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Two-way coupled simulations of stagnation-point ablation with transient material response

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ABSTRACT

Ablative materials are extensively used in aerospace applications to protect the integrity of the spacecraft during atmospheric entry. Both thermal and mechanical stresses have to be withstood in the severe operating conditions typical of space missions. An accurate modeling of the phenomena taking place when these materials are exposed to such a harsh environment is crucial to ensure the success of future, more demanding, missions. This study aims to couple two tools able to handle two different aspects of the ablative material modeling: a stagnation-line flow solver featuring an integrated ablative boundary condition, and a material response code. The coupling algorithm allows for time accurate solutions of the ablative material thermal response accounting for detailed surface chemistry, in-depth material behavior, and surface recession. Two different coupling strategies have been implemented, based either on a direct or an iterative procedure. The developed tool is used to rebuild plasma wind tunnel experiments performed in the von Karman Institute Plasmatron facility. The outcomes of the two strategies are compared, showing a satisfactory agreement with the experimental data. Among the two analyzed coupling procedures, the direct coupling proved to be computationally less expensive, while conserving the same accuracy of the more complex iterative procedure for the analyzed cases. A sensitivity analysis is also conducted to understand the discrepancy with experimental data and show the effects of four uncertain material parameters: thermal conductivity, density, emissivity, and catalytic efficiency.

1. Introduction

There are tremendous challenges in the prediction of spacecraft in atmospheric entry to simulate the response of the ablative Thermal Protection System (TPS). This thermal response strongly depends on the interaction between the ablative material of the heat shield and the high-enthalpy flow surrounding the capsule. Requirements concerning mass efficiency for missions with very high entry velocities have led to the development of new classes of light carbon composite ablators. Currently, new physico-chemical models and computational methods are being developed to understand the material response of these new ablators in a hypersonic flow (see for example the review in Refs. [1–3]).

The common approaches for the macroscopic modeling of the TPS material are mainly of three types. The first approach (i) is based on the one- or multi-dimensional transient computation of the in-depth material behavior [4]. The accurate resolution of all processes taking place inside of the material requires complex physical models [5]. However, simplified boundary conditions are usually used for the gas-solid interface in this kind of approach [4]. For instance, inviscid boundary-layer edge conditions are taken from separate simplified flowfield simulations, and the surface conditions (i.e., temperature or convective heat flux) are obtained by means of semi-empirical relations. Several material-response codes [6–9] use this approach and Lachaud et al. [2] gives a complete overview of each code capabilities. In the second approach (ii), the surface ablation is treated using a dedicated boundary condition in a Computational Fluid Dynamics (CFD) simulation. This approach has been used extensively in a wide range of applications (i.e., heat shields, solid rocket nozzles, etc.) to study both charring and non-charring materials, using either equilibrium or finite-rate surface

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chemistry, giving satisfactory results [10–16]. The last, most complex approach, can be described in short as a combination of the previous two. It can be performed either by coupling together two distinct solvers designed to compute the solid side (first approach) and the gas side (second approach) of problem [17,18], or by directly developing a unified numerical tool capable of computing the flow through the material accounting also for in-depth ablation of the material fibers [9,19]. The latter, in particular, is very promising for the study of highly porous materials for which, under certain conditions, the hypothesis of a mere surface ablation is not justifiable [5].

Two separate codes implementing the approach (i) and (ii) to study the ablative material behavior were developed and tested by the authors. First, a numerical tool was developed to solve the steady-state flow along the stagnation-line of pyrolyzing carbon-based materials accounting for the gas-surface interaction (i.e., ablation) and the pyrolysis gas injection [20,21]. In parallel, a material-response code was developed to simulate the complex in-depth thermal response of the same kind of materials [22,23]. The main objective of the present work is to perform and test the implementation of a tool, based on these two codes, capable of performing the third kind of the described approaches (coupled).

The manuscript is organized as follows. In the first part, the capabilities of each code are summarized and the implemented models are reviewed. Then, different coupling strategies are described, tested, and compared using as test cases the experiments performed in the inductively coupled Plasmatron facility at the von Karman Institute (VKI). Finally, a sensitivity analysis is performed to put forward the most influencing parameters.

2. Numerical tools

In this section, the two numerical tools (i.e., flow solver and material-response code) used in the analysis are described. The respective models, the boundary conditions, and a verification test case for each code are presented.

2.1. Flow solver

The surface ablation model used in this study has been implemented in the VKI stagnation-line code [20,21]. The development state of this tool allows CFD steady-state simulations of the flow along the stagnation-line of pyrolyzing carbon-based materials. Only the information relevant for the present gas-surface interaction study are given in the following, interested readers are referred to [20,24] for a more general description of this tool.

2.1.1. Model

The stagnation-line governing equations for spherically shaped blunt bodies can be obtained, as described in Ref. [25], by taking the following steps: (i) perform a coordinate transformation to recast the original equations (i.e., cartesian reference frame) in spherical coordinates originating in the body center; (ii) apply a separation $\theta \to 0$ of variables (i.e., $\hat{\phi}(r, \theta) = \overline{\phi}(\theta)\,\phi(r)$); (iii) take the limit $\theta \to 0$. In the case of flows in thermal equilibrium and chemical non-equilibrium these equations read

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}}{\partial r} - \frac{\partial \boldsymbol{F^d}}{\partial r} = \widetilde{\boldsymbol{S}}, \tag{1}$$

where the vectors of the conservative variables ($\boldsymbol{U}$), the inviscid fluxes ($\boldsymbol{F}$), and the diffusive fluxes ($\boldsymbol{F^d}$) are

$$\boldsymbol{U} = [\rho_i \quad \rho u \quad \rho v \quad \rho E]^{\mathrm{T}} \quad i = 1, N_s, \tag{2}$$

$$\boldsymbol{F} = [\rho_i u \quad p + \rho u^2 \quad \rho u v \quad \rho u H]^{\mathrm{T}}, \tag{3}$$

$$\boldsymbol{F^d} = [-\rho_i u_i^d \quad \tau_{rr} \quad \tau_{r\theta} \quad \tau_{rr} u - Q]^{\mathrm{T}} \quad i = 1, N_s. \tag{4}$$

The vectors in Eqs. (2)–(4) are unaltered with respect to the original system with the following exception: (i) the variables u, v, u_i^d, τ_{rr}, and $\tau_{r\theta}$ only include the part of the original generic variable $\hat{\phi}(r, \theta)$ that depends only on the radial coordinate i.e. $\phi(r)$; (ii) only the radial component of the viscous fluxes is considered because of the flow-field symmetry constraints taken in the ansatz derivation [25]. The source term vector on the right-hand side of Eq. (1) contains, together with the chemical source terms, also the convective and diffusive metric terms arising from the transformation in spherical coordinates.

The original derivation of the stagnation-line equations given in Ref. [25] assumed the Newtonian theory to express the pressure distribution around the body

$$p - p_\infty = \frac{1}{2}\rho_\infty u_\infty^2 \cos^2\theta. \tag{5}$$

This assumption provides a good approximation only in the case of hypersonic flows ($Ma \gg 1$). However, the subsonic pressure distribution around a sphere derived from potential flow theory is

$$p - p_\infty = \frac{1}{2}\rho_\infty u_\infty^2 \left(\cos^2\theta - \frac{5}{4}\sin^2\theta\right), \tag{6}$$

and Eq. (6) reduces to Eq. (5) on the stagnation line ($\theta \to 0$). Therefore, Eq. (1) still holds in the case of subsonic flows.

The stagnation-line code is coupled with the Mutation^{++} library [26]. The library is used for the computation of the thermodynamic and transport properties, as well as for the evaluation of the gas-phase chemical source terms. Species thermodynamic properties for the present analysis are obtained from the NASA polynomials [27], and relative mixture quantities are derived from pure species quantities through mixing rules. The transport properties are derived from kinetic theory. The chemical production rates for species, based on elementary chemical reactions including third body, are calculated by taking the forward reaction rate coefficients specified by the user in an Arrhenius law form. The backward rate coefficient is determined by satisfying the equilibrium relation.

2.1.2. Boundary conditions

The boundary condition accounts for the injection of the products of both heterogeneous surface reactions (ablation) and in-depth material decomposition (pyrolysis). The model is based on the following hypotheses: (i) the interaction between the material and the impinging flow takes place only on the surface (no volumetric ablation); (ii) surface mass and energy balances are applied to compute the mass blowing flux and the surface temperature; (iii) the steady-state ablation hypothesis allows to approximate the conductive heat flux through the TPS in order to close the surface energy balance; (iv) the steady-state ablation also permits the evaluation of the pyrolysis mass flow rate as a fixed portion of the mass blowing flux (i.e., at steady state the recession of the surface and that of the char line proceed at the same speed, so the char layer thickness is a constant value); (v) the pyrolysis gas has a prefixed elemental composition and it is injected in thermo-chemical equilibrium at the actual surface conditions (pressure and temperature).

The surface balances over the pyrolyzing ablative material are then given by

$$(\rho_i u)_{\mathrm{w}} + (\rho_i u_i^{\mathrm{d}})_{\mathrm{w}} = \dot{\omega}_{i_{\mathrm{w}}} + \dot{\omega}_{i_{\mathrm{g}}}, \tag{7}$$

$$\underbrace{k_{\mathrm{w}} \frac{\partial T}{\partial r}\Big|_{\mathrm{w}} - \sum_i^{N_s} (h_i \rho_i u_i^{\mathrm{d}})_{\mathrm{w}}}_{q_{\mathrm{conv}}} + \dot{m}_{\mathrm{c}}(h_{\mathrm{c}} - h_{\mathrm{w}}) + \dot{m}_{\mathrm{g}}(h_{\mathrm{g}} - h_{\mathrm{w}}) - \sigma\,\varepsilon_{\mathrm{w}}\,T_{\mathrm{w}}^4 = q_{\mathrm{cond,s}}, \tag{8}$$

where the subscripts g, c, and w indicate the terms that belong to the pyrolysis gas, the charred material, and the gas adjacent to the wall, respectively. Equation (7) is the species surface mass balance ($i = 1, N_s$). In Eq. (7), the species convective flux ($\rho_i u$) is triggered by