitivity and gradient analysis applications**.** The new program obtained is called the differentiated program. Automatic differentiation with adjoint models and gradients computations are used in many fields of science such as pioneering work in meteorology**.**
The derivatives of the instructions of a program (elemental operations) are combined according to the chain rule of differential calculus, leading to the two major modes of computing derivatives with AD, the so-called forward (tangent-linear) mode and reverse (cotangent-linear or adjoint) mode.

- The forward mode uses directional derivatives on a given direction vector in the input space (tangent approach. It is appropriate to derive functions with small numbers of independent variables (input).
- The reverse mode uses derivatives starting with the dependent variables (output) and proceeding toward the independent variables (input), and it is computed in the reverse of the original program's order. It is appropriate for functions with small numbers of dependent variables (output) and lots of input independent variables. The reverse mode of automatic differentiation is functionally equivalent to hand written discrete adjoint codes.

The implementation of robust and effective automatic differentiation tools requires advances in compiler technology, graph algorithms, and automatic differentiation theory, and compared with other methods to compute adjoint and gradients, automatic differentiation offers a number of advantages:

- Accuracy: derivatives computed via automatic differentiation exhibit no truncation error.
- Reduced software costs: automatic differentiation eliminates the time spent developing and debugging derivative code by hand, or experimenting with step sizes for finite difference approximations.

The adjoint code in φ variables is built by automatic backward differentiation of the output J versus W direct state variables, following and analyzing the flow of instructions in the direct program, and the dependences in W . The gradient computation of $J(p)$ versus p parameter is built by automatic backward differentiation of the output $J(p)$ versus p parameter, also following the flow of instructions in the direct program and analyzing the flow dependences in p . It can be shown again that the gradient result depends on the W direct state variable and the φ adjoint state variable.

2. Numerical results

Synthetic test case

Some applications of time domain surface heat convection coefficient inverse problem for thermally degradable material are now presented. The material is a one-dimensional slab of thickness e, and time domain temperature measurements are used below the boundary surface, at a given thermocouple position, during a time interval. We start the minimization loop by an initial guess on convection coefficient and try to identify or reconstruct the good convection coefficient. In all the following curve results legends, INI stands for initial guess of the convection coefficient, NUM for reconstruction obtained at the end of optimization process, and OBS for the reference solution of the convection coefficient. The final time is denoted by t_f . The estimated temperatures are obtained from the solution of the direct problem, by using a given well known convection coefficient $\alpha_0(t)$. We want to restitute by inversion this coefficient.

Moreover, we define now two similar quality estimators for inverse problem :

- A good estimator for the quality of restitution of temperature measurements is the RMS_T error between the θ_m^n measured temperature and the reconstructed temperature $Topt_m^n$, at sensor m, at optimal inverse solution p_{opt} :

$$RMS_T = EQM = \sqrt{\frac{\sum_{n=1}^{N}\left(Topt_m^n - \theta_m^n\right)^2}{N}} \quad (14)$$

- A good estimator for the quality of restitution/identification of convection coefficient is the RMS_p error between the reference α_0 convection coefficient and the reconstructed optimal p_{opt} :

$$RMS_p = \sqrt{\frac{\sum_{n=1}^{N}\left(p_{opt}^n - \alpha_0{}^n\right)^2}{N}} \quad (15)$$

<u>Identification of High Flux with ablation, Carbon/Resin material , x0=2.6 mm</u>

It is a quite difficult test case, containing high fluxes. In Fig. 1, good results are obtained in the reconstructed convection coefficient, except at final time, with initial half guess and using synthetic data (errorless measurements). The RMS error on the flux is 0.06.

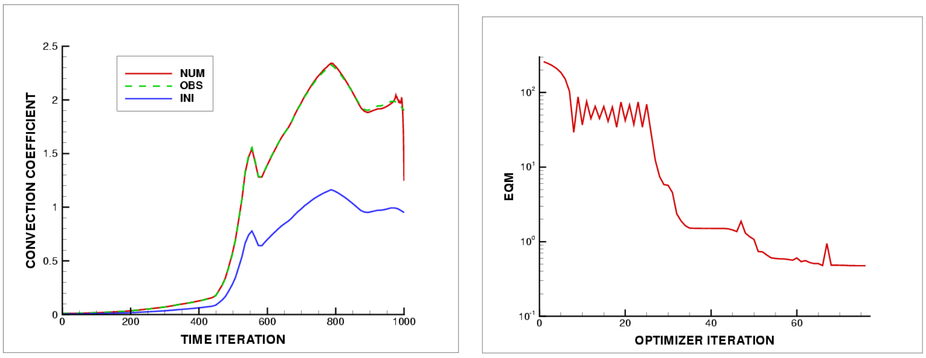

Figure 1 Identification of High Flux with ablation, x0=2.6 mm

Fig. 1 shows also that the RMS error on measured temperature, at the end of optimization process, is very low (0.7), after 70 optimizer iterations. RMS (EQM) error on temperatures
Fig. 2 shows results in the convection coefficient obtained, with initial half of the value, additive, uncorrelated, normally distributed, zero mean and known standard deviation (2%) noise, and uniform distributed, zero mean and known standard deviation (5%) noise. The RMS error on the flux is 0.105 and 0.125., which is satisfactory.

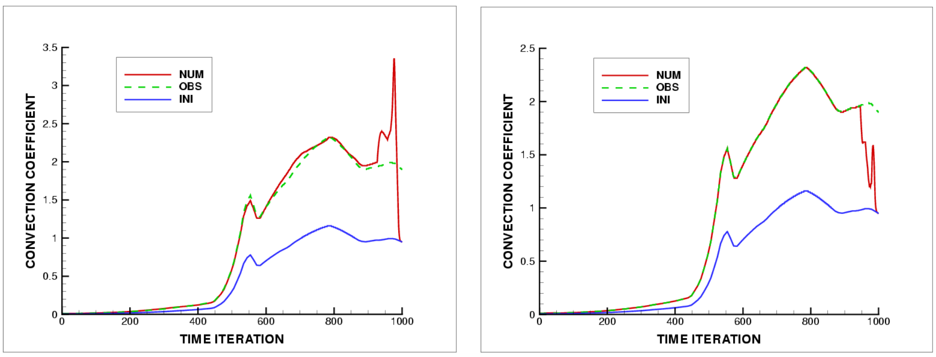

Figure 2: Identification of High Flux with ablation, with 2% normal / 5% uniform noise , x0=2.6 mm

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 used with four coupled plasma torchs.
The measurements of sensors 1 to 4 (among the 8 sensors available at different depth) are treated all together in a multi-sensors inversion process, with high ablation and high fluxes experiments conditions. We analyze the heat flux restitution obtained
We show Fig. 3 the sensitivity to the inverse convection coefficient problem, for two different initial guess on the flux. The shape of the different convection coefficients results (Num, Num 2) seems quite robust to the two different initial guess (Init, Init 2).

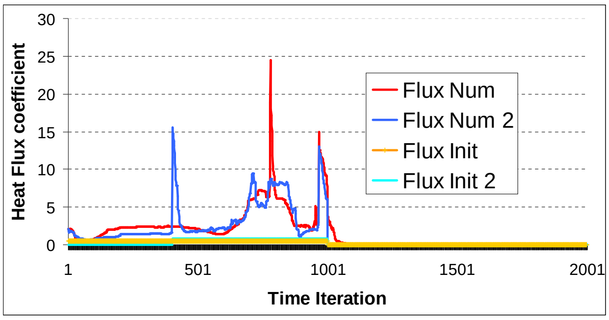

Figure 3 Flux identification
Two different initial guess (Init, Init 2) and Two different flux results (Num, and Num 2)

We show Fig. 4 the comparisons between the measurements (TC Obs) of temperature and the simulated (TC Num) temperatures obtained after the optimization process, on the thermocouple sensors N°1 to 4. The agreement is quite good, from sensors close to the surface (N°1) to sensor more deeply located in the slab (N°4). The final quadratic cost (eqm) is equal to 262, with a total of 150 optimizers iterations (gradient + quasi Newton optimization).

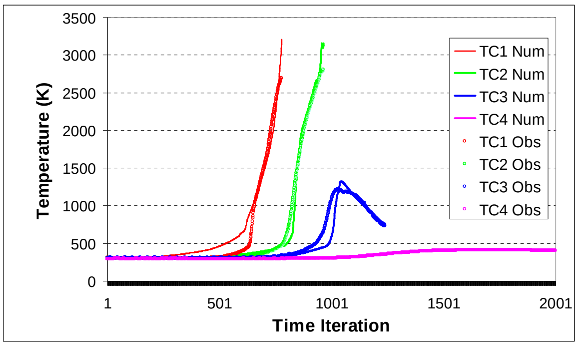

Figure 4: simulated (Num) and measured (obs) levels of temperatures at the sensors N°1 to 4, for the identified convection coefficient (Num)

Using the common information of the four sensors, we can see that the simulated ablation values (for heat flux Num) and the restitution of surface temperature are quite comparable to the measured ones (Fig. 5). The respective comparison to pyrometer measurements and surface temperature measurements are encouraging. An other source of error lies in the experimental process and in the 1D Monopyro model, taking into account the conduction and diffusion effect between all the sensors.

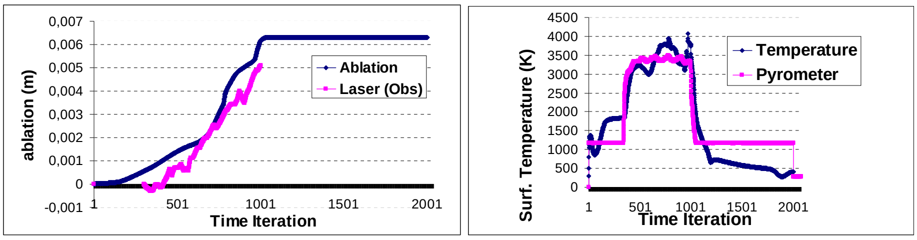

Figure 5 : simulated (num) and measured (Laser Obs) levels of ablation. Simulated (Temp) and measured (Pyrometer) levels of surface temperatures.

3. 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.
The inverse problem is formulated as a minimization problem involving a least square problem functional, through an optimization loop. An optimal control formulation (Lagrangian, adjoint and gradient computations) is then applied and developed, using an inverse software Monopyro which was developed at EADS ASTRIUM-ST Les Mureaux, and which is a transient one-dimensional thermal code, with ablative surface and Gear integration scheme.
Several validation test cases, using synthetic, noisy on-ground and in-flight data temperatures measurements are carried out, by applying the results of the minimization algorithm. Main results are:

- Validity of the inverse formulation for the description of 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 high heat fluxes and large magnitudes, ablation effects, and operational data
- Encouraging results with an automatic differentiation tool are also obtained, without ablation
- Implementation of the automatic differentiation tool to generate the inverse code,

Current works have started and have to be extended on the:

- Robustness to initial guess, sensitivity to measurements, number and position of sensors, and application of regularization methods to stabilize noise errors on measurements,
- Thermal model uncertainties influences on the accuracy of extracted flight heat flux, athermanous enthalpy identification,
- Validations on new implicit non linear Monopyro solver and aerothermal flight measurements

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