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A numerical approach for the study of the gas–surface interaction in carbon–phenolic solid rocket nozzles

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ABSTRACT

In the present study, surface mass and energy balances have been implemented in the ablative boundary condition of a two-dimensional full Navier–Stokes solver, to take into account the pyrolysis gas injection. A finite-rate ablation model is used, with steady-state ablation approximation to obtain the surface temperature. With this approximation, the conductive heat flux entering the wall is directly computed without a coupling with a solid conduction solver and the pyrolysis gas mass flow rate is a known fraction of the char mass flow rate. Simulations of carbon–phenolic solid rocket motor nozzle have been carried out to validate the model and to investigate the role of the most uncertain parameters. Results show the influence of the pyrolysis gas composition and of the ratio between pyrolysis gas and char mass fluxes, over the final erosion.

1. Introduction

Ablative materials are used as thermal protection systems (TPS) in several aerospace applications (solid rocket motor nozzle, reentry heat shield, etc.). These materials can be distinguished in two main categories: pyrolyzing and non-pyrolyzing. A pyrolyzing (charring) material is made of a filler (resin) and a reinforcing material (carbon, silica, etc.). When heated, the resin experiences a series of chemical reactions that release gaseous by products leaving a porous layer of *char* or residue. Although in case of carbonaceous materials (graphite, carbon–carbon, carbon–phenolic) the surface recession is due essentially to the thermochemical erosion caused by the gaseous oxidizing species, when a pyrolyzing material is used, the response could be strongly different due to the pyrolysis gas injection.

The common approaches to study the ablation of a TPS material are substantially of two different types.

The first approach, which only requires limited computational resources and has the merit to provide quick results, is based on the one- or multi-dimensional transient computation of the conduction inside the material by enforcing a raw boundary condition at the gas–solid interface [8]. Basically, the flow is considered inviscid and surface conditions, i.e. temperature or convective heat flux, are obtained by means of semi-empirical relations. The second approach treats the erosion using accurate "ablative" boundary conditions for the CFD simulation of viscous flows [3,25]. The latter approach has been used to study the thermochemical erosion of non-pyrolyzing ablative TPS materials (e.g.: graphite and carbon–carbon). In this case, the conduction inside the solid material, when coupling with a solid conduction solver is not available, is treated in a simplified manner.

The use of such an approach in case of pyrolyzing ablative TPS materials requires to take into account the pyrolysis gas injection [16]. In fact, as the pressure rises inside the residual char, the gaseous pyrolysis products are forced to flow through the char up to the solid–flow interface. Thus, the pyrolysis gas injection needs to be accurately modeled to correctly predict the gas–surface interaction over such a material.

The objective of this study is to extend a model developed for non-pyrolyzing ablative TPS [2–4] to the case of pyrolyzing materials. Hence, modified surface mass and energy balances have been implemented to take into account the pyrolysis mass injection in case of steady-state ablation.

Furthermore, to evaluate the role of the uncertainties about the resin decomposition process modeling, a sensitivity analysis has been carried out for the most uncertain parameters.

2. Physical and theoretical modeling

The goal of developing a flow solver with ablating boundary conditions has been achieved by considering that the surface energy and mass balances, coupled with an ablation model, provide complete surface conditions to solve the coupled flow/ablation

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problem [5,16]. The present model uses the so-called steady-state ablation approximation to manage the conduction heat flux entering the wall, which is needed to solve the surface energy balance and to obtain the surface temperature. It is worth noting that the steady-state ablation can be considered as a good approximation when a coupling with a material-response code is not available, and materials are exposed to high heat fluxes for a sufficiently long time. Rocket-nozzle environments typically ensure such conditions [10].

In case of pyrolyzing materials, both the surface and the in-depth balances have to take into account of the mass and energy terms due to the pyrolysis gas injection.

2.1. Boundary conditions

The surface mass balance in case of pyrolyzing material, for each species $i = 1, N_c$, can be expressed as in [16]:

$$\rho D_{im} \frac{\partial y_i}{\partial \eta}\bigg|_w = (\rho v)_w y_i - \dot{m}_{i,c} - \dot{m}_g y_{i,g} \tag{1}$$

where the term on the left-hand side is the mass flux due to diffusion, D_{im} is the effective diffusion coefficient of the ith species in the mixture, ρ is the gas density, η is the normal to the wall in the outward direction (from surface to gas) and y_i is the mass fraction of the ith species; the terms on the right-hand side are respectively due to blowing (v is the velocity normal to the wall), heterogeneous surface reactions ($\dot{m}_{i,c}$ are positive for ablation products and negative for the species which are consumed in the ablation process) and pyrolysis gas injection. The term $y_{i,g}$ represents the mass fraction of the ith species in the pyrolysis gas.

The heterogeneous surface reactions are modeled with a finite-rate chemistry approach [4]. The overall rate of these reactions depends on their kinetics as well as on the rate at which the oxidizing species diffuse across the boundary layer to the nozzle surface. If the kinetic rates are much higher than the diffusion rates, the recession rate is determined primarily by the diffusion mechanism of oxidizing species (diffusion-limited). The other extreme situation is that of high diffusion rates and low kinetic rates, in which case the recession is predominantly determined by the chemical kinetics (kinetic-limited).

Summing Eq. (1) over all species and noting that the heterogeneous surface reaction term sums to the mass consumed by the ablation process ($\dot{m}_c$), the surface mass balance becomes:

$$(\rho v)_w = \dot{m}_c + \dot{m}_g = \dot{m} \tag{2}$$

Taking into account Eq. (2), the surface energy balance is:

$$\begin{aligned} &k\frac{\partial T}{\partial \eta}\bigg|_w + \sum_{i=1}^{N} h_{i_w} \rho D_{im} \frac{\partial y_i}{\partial \eta}\bigg|_w + \alpha \dot{q}_{rad} - \varepsilon \sigma T_w^4 \\ &\quad = \dot{m} h_w - \dot{m}_c h_{c_w} - \dot{m}_g h_{g_w} + \dot{q}^{ss}_{cond} \end{aligned} \tag{3}$$

The terms on the left-hand side are conduction from gas, diffusion, radiation and re-radiation from the surface; on the right-hand side are the terms due to blowing, surface recession, pyrolysis gas injection and steady-state conduction.

2.2. In-depth behavior

By integrating the mass conservation equation between the back surface (virgin state) and the gas–solid interface of a pyrolyzing ablative material, and considering the steady-state solution, the mass conservation equation in a moving coordinate system tied to the receding surface is [6,8]:

$$\dot{m}_g + \dot{m}_c = \rho_v \dot{s} \tag{4}$$

where the term $\dot{s}$ represents the recession rate and the subscripts v, c and g indicate, respectively: virgin material, charred material and pyrolysis gaseous products. Looking at Eq. (4), it can be stated that in the steady-state condition the pyrolysis gas mass flow rate is a known fraction, ϕ, of the char mass flow rate:

$$\phi = \frac{\dot{m}_g}{\dot{m}_c} = \left(\frac{\rho_v}{\rho_c} - 1\right) \tag{5}$$

The general form of the in-depth energy balance in case of pyrolyzing material can be formulated as follows [18]:

$$\frac{\partial}{\partial t}(\rho_s h_s A) = \frac{\partial}{\partial \eta}\left(A k_s \frac{\partial T}{\partial \eta}\right) - \dot{s}\frac{\partial}{\partial \eta}(\rho_s h_s A) - \frac{\partial}{\partial \eta}(\dot{m}_g h_g) \tag{6}$$

where the terms (from left to right) represent: the time variation of the material sensible energy, the net conduction inside the material, the convected energy due to the coordinate motion and the energy entering the control volume due to the pyrolysis gas injection.

Thus, integrating Eq. (6) between the gas–wall interface (w) and a point inside the material (assuming adiabatic condition at the inner surface) where the material is still in the virgin state (in) and, therefore, the term $(\dot{m}_g h_g)_{in}$, related to the energy due to the pyrolysis gas injection, is null, the steady-state solution is:

$$\dot{q}^{ss}_{cond} = (\dot{m}_g h_g)_w - \dot{s}(\rho_{v_{in}} h_{v_{in}} - \rho_{c_w} h_{c_w}) \tag{7}$$

Hence, substituting Eq. (4) into Eq. (7), the final steady state conduction term can be rewritten as [16]:

$$\dot{q}^{ss}_{cond} = \dot{m}_c h_{c_w} + \dot{m}_g h_{g_w} - (\dot{m}_c + \dot{m}_g) h_{v_{in}} \tag{8}$$

At this point, substituting Eq. (8) into Eq. (3), gives the final steady-state surface energy balance:

$$\begin{aligned} &k\frac{\partial T}{\partial \eta}\bigg|_w + \sum_{i=1}^{N} h_{i_w} \rho D_{im} \frac{\partial y_i}{\partial \eta}\bigg|_w + \alpha \dot{q}_{rad} - \varepsilon \sigma T_w^4 \\ &\quad = \dot{m}(h_w - h_{v_{in}}) \end{aligned} \tag{9}$$

It can be noted that the terms related to the pyrolysis gas and char enthalpy in Eq. (3) have vanished in Eq. (9).

2.3. Pyrolysis gas composition

During the decomposition of a pyrolyzing material, the gaseous pyrolysis products rise the pressure inside the char, forcing these products to flow through this porous media. Of course, the residence time of the pyrolysis gas inside the material and the chemical interactions between the pyrolysis gas and the char can strongly modify the composition and the properties of both the char and the gas [27].

In the present model, the pyrolysis gas composition injected into the main flow is treated in a simplified manner. In fact, this gas is considered to be in chemical equilibrium at the wall temperature and pressure. Under this hypothesis its composition can be calculated by a chemical equilibrium code [12] and stored in a database containing the pyrolysis gas composition at different values of pressure and temperature.

The elemental composition of the phenolic resin, to be used in the chemical equilibrium code, has been calculated starting from a simple phenol molecule (C_6H_6O) and assuming that the resin char contains only carbon (the carbon cloth plus condensed phase carbon formed in resin pyrolysis). Hence an assigned percentage of the carbon mass fraction of the resin is assumed to remain as solid in the char [26]. The amount of this percentage has been calculated performing chemical equilibrium calculations by means