Numerical Analysis of Heating and Ablating Non–Pyrolitic Materials

A. Davidy

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Research Objectives

1) Development a new and flexible tool in order to check out transient numerical computations testing of heat transfer equation of ablative material.

2) Implement COMSOL software modules (Heat Transfer and ALE) in order to solve the heat transfer equation of non pyrolytic material (such as C/C).
Graphite and carbon-carbon composites have excellent thermal and physical properties as well as low densities, are widely used as materials for rocket nozzles.

One of the serious problems is the erosion of the rocket nozzle material. The nozzle is exposed to the hot propellant combustion products which form a turbulent boundary-layer over the nozzle surface. The hot products transfer energy to the nozzle wall, causing the surface temperature to rise.
Physical and Chemical Processes Associated with the Rocket Nozzle Erosion

Convective Stream of Hot Combustion Products
- Gas-phase reaction in boundary layer
- Convective & radiative heating
- Liquid particle impact and deposition on surface
- Conductive heat transfer
- Subsurface phase transformation, grain growth, coarsening, creep due to rapid heating

Formation of superficial scales
- Removal of molten material by shear flow
- Diffusion of gas-phase chemical species
- Heterogeneous reaction
- Adsorption of chemical species at surface
- Pyrolysis & evaporation
- Spallation of damaged material
- Subsurface thermal profile
- Formation of oxides, carbides, and nitrides near surface
- Thermal stresses induced microstructural damage (microcracks) in the matrix of nozzle material

Ragini A. & Kuo, K.K., Effect of Pressure and Propellant Composition on Graphite Rocket Nozzle Erosion Rate, Journal of Propulsion and Power, Vol. 23, No. 6, 2007,
(1) Problem Formulation

The heat conduction equation within the solid is:

\[
\rho_s c_{ps} \left( \frac{\partial T_s}{\partial t} \right)_{x'} = \lambda_s \left( \frac{\partial^2 T_s}{\partial x'^2} \right) + a_s \dot{Q}_r \varphi e^{-a_s x'}
\]  \(1\)

For a coordinate system \(x-0-y\) moving with the melting front.

\[
x' = x + \int_0^t vdt
\]  \(2\)

Thus, in a reference frame that moves with the regressing surface, the solid phase heat conduction equation become:

\[
\frac{\partial T_s}{\partial t} = \kappa_s \left( \frac{\partial^2 T_s}{\partial x^2} \right) + v \left( \frac{\partial T_s}{\partial x} \right)_t + \frac{a_s \varphi \dot{Q}_r e^{-a_s x}}{\rho_s c_{ps}}
\]  \(3\)
(1.a) Boundary and Initial Conditions

The boundary condition of Eq. (3) are:

\[ T_s(x = 0, t) = T_m \]
\[ T_s(x \rightarrow \infty, t) = T_a \]  \( )4( \)

The initial condition of Eq. (3) is:

\[ T_s(x, t = 0) = T_a \]  \( )5( \)

The solution of the heat conduction equation is split into two parts:

\[ T_s(x, t) = \theta_s(x) + \theta_h(x, t) \]  \( )6( \)
(1.b) Analytical Solution Process:

1) Solution of the Steady-State heat conduction equation

2) Solution of the Transient conduction equation.
   a) Derivation of homogeneous conduction equation by using exponential transformation
   b) Solution of the homogeneous heat transfer equation by using Green function.

3) Combination of the Steady state and Transient solutions.
(1.c) Temperature Distribution

The temperature distribution is given by:

\[
T_s(x, t) = \frac{1}{2} \left[ T_a - T_m + \frac{\dot{Q}_r \varphi}{\rho_s c_p, s (v - a_s \kappa_s)} \right] \exp \left[ -\frac{vx}{\kappa_s} \right] \text{erfc} \left( -\frac{x}{2\sqrt{\kappa_s t}} + \frac{v}{2\kappa_s} \sqrt{\kappa_s t} \right) + \\
\frac{1}{2} \left[ T_a - T_m + \frac{\dot{Q}_r \varphi}{\rho_s c_p, s (v - a_s \kappa_s)} \right] \text{erfc} \left( \frac{x}{2\sqrt{\kappa_s t}} + \frac{v}{2\kappa_s} \sqrt{\kappa_s t} \right) \\
- \frac{\dot{Q}_r \varphi}{2\rho_s c_p, s (v - a_s \kappa_s)} \exp \left[ -a_s x - (va_s - a_s^2 \kappa_s) t \right] \text{erfc} \left( -\frac{x}{2\sqrt{\kappa_s t}} - \left( \frac{v}{2\kappa_s} - a_s \right) \sqrt{\kappa_s t} \right) \\
- \frac{\dot{Q}_r \varphi}{2\rho_s c_p, s (v - a_s \kappa_s)} \exp \left[ \left( -\frac{v}{\kappa_s} + a_s \right) x - (va_s - a_s^2 \kappa_s) t \right] \text{erfc} \left( \frac{x}{2\sqrt{\kappa_s t}} - \left( \frac{v}{2\kappa_s} - a_s \right) \sqrt{\kappa_s t} \right) \\
+ T_a + \left[ T_m - T_a - \frac{\dot{Q}_r \varphi}{\rho_s c_p, s (v - a_s \kappa_s)} \right] e^{-\frac{vx}{\kappa_s}} + \frac{\dot{Q}_r \varphi e^{-a_s x}}{\rho_s c_p, s (v - a_s \kappa_s)}
\]
This model demonstrates the use of the Moving Mesh (ALE) application mode.

. Thermophysical Properties of the C/C and Silica Glass (backup material) used in the calculations.

<table>
<thead>
<tr>
<th>Thermal Conductivity</th>
<th>Heat Capacity</th>
<th>Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>31.5 [W/(m K)]</td>
<td>2,093 [J/kg K]</td>
<td>1,900 [kg/m^3]</td>
</tr>
<tr>
<td>1.38 [W/(m K)]</td>
<td>703 [J/kg K]</td>
<td>2,203 [kg/m^3]</td>
</tr>
</tbody>
</table>
(2.c) Comparison Between Analytical and COMSOL Numerical Results

![Graph comparing Analytical Solution and COMSOL Finite Element Solution](image)

- Analytical Solution
- COMSOL Finite Element Solution

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**x [m]**

- 0
- 0.002
- 0.004
- 0.006
- 0.008
- 0.01
- 0.012
- 0.014
- 0.016
- 0.018
- 0.02

**T [K]**

- 0
- 500
- 1000
- 1500
- 2000
- 2500
- 3000
C/C Nozzle Regression Approach

Temperature field and erosion of nozzle throat material after firing
Concluding Remarks

• A preliminary transient model was developed to describe the spatial temperature distribution inside C/C.

• Solution of the heat conduction equation in the material is split up into steady state solution and transient solution. The transient solution is based on Green functions. A heat flux profile of general spatial shape may be employed in the model.

• The COMSOL numerical results of the present model compare favorably with Analytical results.
Future Modeling Work

• Solving the diffusion and Energy equation of gaseous oxidizing species by using Chemical Engineering Module.

• Calculation of the ablation heat flux at the receding surface.

• Calculation of gaseous pressure buildup in the backup phenolic material as a result of it’s decomposition.
Thank You for Your Attention

Questions?