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Numerical Analysis of Heating and Ablating Non– Pyrolitic Materials

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Abstract: A two dimensional time dependent model is developed and assessed to describe the interrelated processes of conduction, convective heating and ablation of Carbon-Carbon ablative material. An aerothermochemical analysis for the process of non-pyrolitic composite material regression in large advanced solid-propellant rocket motors has been conducted. The analytical approach is similar in spirit to the approach of Borie, with the main idea of the nozzle regression being due to the carbon-carbon chemical attack by H_2O. The different steps of the work have consisted of the development and applications of several numerical codes substantiated by experimental results concerning the regression rate and the surface roughness of a carbon-carbon material.

Keywords: Nozzle**,** Throat, Graphite, Carbon-Carbon, Heat Transfer, Heat Conduction Ablation, Convective Heating, recession.

1. Introduction

The drive towards higher and higher energy solid propellants in rocket motors has created a need for materials, which can withstand the severe temperatures and pressures associated with their burning. Graphite and Carbon-Carbon, on account of their excellent high temperature stability and low densities, have found increasing application as nozzle materials in high energy, solid-propellant rocket motors. However, some complex associated with use of such materials have not yet been completely solved. One of these is the loss of nozzle material during motor operation, referred to as nozzle recession increases the nozzle throat area and thereby alters the expansion ratio and diminishes the thrust. This reduction in thrust must be estimated and incorporated in the rocket motor design. Recession, by weakening the nozzle may cause its structural failure under the high pressure encountered in rocket motors[1]. The hostile thermochemical environment resulting from the high-performance solid propellants poses many problems to such materials. One of the serious problems is the erosion/recession of the rocket-nozzle material. During the motor operation, the temperature of the nozzle material increases rapidly because of the high heat-transfer rate to the nozzle wall from the hot combustion exhaust. At high surface temperatures, heterogeneous chemical reactions occur between the nozzle material and oxidizing species such as H_2O, OH, and CO_2, present in the combustion stream[2]. The heterogeneous reactions cause the surface to recede, resulting in the thermochemical erosion of the nozzle. In addition to thermochemical erosion, the graphite material can also be consumed by a mechanical erosion mechanism. However, for high-density graphite with excellent mechanical properties, the mechanical erosion could be considered to be secondary to thermochemical erosion. The physical and chemical processes of graphite nozzle erosion are extremely complicated, as shown in Figure 1 [3]. Such erosion is most severe at the throat due to the maximum heat-transfer rate in that region. The increase in the nozzle throat area decreases the thrust and reduces the motor performance significantly in long-duration firings.

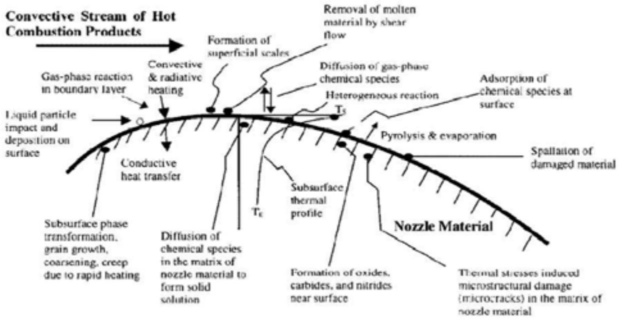

Figure 1. Physical and chemical processes associated with the rocket nozzle erosion[3].

Keswani[1] conducted theoretical studies to predict recession of graphite nozzles in different rocket motors, with different nozzle geometries and materials (carbon-carbon composites and bulk graphite), at different operating pressures and temperatures, and in wide range of propellant formulations. Recession was found to be strongly influenced by propellant composition, chamber pressure, and motor geometry, and the analysis showed that recession is due to primarily to the oxidation of carbon to carbon monoxide by H_2O and CO_2. The analysis also showed that the influence of chemical kinetics is predominant only when the surface temperature is low and that the recession rate is largely determined by the diffusion rate of oxidizing species when the nozzle surface temperature has reached about 2500 K. The other major conclusions of these works were: the total recession increases as material density decreases, as surface roughness increases, or as carbon thermal conductivity decreases

2. Model Formulation

The overall description for the regression phenomena is as follows: as the propellant burns in the rocket chamber, the resulting hot combustion gases flows in the nozzle and form a boundary layer (laminar or turbulent, depending on the conditions) over the lower temperature nozzle surface. The aggressive chemical species, principally H_2O, present in large quantities in the core flow, diffuse across the boundary layer to the nozzle surface, where heterogeneous reactions with carbon-carbon material occurs, including regression. At the beginning of the motor operation, the surface temperature is low, the surface reaction rates are lower compared to the aggressive species diffusion across the boundary layer, and the overall regression phenomenon is controlled by the kinetics of heterogeneous surface reactions. When the motor progressively reaches its equilibrium operating conditions, the surface temperature increases, the surface reaction rates become of the same order as the diffusion rates, and the regression phenomenon becomes controlled by both mechanisms, with a major influence for the process that has the slower rate. Figure 2 presents a summary of the different steps of the analysis, consisting of several calculations and a carbon-carbon attack description substantiated by experimental results concerning the regression rate and the increase of transfer coefficients due to surface roughness for one carbon-carbon material[4].

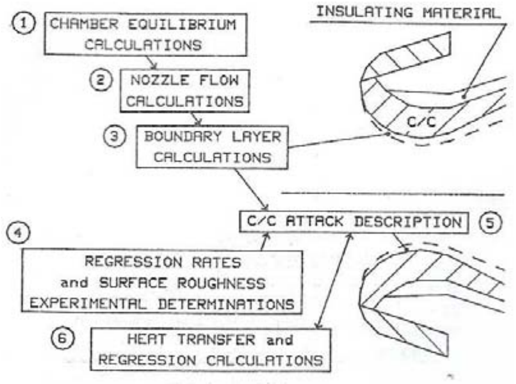

Figure 2. Summary of carbon-carbon nozzle regression approach[4].

3. Chamber Equilibrium Calculations

Because all previous studies have confirmed that propellant composition greatly influences nozzle regression, it is vital to identify the major products that constitute the propellant exhaust gases, hence, the first calculations of the analysis have been made to provide the characteristics of typical propellant exhaust gases in the combustion chamber.

4. Nozzle Flow Calculations

The calculation for the hot combustion gas flow in the nozzle is carried out through division of the flow into two zones: the flow-wall interaction zone (boundary layer flow), where the viscous force action and the heat – and mass –transfer processes are concentrated, and the non-viscous zone (inviscid core flow). The thermodynamic flow properties of the flow (pressure, temperature, density) has been calculated at the outer edge of the boundary layer by use of a numerical procedure allowing for equilibrium composition effects between motor chamber and geometric throat of the nozzle.

5. Boundary layer Calculations

Because of the complexity of the problems, the boundary layer calculations giving the heat and mass convective flux at the wall have been made by MEIT methodology. The MEIT methodology solves both the boundary layer integral momentum and energy equations. The required inputs are surface shape, boundary layer edge conditions, boundary layer gas properties and wall conditions. To solve these two equations, the local shape factor, recovery factor, Stanton number and friction coefficient must be defined. The effects of surface roughness, acceleration, and boundary layer properties are taken into account in terms of influence coefficients. These influence coefficients are included in the formulation of both the local the local Stanton number and friction coefficient. The solution procedure is carried out by an explicit finite difference scheme. Although MEIT is designed primarily for rocket environment, which consists of turbulent flow; both laminar and transitional flow situations are also included. The two boundary layer integral equations solved by MEIT are[5]:

$$\frac{1}{r\rho_e u_e^2}\frac{d}{ds}\left(r\rho_e u_e \theta\right) = \frac{C_f}{2} + \frac{(\rho v)_w u_e}{\rho_e u_e^2} + \frac{H\theta}{\rho_e u_e^2}\frac{dp}{ds} \tag{1}$$

$$\frac{1}{r\rho_e u_e\left(h_{t,e} - h_w\right)}\frac{d}{ds}\left(r\rho_e u_e\left(h_{t,e} - h_w\right)\phi\right) = C_H\left(\frac{h_r - h_w}{h_{t,e} - h_w}\right) + \frac{(\rho v)_w\left(h_{t,e} - h_t\right)}{\rho_e u_e\left(h_r - h_w\right)} \tag{2}$$

Where the momentum and energy thicknesses are respectively:

$$\theta \equiv \int_0^\infty \frac{\rho u}{\rho_e u_e}\left(\frac{u_e - u}{u_e}\right)dy \tag{3}$$

$$\phi \equiv \int_0^\infty \frac{\rho u}{\rho_e u_e}\left(\frac{h_{t,e} - h_t}{h_{t,e} - h_w}\right)dy \tag{4}$$

The boundary layer shape factor, H, is defined as:

$$H = \frac{\delta^*}{\theta} \tag{5}$$

Where δ^*, the displacement thickness is given by:

$$\delta^* = \int_0^\infty \left(1 - \frac{\rho u}{\rho_e u_e}\right)dy \tag{6}$$

The total enthalpy at the boundary layer edge is defined by:

$$h_{t,e} \equiv h_e + \frac{u_e^2}{2} \tag{7}$$

While the recovery enthalpy is given by

$$h_r = h_e + F\frac{u_e^2}{2} \tag{8}$$

Where F is the recovery factor. The heat transfer rate and skin friction are related to the Stanton number and friction coefficient respectively by

$$\tau_w = \rho_e u_e^2 \frac{C_f}{2} \tag{9}$$

$$\dot{q}_w = \rho_e u_e C_H\left(h_r - h_w\right) \tag{10}$$

In order to facilitate the solutions of Equations (1) and (2), the local shape factor, recovery factor, Stanton number and friction coefficient have to be defined, and this is described in[5].

6. Heat Transfer and Regression Calculations

The final step in the analysis of Carbon- Carbon regression has been the calculation of the thermal response and the regression of the nozzle throat material. This step has been carried out using mono-dimensional heat transfer model in the material in the radial direction, with integration of the un stationary heat transfer equation between moving ablating surface material and insulting material with material thermophysical properties (heat capacity and thermal conductivity) variable with respect to temperature.

The initial condition was constant ambient temperature and the boundary conditions were heat flux calculated after the preceding description at the surface. The further assumption of a flow transition between laminar boundary layer existing on the "smooth" virgin carbon-carbon material at the firing start and a turbulent boundary layer existing on the very rough ablative carbon-carbon surface during stabilized motor operation has been made. This is because an important delay has been observed on the start of the regression, not explainable by several other assumptions: thermal dilation of the nozzle throat, giving only a few tenths of a millimeter, two dimensional heat transfer, giving only a few degrees of difference at the nozzle throat, and the presence of a protective alumina coating, not seen in large scale nozzle tests, interrupted at about 13 s. Figure 3 shows the experimental regression data corresponding predicted regression as a function of time for a carbon-carbon nozzle throat of interest and for indicated conditions (p_{ch}=4.9 Mpa, use of carbon –carbon regression rate kinetics, alumina segregation, and roughness transition assumptions), We can observe the large delay at the beginning of the recession and the agreement between measured and predicted recession at all times.

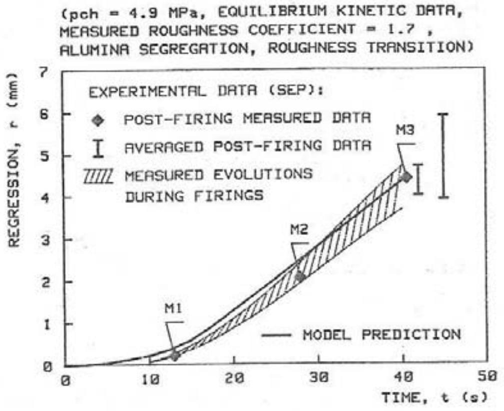

Figure 3. carbon-carbon regression evolutions at the nozzle throat[4].

7. Use of COMSOL Multiphysics

The formulation of the theoretical model involves the general conservation equations for the gas and the solid phase. The gas phase conservation equations are comprised of equations for the viscous boundary layer region and the core-flow region. The solid phase conservation equation is the transient heat conduction equation for the nozzle material. The heat conduction equation of carbon-carbon ablating material is solved by using COMSOL – Heat Transfer Module. The Heat Transfer Module consists of a number of application modes that describe the temperature field of a non-isothermal system. These application modes treat problems that involve heat transfer by conduction, convection, and radiation. In addition to the application modes that describe the temperature field. With this application mode you can describe the convective field of a heat transfer problem[5]. The surface recession rate is specified with a moving mesh boundary condition enabled through the “Moving Mesh Application Mode” of the COMSOL Multiphysics software. The program has a pre-packaged feature described as the Arbitrary Lagrangian-Eulerian (ALE) method; it permits moving boundaries without the need for the mesh movement to follow the material[6]. It has been assumed that the gaseous temperature is 3840 K. The thermophysical properties of Carbon-Carbon used in the calculation is shown in Table 1. The thermophysical properties of backup material (Silica Glass) used in the calculation is shown in Table 2.

Table 1: Thermo-physical Properties of Carbon-Carbon used in calculations.

Parameter	Value	Unit
ρ_s	1,900	$\mathrm{kg/m^3}$
$c_{p,s}$	2093.4	$\mathrm{J/kg\,K}$
λ_s	31.5	$\mathrm{w/(m\cdot K)}$

Table 2: Thermo-physical Properties of backup-material (Silica Glass) used in calculations.

Parameter	Value	Unit
ρ_b	2,203	$\mathrm{kg/m^3}$
$c_{p,b}$	703.0	$\mathrm{J/kg\,K}$
λ_b	1.38	$\mathrm{w/(m\cdot K)}$

Figure 4 shows the convergence curve.

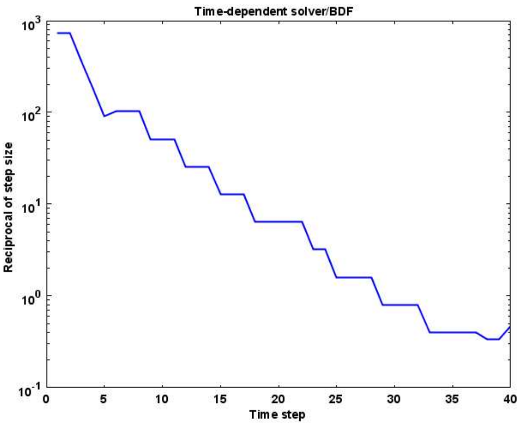

Figure 4. Convergence curve.

It can be seen from Figure 4 that the calculation results has been converged. Figure 5 shows the temperature field and nozzle contour after 30 sec from ignition

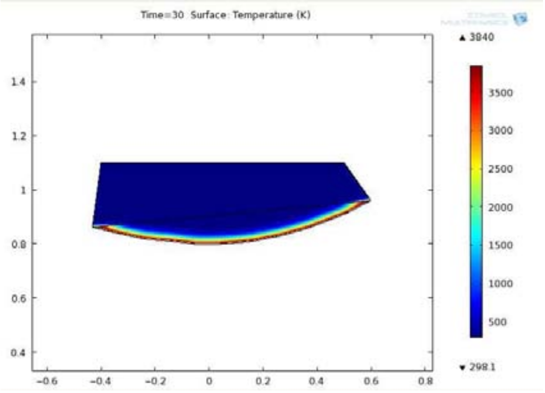

Figure 5. Temperature field and erosion of nozzle throat material after firing.

It can be seen from Figure 5 that the backup material has low temperature after the 30 sec from the ignition.

9. Conclusions

An aerothermochemical analysis for the process of non pyrolitic composite material regression in large advanced solid-propellant rocket motors has been conducted. The analytical approach is similar in spirit to the approach of Borie, with the main idea of the nozzle regression being due to the carbon-carbon chemical attack by H_2O. The different steps of the work have consisted of the development and applications of several numerical codes substantiated by experimental results concerning the regression rate and the surface roughness of a carbon-carbon material. The heat conduction equation of Carbon-Carbon ablating material is solved by using COMSOL – Heat Transfer Module. The Heat Transfer Module consists of a number of application modes that describe the temperature field of a non-isothermal system. These application modes treat problems that involve heat transfer by conduction, convection, and radiation. In addition to the application modes that describe the temperature field. With this application mode you can describe the convective field of a heat transfer problem[5]. The surface recession rate is specified with a moving mesh boundary condition enabled through the "Moving Mesh Application Mode" of the COMSOL Multiphysics software. The program has a pre-packaged feature described as the Arbitrary Lagrangian-Eulerian (ALE) method; it permits moving boundaries without the need for the mesh movement to follow the material[6].

8. References

1. Santosh T. Keswani, Recession of Graphite Nozzles in Rocket Motors, *A Thesis in Mechanical Engineering*, *The Pennsylvania State University*, *The Graduate School Department of Mechanical Engineering* (1984).

2. Piyush Thakre & Vigor Yang, A Comprehensive Model to Predict and Mitigate the erosion of Carbon-Carbon/Graphite Rocket Nozzles, *43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit 8-11 July 2007*, Cincinnati, OH, AIAA 2007-5777.

3. Ragini Acharya & Kenneth K. Kuo, Effect of Pressure and Propellant Composition on Graphite Rocket Nozzle Erosion Rate, *Journal of Propulsion and Power*, 23, 1242-1254 (2007).

4. Borie, V., Brulard, J., & Lengelle, G., Aerothermochemical Analysis of Carbon-Carbon Nozzle Regression in Solid-Propellant Rocket Motors, *Journal of Propulsion*, **5**, No. 6, 665-673 (1989)

5.Kwong, K., Suchsland, K. & Tong, H., Momentum/Energy Integral Technique (MEIT) User's Manual, Approved for public release, distribution unlimited, Acurex UM-78-86, (1978).

6.Anonymous, COMSOL Multiphysics - Modeling Guide. Version 4.0a, August 2010.