UNCERTAINTY QUANTIFICATION FOR CHARACTERIZATION OF HIGH ENTHALPY FACILITIES

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The postflight analysis of a space mission requires accurate determination of the free-stream conditions for the trajectory. The Mach number, temperature, and pressure conditions can be rebuilt from the heat flux and pressure measured on the spacecraft by means of a Flush Air Data System (FADS). This instrumentation comprises a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and heat flux (calorimeters). Knowing that experimental data suffer from errors, this methodology needs to integrate quantification of uncertainties. Epistemic uncertainties on the models for chemistry in the bulk and at the wall (surface catalysis) should also be taken into account. To study this problem it is necessary to solve a stochastic backward problem. This paper focuses on a preliminary sensitivity analysis of the forward problem to understand which uncertainties need to be accounted for. In section 2, the uncertainty quantification methodologies used in this work are presented. Section 3 is dedicated to the one-dimensional (1D) simulations of the shock layer to identify which chemical reactions of the mechanism need to be accounted for in the Uncertainty Quantification (UQ). After this triage procedure, the two-dimensional (2D) axisymmetric flow around the blunt nose was simulated for two trajectory points of EXPERT (EXPERimental Reentry Test-bed) is simulated and the propagation of the uncertainties on the stagnation pressure and heat flux has been studied. To do this study, the open source software DAKOTA from Sandia National Laboratory [1] is coupled with two in-house codes: SHOCKING that simulates the evolution of the chemical relaxation in the shock layer [2], and COSMIC that simulates axisymmetric chemically reacting flows [3].

1 INTRODUCTION

Many achievements in the rocket science have been made since Apollo, but the prediction of the heat flux to the surface of a spacecraft remains an imperfect science, and inaccuracies in these predictions can be fatal for the crew of a spacecraft or the success of robotic missions. This quantity is estimated during the design phase for the heat shield used to protect the payload and astronauts. Predicting an accurate heat-flux is a particularly complex task, regarding the uncertainty on the models for the complex multiphysics phenomena involved in hypersonic flows as well as the uncertainty on atmospheric properties such as the density and the temperature. Hence, it is difficult to establish “error bars” on the heat-flux prediction. To avoid a space mission failure and to ensure the safety of the astronauts and the payload, engineers resort to safety factors to determine the heat shield thickness, at the expense of reducing the mass of the embarked payload. The design of Apollo, Galileo, and Huygens are famous examples of a “lucky” heat shield design with a barely enough safety factor [4].

Uncertainty Quantification is a systematic approach to establish “error bars.” At the interface of physics, mathematics, and statistics, UQ tools aim at developing rigorous methods to characterize the impact of the “limited knowledge” on quantities of interest (QOIs), such as the heat flux. This limited knowledge arises from uncertainties related to the inputs of any computation attempting to represent a physical system. The uncertainties are naturally associated to the choice of the physical models and to the specification of the input parameters required for performing an analysis. As an example, numerical simulations require a precise specification of boundary conditions and, typically, only limited information is available from corresponding experiments and observations. Errors associated to the translation of a mathematical formulation into a numerical algorithm (and a computational code) are not considered here as uncertainties.

The postflight analysis of a space mission requires an accurate determination of the free-stream conditions for the trajectory. The Mach number, temperature and pressure conditions can be rebuilt from the heat flux and pressure measured on the spacecraft by means of a FADS. This instrumentation comprises a set of sensors flush mounted in the thermal protection system to measure the static pressure (pressure taps) and the heat flux (calorimeters). Knowing that experimental data suffer from errors, this methodology needs to integrate the quantification of uncertainties. Epistemic uncertainties on the models for chemistry in the bulk and at the wall (surface catalysis) should also be taken into account. Rebuilding the free stream conditions from the FADS data amounts to solving a stochastic inverse problem. As shown in [5], the state-of-the-art techniques for free-stream characterization rely on several approximations, such as the equivalent specific heat ratio approximation, which means that one replaces a complex high temperature effect including thermochemical nonequilibrium by

Table 1 Free stream conditions for two trajectory points of the EXPERT vehicle

Flow conditions	Altitude, km	p_∞ , Pa	T_∞ , K	M_∞
Chemical nonequilibrium	60	20.3	245.5	15.5
Chemical equilibrium	30	1200	220	12.3

an “equivalent” calorically perfect gas. This approximation is then used, starting from Pitot measurements, to reconstruct the stagnation pressure, the free stream conditions and to prescribe the error intervals on these quantities. This methodology cannot take into account the heat flux contribution nor the various uncertainties related to measurement errors. It is known that a correct knowledge of the heat flux drives more complex models such as the gas–surface interaction. This paper is the first step to the design of an improved methodology for rebuilding the free stream conditions based on a stochastic inverse problem. The forward problem is studied here. Two points of the trajectory of the European EXPERT vehicle, which has been developed by the European Space Agency as a part of its General Technological Research Program, are investigated. The first trajectory point corresponds to chemical nonequilibrium flow conditions, and the second one — to chemical equilibrium conditions, as reviewed in Table 1. The aim is to study how the uncertainty on the free stream conditions and on the chemical mechanism propagates to two QOIs: the pressure and the heat flux at the stagnation point.

In section 2, the uncertainty quantification methodologies used in this work are presented. Section 3 is dedicated to 1D simulations of the shock layer to identify which chemical reactions of the mechanism need to be accounted for in the UQ. After this triage procedure, in section 3, the 2D axisymmetric flow around the blunt nose for two trajectory points of EXPERT is simulated and the propagation of the uncertainties on the QOIs is studied. The open source software DAKOTA from Sandia National Laboratory [1] is coupled with two in-house codes: SHOCKING that simulates the evolution of the chemical relaxation in the shock layer [2], and COSMIC that simulates axisymmetric chemically reacting flows [3].

2 UNCERTAINTY QUANTIFICATION

To apply UQ tools to the problem, the first step is to define QOIs (or outputs): the pressure p_{st} and the heat flux q_{st} at the stagnation point. Next, possible sources of uncertainty on these QOIs are searched. The following random variables (or inputs) are selected: the free stream Mach number M_∞ , the free stream

pressure p_∞ , the preexponential factor A_r of the reaction rate coefficients for the gas-phase reactions, and the effective catalytic recombination coefficient γ for the gas-surface interaction. Then, uncertainty quantification methods can be used to compute error bars on the QOIs and correlations between the inputs and outputs. In this paper, two kinds of methodology are used: sampling and stochastic expansion. In this section, these methodologies and the statistical data that they allow to compute are presented.

2.1 Sampling

In this case, the quantity of interest y is computed for a given number of samples of the input data. Two sampling methods are considered for the random variables:

- random sampling based on a Monte-Carlo method; and
- Latin Hypercube Sampling (LHS): the range of each random variables is divided in intervals with equal probability, leading to hypercubes in the stochastic space. Then, one sample is chosen for each hypercube.

In the following section, the LHS is used. If N_s is the number of sampling and y_i is the value of the quantity of interest at the i th sample, the following statistical data can be computed based on these sampling methods:

- the expected value:

$$E(y) = \frac{1}{N_s} \sum_{i=0}^{N_s} y_i ; \quad (1)$$

- the variance:

$$\text{Var}(y) = \frac{1}{N_s} \sum_{i=0}^{N_s} [y_i - E(y)]^2 ; \quad (2)$$

- from the variance, the standard deviation can be deduced:

$$\sigma = \sqrt{\text{Var}(y)} ; \quad (3)$$

- the Pearson correlation coefficient between the input x and y :

$$\text{Pear}(x, y) = \frac{\sum_{i=0}^{N_s} [x_i - E(x)] [y_i - E(y)]}{\sqrt{\sum_{i=0}^{N_s} [x_i - E(x)]^2 [y_i - E(y)]^2}} . \quad (4)$$

The Pearson correlation coefficients give only a rough indication of the influence of x on y . In particular, it measures how close to a line are the points of coordinates (x, y) . The values obtained by means of Eqs. (1)–(4) are reliable only if the number of samples N_s is large enough. Hence, in the case of 2D computational fluid dynamics (CFD) simulations, this method is computationally expensive. For this reason, the stochastic expansion methods with a lower computational cost was also used.

2.2 Stochastic Expansion: Polynomial Chaos

This method is similar to the finite element method used for deterministic problems: Askey polynomials [6] are used to discretize the aleatory variables. This group of polynomial has the advantage of providing a class of optimal polynomial for each kind of Probability Distribution Function (PDF) (for instance, a Gaussian function will be adequately discretized by means of a combination of Hermitian polynomials). Let us consider a problem with two aleatory variables $(\xi_0; \xi_1)$, the discretization of order 1 of the output $y(\xi_0, \xi_1)$ is as follows:

$$y = \sum_{i=0}^2 \alpha_i \Psi_i$$

where the functions

$$\begin{aligned} \Psi_0 &= \psi_0(\xi_0)\psi_0(\xi_1); \\ \Psi_1 &= \psi_1(\xi_0)\psi_0(\xi_1); \\ \Psi_2 &= \psi_0(\xi_0)\psi_1(\xi_1) \end{aligned}$$

are based on orthogonal polynomials ψ_1 and ψ_0 of the order 0 and 1 that have been chosen to discretize the aleatory variables. To compute the α_i coefficients, a spectral projection is used:

$$\alpha_i = \frac{\langle y, \Psi_i \rangle}{\langle \Psi_i, \Psi_i \rangle}$$

In this formula, the denominator can be computed analytically, and it is only necessary to compute the numerator, for instance, by using quadrature rules or a sparse grid of Smolyak [7]. Using the discretization of the response, it is possible to compute its expected value:

$$E(y) = \int f(y)y \, dy = \sum_k y_k w_k$$

where symbol f stands for the PDF of y and symbol w_k for the weights of the quadrature rule in which f is included. The total variance is given by the relation:

$$\text{Var}(y) = E([y - E(y)]^2).$$

Finally, the Sobol indices [8] can be computed to study the sensitivity of y to each random variables. They compare the variance of the conditional expectation $\text{Var}_{\xi_i}[E(y|\xi_i)]$ against the total variance $\text{Var}(y)$. The formula for the Sobol indices is:

$$S_i = \frac{\text{Var}_{\xi_i}[E(y|\xi_i)]}{\text{Var}(y)} \quad (5)$$

where, for instance, the conditional expectation is

$$E(y|\xi_0) = \int f(\xi_0, E(\xi_1))y(\xi_0, E(\xi_1)) d\xi_0.$$

Higher order Sobol indices can also be defined with conditional expectation based on several variables (provided that the stochastic dimension is larger than 2). The main drawback of the stochastic expansion is that the dimension of the stochastic space is limited by the computational time, this is called the curse of dimensionality. For this reason, the triage of the chemical reactions follows two steps. First, the chemical reactions that influence the most of the gas compositions at the boundary layer edge are found using the LHS method. Then, when the main contributions are determined, Polynomial Chaos (PC) is used to get a more accurate calculation of the correlations, since Pearson's correlation coefficients are used in LHS instead of variance-based coefficients in PC.

3 STUDY OF THE GAS COMPOSITION AFTER A SHOCK

3.1 Background

In this section, the QOIs are the concentration of nitrogen $[N]_w$, and oxygen $[O]_w$ at the distance from the shock corresponding to the stand-off distance of the two trajectory points. This choice of QOI is motivated by the major influence of the recombination of atoms at the surface on a reusable thermal protection material. To compute the evolution of the chemical composition of the gas after the shock, we use the SHOCKING code [2]. The population of electronic energy levels are obtained from detailed chemistry mechanism for electronic energy levels of atoms and the rotational/vibrational energy levels of molecules based on Boltzmann distributions. The code computes the downstream flow field using the 1D conservation equations of mass, momentum and global energy plus the conservation of vibrational energy of the nitrogen molecules. This code does

not account for the deceleration due to the body and the stand-off distance is imposed a priori to an approximate value equal to 3.8 cm. The chemical model is the one of Park *et al.* [9] for a mixture of eleven species.

Following the suggestion of [10], the random variable for the chemical reactions is the preexponential factor A_r of the Arrhenius rate equation: $k_r = A_r T^b \exp(-C_r/T)$. Indeed, other parameters such as the activation energy are known with higher accuracy. The preexponent coefficients are assumed to vary following a logarithmic normal distribution with a probability distribution defined by:

$$P(k_r) \propto \exp \left[-\frac{1}{2} \left(\frac{\log_{10}(k_r/k_r^0)}{\sigma} \right)^2 \right] \quad (6)$$

where k_r^0 represent the mean value and σ is the standard deviation of k_r given in Table 1. The free stream parameters are not considered here as random variables in this section, because the goal of this step is to simplify the stochastic problem by selecting the gas reactions which contribute the most to the error on the pressure and the heat flux at the stagnation point. Here, only the results obtained for the trajectory point corresponding to a chemical nonequilibrium flow given in Table 3 are shown. The influence of the reaction rate coefficients is, certainly, not studied for the equilibrium situation.

Table 1 Standard deviation for the reaction rate coefficients preexponential factors

Gas reaction	Deviation σ
$O_2 + M \rightarrow 2O + M$ $M = O_2, NO, N_2, O, N$	0.10
$NO + M \rightarrow N + O + M$ $M = O_2, NO, N_2, O, N$	0.12
$N_2 + M \rightarrow 2N + M$ $M = O_2, NO, N_2$	0.11
$N_2 + M \rightarrow 2N + M$ $M = O_2, NO, N_2$	0.11
$N_2 + M \rightarrow 2N + M$ $M = O, N$	0.15
$N_2 + O \rightarrow NO + N$ $O_2 + N \rightarrow NO + O$	0.10
$N + O \rightarrow NO^+ + em$	0.13
$N + N \rightarrow N_2^+ + em$ $O + O \rightarrow O_2^+ + em$	0.10
$O + em \rightarrow O^+ + 2em$	0.12
$N + em \rightarrow N^+ + 2em$	0.09
$NO^+ + O \rightarrow N^+ + O_2$	0.10
$O_2^+ + N_2 \rightarrow N_2^+ + O_2$ $O^+ + NO \rightarrow N^+ + O_2$	0.13
$O_2^+ + N_2 \rightarrow N_2^+ + O_2$	0.14
$O_2^+ + N_2 \rightarrow N_2^+ + O_2$ $NO^+ + N \rightarrow O^+ + N_2$ $NO^+ + O_2 \rightarrow O_2^+ + NO$ $NO^+ + O \rightarrow O_2^+ + N$ $O^+ + N_2 \rightarrow N_2^+ + O$ $NO^+ + N \rightarrow O_2^+ + O$	0.10

Table 3 Postshock flow field characteristic

N_2	O_2	p_∞ , Pa	V_∞ , m/s	T_∞ , K
79%	21%	20	5000	256

3.2 Results

3.2.1 Latin hypercube sampling

First, the LHS method to select the 10 most important reactions is used. To quantify the convergence of the stochastic method, the standard deviation of the concentrations $[N]_w$ and $[O]_w$ is used. In Fig. 1, the deviation of both QOIs is plotted with respect to the number of samples used by the LHS method. As can be observed, after 30 000 samples, the deviation reaches a plateau, meaning that the LHS has converged. Next, the results obtained with 50 000 samples are analyzed. Figure 2 makes it clear that the 4 main contributors to the error on

Figure 1 Convergence of the LHS on the deviations for the concentrations $[N]_w$ (a) and $[O]_w$ (b)

Figure 2 Correlation between the reaction rate coefficients and the concentrations of $[N]_w$ (a) and $[O]_w$ (b). Numbers refer to the number of reaction in Tables 4 and 5

Table 4 Sobol indices of $[N]_w$

No.	Reaction	First order	Second order
1	$\text{NO} + \text{O} \rightarrow \text{N} + \text{O} + \text{O}$	$8.83 \cdot 10^{-1}$	$8.81 \cdot 10^{-1}$
2	$\text{NO} + \text{N} \rightarrow \text{N} + \text{O} + \text{N}$	$4.25 \cdot 10^{-2}$	$4.40 \cdot 10^{-2}$
3	$\text{O}_2 + \text{O} \rightarrow \text{O} + \text{O} + \text{O}$	$4.00 \cdot 10^{-2}$	$4.06 \cdot 10^{-2}$
4	$\text{O}_2 + \text{N}_2 \rightarrow \text{O} + \text{O} + \text{N}_2$	$1.35 \cdot 10^{-2}$	$1.35 \cdot 10^{-2}$
5	$\text{NO} + \text{NO} \rightarrow \text{N} + \text{O} + \text{NO}$	$9.35 \cdot 10^{-3}$	$1.01 \cdot 10^{-3}$
6	$\text{NO} + \text{N}_2 \rightarrow \text{N} + \text{O} + \text{N}_2$	$7.77 \cdot 10^{-3}$	$8.26 \cdot 10^{-3}$
7	$\text{N}_2 + \text{O} \rightarrow \text{NO} + \text{N}$	$1.64 \cdot 10^{-3}$	$2.25 \cdot 10^{-3}$
8	$\text{O}_2 + \text{N} \rightarrow \text{O} + \text{O} + \text{N}$	$1.34 \cdot 10^{-3}$	$1.42 \cdot 10^{-3}$
9	$\text{N}_2 + \text{O} \rightarrow \text{N} + \text{N} + \text{O}$	$3.07 \cdot 10^{-4}$	$3.66 \cdot 10^{-4}$
10	$\text{O}_2 + \text{O}_2 \rightarrow \text{O} + \text{O} + \text{O}_2$	$9.97 \cdot 10^{-5}$	$1.20 \cdot 10^{-4}$

Table 5 Sobol indices of $[\text{O}]_w$

No.	Reaction	First order	Second order
1	$\text{NO} + \text{O} \rightarrow \text{N} + \text{O} + \text{O}$	$8.75 \cdot 10^{-1}$	$8.752 \cdot 10^{-1}$
2	$\text{O}_2 + \text{N}_2 \rightarrow \text{O} + \text{O} + \text{N}_2$	$4.49 \cdot 10^{-2}$	$4.670 \cdot 10^{-2}$
3	$\text{NO} + \text{N} \rightarrow \text{N} + \text{O} + \text{N}$	$4.27 \cdot 10^{-2}$	$4.540 \cdot 10^{-2}$
4	$\text{O}_2 + \text{O} \rightarrow \text{O} + \text{O} + \text{O}$	$1.45 \cdot 10^{-2}$	$1.490 \cdot 10^{-2}$
5	$\text{NO} + \text{NO} \rightarrow \text{N} + \text{O} + \text{NO}$	$9.27 \cdot 10^{-3}$	$1.060 \cdot 10^{-2}$
6	$\text{NO} + \text{N}_2 \rightarrow \text{N} + \text{O} + \text{N}_2$	$7.79 \cdot 10^{-3}$	$8.570 \cdot 10^{-3}$
7	$\text{O}_2 + \text{N} \rightarrow \text{O} + \text{O} + \text{N}$	$1.59 \cdot 10^{-3}$	$1.690 \cdot 10^{-3}$
8	$\text{N}_2 + \text{O} \rightarrow \text{NO} + \text{N}$	$1.98 \cdot 10^{-4}$	$3.750 \cdot 10^{-4}$
9	$\text{N}_2 + \text{O} \rightarrow \text{N} + \text{N} + \text{O}$	$2.55 \cdot 10^{-4}$	$3.010 \cdot 10^{-4}$
10	$\text{O}_2 + \text{O}_2 \rightarrow \text{O} + \text{O} + \text{O}_2$	$9.74 \cdot 10^{-5}$	$1.190 \cdot 10^{-4}$

Figure 3 Correlation between the reaction rate coefficients $\text{NO} + \text{O} \rightarrow \text{N} + \text{O} + \text{O}$ and the concentrations of $[N]_w$ (a) and $[O]_w$ (b)

$[N]_w$ and $[O]_w$ are identical but with a different ranking keeping the dissociation reaction $\text{NO} + \text{O} \rightarrow \text{N} + \text{O} + \text{O}$ as a major contributor for both uncertainties. This strong correlation is confirmed based on Fig. 3 where the cloud of samples is presented.

3.2.2 Polynomial chaos

The results obtained with the LHS method allow to determine the more important reactions. In Tables 4 and 5, the Sobol indices obtained with the first-order PC confirmed that the major contribution is the reaction $\text{NO} + \text{O} \rightarrow \text{N} + \text{O} + \text{O}$. The other reactions have a very small contribution to the uncertainty of the gas composition at the boundary layer edge. Moreover, comparing the results obtained with a second-order PC to those obtained with a first-order discretization, very similar Sobol indices are observed. This means that there are no major cross influence and that the reaction rate of $\text{NO} + \text{O} \rightarrow \text{N} + \text{O} + \text{O}$ is linearly correlated to the gas composition near the body. This is in agreement with Fig. 3.

4 INFLUENCE OF MEAN FLOW CONDITIONS
AND CHEMICAL MODEL
ON PRESSURE AND HEAT FLUX
AT THE STAGNATION POINT

4.1 Background

Table 6 Stagnation point heat flux obtained by means of different mixtures

Mixture	q_{st}
air5	$3.6 \cdot 10^6$
air7	$3.7 \cdot 10^6$
air11	$3.7 \cdot 10^6$

The results of the former section allow studying the impact of the chemical model and of the mean flow characteristics on the pressure and the heat-flux measured at the stagnation point of the EX-PERT vehicle. To compute these QOIs, the in-house code COSMIC [3], a cell-centered finite volume 2D axisymmetric Navier–Stokes solver is used. It includes a set of physicochemical models to simulate high temperature reacting flows, including the gas–surface interaction. Indeed, the wall of the spacecraft acts as a catalyzer and promotes recombination of atoms. This phenomenon is modeled by a catalytic wall at radiative equilibrium where quantity γ represents the proportion of gas impinging the body that will recombine, the so-called effective catalytic recombination coefficient. In order to choose a reduced mixture of species suitable for the considered application, the simulations were carried out using mixtures with, respectively, 5, 7, and 11 species. In Table 6, it is verified that the stagnation point heat flux obtained by means of the 5-species mixture was accurate enough

Figure 4 Pressure field for the CFD simulation of the point at nonequilibrium (a) and at equilibrium (b) trajectory points.

with respect to the one obtained by means of 7 and 11 species. Then, it is possible to use a mixture of 5 of the following species: N_2 , O_2 , N , O , and NO and the corresponding Park chemical mechanism.

Finally, the two trajectory points of Table 1 are considered. Figure 4 shows the pressure contours of the simulation of the two points.

4.2 Results

For this study, the random variables are the free stream Mach number M_∞ and the pressure p_∞ , the gas reaction rate coefficients of $\text{NO} + \text{O} \rightarrow \text{N} + 2\text{O}$, $\text{NO} + \text{N} \rightarrow 2\text{N} + \text{O}$, $\text{O}_2 + \text{O} \rightarrow 2\text{O} + \text{O}$ and $\text{O}_2 + \text{N}_2 \rightarrow 2\text{O} + \text{N}_2$, and the effective catalytic recombination coefficient γ . The reaction rate coefficients follow the same distribution as in Table 1. Concerning the free stream parameters and the recombination factor, their probability distribution are detailed in Table 7. The free stream Mach number and pressure are assumed to follow a Gaussian distribution. Finally, given the recombination conditions, the uncertainty on γ is due to a lack of knowledge, it is usual to consider its PDF as uniform.

As can be seen in Table 8, the quantities M_∞ and p_∞ have the largest impact on p_{st} with an equivalent magnitude. The reaction rate coefficients and the effective recombination factor do not have any effect on the the pressure uncertainty.

Table 7 Distribution of the random variables for the flow at nonequilibrium (left) and at equilibrium (right) trajectory points

Variable	Distribution	Mean	Deviation	Max	Min
M_∞	Gaussian	15.5/12.03	0.875/0.875	—	—
p_∞ , Pa	Gaussian	20.3/1394.0	2/80	—	—
γ	Uniform	—	—	0.002/0.002	0.001/0.001

Table 8 Sobol indices of p_{st}

Parameter/reaction	Nonequilibrium	Equilibrium
M_∞	$5.76 \cdot 10^{-1}$	$8.62 \cdot 10^{-1}$
p_∞	$4.23 \cdot 10^{-1}$	$1.30 \cdot 10^{-1}$
$O_2 + N_2 \rightarrow 2O + N_2$	$2.14 \cdot 10^{-5}$	$3.54 \cdot 10^{-6}$
$O_2 + O \rightarrow 2O + O$	$3.75 \cdot 10^{-5}$	$2.67 \cdot 10^{-6}$
$NO + O \rightarrow N + O + O$	$5.36 \cdot 10^{-5}$	$1.68 \cdot 10^{-6}$
$NO + N \rightarrow N + O + N$	$2.69 \cdot 10^{-6}$	$1.38 \cdot 10^{-9}$
γ	$1.76 \cdot 10^{-8}$	$1.44 \cdot 10^{-8}$

This result was expected, as usually the chemistry only influences the heat flux. Indeed, the results are rather different when the heat-flux is considered. As shown in Table 9, the most important contribution comes from M_∞ , then with one order of magnitude less, is the the pressure p_∞ and γ . The chemical reaction rate coefficients have still very low effects on the uncertainty of the heat flux and the pressure at the stagnation point, but the Sobol indices are higher than for the stagnation pressure p_{st} . There could have been expected a stronger effect of the chemistry on the heat flux, an explanation to this result being that the flow considered here is at a moderate temperature and, if even the catalytic effects need to be accounted to compute the heat flux, it does not represent the biggest part of it. Moreover, γ is rather low and a smaller uncertainty is chosen than in [11].

The choice for this uncertainty is justified by a preliminary study on the uncertainty on the identification of the catalytic properties [12]. Finally, when the flow is at the chemical equilibrium, it is seen that the main contributor to the uncertainty on p_{st} are the free stream conditions M_∞ and p_∞ . The pressure p_∞ has a lower influence than in the case of a nonequilibrium flow. This is confirmed by the value of the Sobol indices of γ and of the reaction rates, which are almost null. The same behavior is present concerning the heat-flux. Finally, the error bars on the pressure and on the heat flux in Table 10 are examined. Concerning p_{st} , the uncertainty is of 50% for both types of the flow, whereas the error on q_{st} is bigger in the case of the flow in equilibrium.

Table 9 Sobol indices of q_{st}

Parameter/reaction	Nonequilibrium	Equilibrium
M_∞	$8.79 \cdot 10^{-1}$	$9.780 \cdot 10^{-1}$
p_∞	$8.53 \cdot 10^{-2}$	$3.453 \cdot 10^{-3}$
$O_2 + N_2 \rightarrow 2O + N_2$	$9.42 \cdot 10^{-4}$	$6.430 \cdot 10^{-5}$
$O_2 + O \rightarrow 2O + O$	$3.13 \cdot 10^{-3}$	$1.010 \cdot 10^{-4}$
$NO + O \rightarrow N + O + O$	$9.23 \cdot 10^{-3}$	$5.200 \cdot 10^{-5}$
$NO + N \rightarrow N + O + N$	$1.27 \cdot 10^{-3}$	$2.120 \cdot 10^{-8}$
γ	$2.12 \cdot 10^{-2}$	$1.740 \cdot 10^{-2}$

Table 10 Error bars for nonequilibrium (left) and equilibrium (right) flows

Parameter	Expected value	Relative error
p_{st} , Pa	$6.50 \cdot 10^3 / 2.68 \cdot 10^5$	45%/45%
q_{st} , W/m ²	$4.939 \cdot 10^5 / 6.55 \cdot 10^5$	51%/60%

5 CONCLUDING REMARKS

Reviewing the results, it was found that the chemical reaction influencing the most the concentration of N and O at the surface of the body are the nitric oxide dissociation reactions $NO + O \rightarrow N + 2O$, $NO + N \rightarrow 2N + O$, and the oxygen dissociation reactions $O_2 + O \rightarrow 2O + O$ and $O_2 + N_2 \rightarrow 2O + N_2$. Moreover, the free stream Mach number has the larger impact on the error on the pressure and the heat flux at the stagnation point. The influence of the chemistry on p_{st} is rather small, whereas it is a bite greater in the case of q_{st} . When a flow in the chemical equilibrium is considered, the impact of the chemistry is very small, as was expected. In the future, using the experimental uncertainties on the pressure and the heat flux measured at the surface of the body, the Bayesian theory is plotted to be used to reconstruct the free stream quantities using inverse problem methodologies [5].

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REFERENCES

1. Adams, B. M., W. J. Bohnhoff, K. R. Dalbey, J. P. Eddy, M. S. Eldred, D. M. Gay, K. Haskell, P. D. Hough, and L. P. Swiler. 2009. DAKOTA, a multilevel parallel object-oriented framework for design optimization, parameter estimation, uncertainty quantification, and sensitivity analysis: Version 5.0 User's Manual. Sandia Technical Report SAND2010-2183.
2. Magin, T. E., L. Caillault, A. Bourdon, and C. Laux. 2006. Nonequilibrium radiative heat flux modeling for the Huygens entry probe. *J. Geophys. Res. — Planets* 111(E7):E07S12.
3. Barbante, P. F. 2001. Accurate and efficient modelling of high temperature non-equilibrium air flows. Von Karman Institute, Belgium.
4. Park, C. 2008. Frontiers of aerothermodynamics. In: *Non-equilibrium gas dynamics from physical models to hypersonic flights*. RTO-EN-AVT-162.
5. Olivier, H., and P. zur Nieden. 2007. Determination of atmospheric density from reentry flight data. *J. Spacecraft Rockets* 44(2).
6. Askey, R., and J. Wilson. 1985. Some basic hypergeometric polynomials that generalize Jacobi polynomials. *Mem. Amer. Math. Soc.* 319. Providence, RI.
7. Smolyak, S. A. 1963. Quadrature and interpolation formulas for tensor products of certain classes of functions. *Dokl. Akad. Nauk SSSR* 4:240–43.
8. Tang, G., L. P. Swiler, and M. S. Eldred. 2010. Using stochastic expansion methods in evidence theory for mixed aleatory-epistemic uncertainty quantification. *AIAA Non-Deterministic Approaches Conference*. Orlando, FL.
9. Park, C., R. L. Jaffe, and H. Partridge. 2001. Chemical-kinetic parameters of hyperbolic earth entry. *J. Thermophys. Heat Transfer* 15(2-1).
10. Bose, D., M. Wright, and Gökçen. 2004. Uncertainty and sensitivity analysis of thermochemical modeling for titan atmospheric entry. AIAA Paper No. 2004-2469.
11. Bettis, B. R., and S. Hosder. 2011. Uncertainty quantification in hypersonic re-entry flows due to aleatory and epistemic uncertainties. *49th AIAA Aerospace Sciences Meeting Including the New Horizons Forums and Aerospace Exposition*. Orlando, FL.
12. Villedieu, N., F. Panerai, O. Chazot, and T. E. Magin. 2011. Uncertainty quantification for gas-surface interaction in plasmatron facility. *7th Aerothermodynamics Symposium*. Bruges, Belgium.