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Thermochemical ablation modeling forward uncertainty analysis—Part I: Numerical methods and effect of model parameters

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ABSTRACT

Next generation spacecraft will bring back heavier payloads from explored planets. Advance in the modeling of the thermo-chemical ablation of carbon-based thermal protection system materials is fundamental to improve the design capabilities of these vehicles. Computational fluid dynamic approaches are extensively used to model the gas-surface interaction phenomena over ablative materials. The advantage of such kind of approaches is the accurate description of the aerothermal environment obtained through the full resolution of the mechanical, thermal, and chemical boundary layers that develop over an ablative surface when exposed to a high-enthalpy flow. This paper is devoted to the assessment of the uncertainties of such kind of thermo-chemical ablation model and to study their effect on the model final outcomes. A sphere of non-pyrolyzing carbon-based material, exposed to conditions similar to those of a typical plasma wind tunnel test, is the selected test case for the analysis. Two forward non-intrusive uncertainty quantification techniques are used to analyze the influence of the defined set of uncertain parameters on the estimate of steady-state mass blowing flux and surface temperature. Our results show that for the selected conditions, and uncertainty ranges, the surface nitridation reaction probability has the strongest impact on the model outcomes.

1. Introduction

During the past decades space agencies have sent landers to Mars, Venus, and Titan and brought back samples from the Moon, the Sun, comets and asteroids. The common denominator of such kind of probes is that they need protection from the severe aerothermodynamic heating generated flying across the planet's atmosphere, when the high kinetic energy of the spacecraft is transformed into thermal energy [1]. Passive thermal protection systems (TPSs) are commonly used to fulfill the critical task of protecting the spacecraft during this last phase of the mission [2]. In practice, materials capable to survive the harsh thermo-chemical environment, and sustain the predicted heat load, are superimposed to the vital structure of the spacecraft to build-up a physical barrier against the high-enthalpy impinging flow. This barrier is commonly referred to as heat shield. For spacecraft that have to bear severe entry conditions (e.g., velocity and peak heat flux above 10 km/s and 10 W/cm^2, respectively), engineers cannot prescind, since the early ages of space exploration, from using *ablative* materials to build efficient heat shields [2, 3]. In this case, the TPS material is sacrificed during the atmospheric entry, undergoing a series of thermo-chemical and mechanical processes that help to dissipate the incoming energy at the price of its structural integrity [4]. For present and future space exploration missions, advanced ablative TPSs can be mission enabling, significantly impacting the mass of both scientific and instrumental payloads. Therefore, it is of fundamental importance to advance capabilities for their modeling, design and analysis.

Carbon-based materials have been the subject of numerous studies, as they represent the most performing subclass of ablative TPS materials. Numerous experimental efforts have been made to understand and characterize the physical phenomena occurring when these kind of materials are exposed to high-enthalpy flows [5–11]. Simultaneously, a multiplicity of modeling approaches have been developed to study the gas-surface interaction and the material response [12]. Theoretical and numerical models have been developed ad hoc to analyze specific phenomena [13–16], to study particular conditions [17, 18], or to perform global analyses of the TPS material behavior [19–23]. Besides, tools that make use of computational fluid dynamic (CFD) techniques have set. In the CFD

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Nomenclature

$\dot{q}_{\mathrm{rad_{out}}}$	solid radiative heat flux, $\mathrm{W/m^2}$
$\dot{q}_{\mathrm{cond_{net}}}$	conductive heat flux in the solid, $\mathrm{W/m^2}$
$\dot{q}_{\mathrm{rad_{net}}}$	net radiative heat flux, $\mathrm{W/m^2}$
κ	surface reaction velocity, m/s
h	static enthalpy, J/kg
$p_{\mathrm{C,eq.}}$	saturated carbon vapor pressure, Pa
	universal gas constant, 8.314 kJ/(mol K)
$\dot{m}$	surface mass blowing flux, $\mathrm{kg/(m^2 s)}$
Nr	number of surface reactions
N	number of species or dimension of multi-dimensional function
T	temperature, K
υ_i^{d}	diffusive velocity of species i, m/s
υ	velocity, m/s

Greek Symbols

$\dot{\omega}_{\mathrm{iw}}^{r}$	reaction-specific surface source term of species$i$,$\mathrm{kg/(m^2 s)}$
$\dot{\omega}_{\mathrm{iw}}$	overall surface source term of species i,$\mathrm{kg/(m^2 s)}$
γ	reaction probability
λ	thermal conductivity, W/m K
ϕ	generic variable
ρssss	density $\mathrm{kg/m^3}$
σ	Stefan-Boltzmann constant, $5.67 \times 10^{-8}\mathrm{W/(m^2K^4)}$
ε	integral emissivity
$\varepsilon_{\%}$	coefficient of variation

Subscripts

b	back surface of the material
s	solid phase
w	gas-surface interface
i	i^{th} species or generic index
j	generic index

Superscripts

r	r^{th} surface reaction

approach the ablation is treated as a purely surface phenomenon, and its coupling with the external flow field is handled through dedicated boundary conditions in the CFD simulation of the flow field [24]. This tools have been used to analyze the TPS interaction with the surrounding environment. Both charring and non-charring materials, using either equilibrium or finite-rate surface chemistry, have been simulated in a wide range of TPS material applications (e.g., spacecraft heat shields, solid rocket nozzle thermal protections, ground testing of thermal protection materials) [25–33]. The ability of such models to inherently handle the coupling between the operational aerothermodynamic environment and the TPS surface is certainly an asset when the final goal is the numerical reproduction of a real mission, or experiment, to assist the heat shield design. In addition, the possibility of coupling a steady-state CFD model with a transient material response allows to consider both the gas-surface interaction and the in-depth material response [34, 35], with clear benefits in terms of accuracy, particularly when dealing with the analysis of strongly unsteady phenomena.

Numerical simulations are a powerful tool in modern engineering. They allow to predict qualitatively and quantitatively the behavior of generic systems. However, to ensure the reliability of these predictions, a systematic and comprehensive treatment of both the calibration and the validation processes of the developed models is fundamental.

This should also include the quantification of the inherent model uncertainties arising from: the physical simplifications made to obtain a mathematical model representative of the complex phenomena under investigation; the numerical approximations due to the finite discretization used in the numerical solver to approximate the solution of the mathematical model; the lack of knowledge on some of the model parameters. In this context, the growing field of uncertainty quantification (UQ) aims at developing rigorous frameworks and reliable methods to characterize the impact of these uncertainties on the prediction of the quantities of interest (QoI). Investigations that make use of UQ techniques have been embraced with growing enthusiasm in the recent years [36, 37]. Practical applications of these techniques to assess the capabilities of deterministic simulation tools range from simple heat transfer problems [38] to hypersonic flight predictions [39, 40], and have been shown to bring useful information to scientists working in either model development or system design.

This study deals with the analysis of the coupling between a CFD deterministic approach to the ablation modeling, and modern uncertainty quantification techniques. In particular, the work focuses on the numerical study of the forward-stagnation-point ablation of a spherical sample of non-pyrolyzing carbon-based TPS material exposed to a subsonic high-enthalpy flow. Our interest lies in the uncertainties associated to the limited knowledge, or the intrinsic variability, of the input quantities needed to perform the CFD analysis. The deterministic analysis requires, in fact, the precise specification of some model parameters for which typically only limited information is available from experimental observations. The goal is to analyze the model dependencies on some critical parameters, and to quantify how these uncertainties affect the quantitative results of the model.

The article is arranged as follows. Section 2 describes theoretically the ablative boundary conditions, analyzes the model uncertainties and presents the deterministic CFD tool used for the study. Section 3 introduces the basic theory of UQ analysis, discussing the two mathematical approaches selected for the study. In section 4, the UQ analysis on the ablation modeling, applied to a nominal CFD test case, is presented. Two different scenarios, with modified sets of model input uncertainties, are analyzed. Moreover, an investigation on the important aspect of the definition of the input uncertainty distributions is carried out. Finally, section 5 summarizes the outcomes of the analyses and discusses the possible perspectives of the presented approach.

2. Surface ablation modeling

The study of the gas-surface interaction by means of a CFD approach requires the implementation of dedicated boundary conditions. For the present analysis we focus on the case of a non-porous carbon-based non-charring material (e.g., graphite, carbon/carbon, etc…). Moreover the following assumptions are considered [25, 41]: i) the surface ablation is a pure thermo-chemical process (i.e., no material can be removed in condensed phase); ii) the solid