CFD Ablation Predictions with Coupled GSI Modeling for Charring and non-Charring Materials

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OUTLINE

1. CFD and GSI modeling coupling

2. Integration of CFD with GSI modeling

3. Theoretical model
   3.1. Surface Mass Balance (SMB)
   3.2. Surface Energy Balance (SEB)
   3.3. Finite-rate ablation model
   3.4. Pyrolysis model

4. Analysis of results
   4.1. RSRM subscale nozzle test case
   4.2. VEGA Launcher Solid Stages: Zefiro 23 & Zefiro 9A

5. Conclusions
Flow Modeling and Surface Ablation Coupling

- The present state of the art is represented by loose coupling of high-fidelity CFD flow solvers with material thermal response codes
- Three major restrictions still present in these coupled models
  - surface chemical equilibrium assumption
  - non-ablating flow field prediction
  - simplified diffusion modeling based on transfer coefficient

Basic idea
To integrate CFD technology with Computational Surface Thermochemistry (CST) to model material erosion in solid rocket motor nozzle applications

Objectives
1. To account for the effect of surface ablation (charring and non-charring materials)
2. To consider the pyrolysis gas injection (charring materials)
3. To determine surface ablation and temperature as part of the CFD solution under whatever ablation regime (diffusion limited and kinetically limited)
**LOOSE COUPLING: WHERE IT FAILS?**

\[ \rho_e u_e C_h (h_r - h_w)_e - \rho_e u_e C_m [(1 + B') h_w - h_{we}] + \dot{m}_c h_c + \dot{m}_g h_g = q_{rad_{out}} - q_{rad_{in}} + q_{cond} \]

\[ q_{sen} \quad q_{chem} \]

1. **Heat transfer coefficient \((C_h)\)**
   - Evaluated from non-ablative calculation \(\implies\) **Blowing correction** required
   - Depends on the wall temperature (and its profile)

2. **Mass transfer coefficient \((C_m)\)**
   - Evaluated from \(C_h\) \(\implies\) affected by \(C_h\) approximations
   - Related to \(C_h\) throughout **semi-empirical relation**

3. **Mass loss rate \((B')\)**
   - Evaluated from equilibrium tables \(\implies\) kinetically-limited ablation regime?
The “ablative” boundary condition, based on surface mass and energy balances, is grounded on the following hypothesis:

- Steady-state ablation hypothesis:
  - Closed solution of the in-depth energy balance
  - Pyrolysis gas mass flow rate is a known fraction of the char mass flow rate
- Pyrolysis gas in chemical equilibrium at the wall temperature and pressure

The following assumptions are made in the analysis:

- Flow is axisymmetric and steady
- Radiation heat transfer is negligible
- Negligible effect of gas-phase reactions on ablation (due to small concentration of oxygen)

**Code Specifications:**

- RANS 2-D axisymmetric solver
- Finite difference method (λ scheme)
- Spalart-Allmaras turbulence model
- Multicomponent diffusion model
- Thermodynamic and transport properties described by curve fits (Gordon & McBride)
Surface Mass Balance (SMB)

- **SMB for the $i^{th}$ species**:

$$\rho D_{im} \frac{\partial y_i}{\partial \eta} \bigg|_w + \dot{m}_g y_{i,g} + \dot{m}_{i,c} = (\rho v)_w y_{i,w} \quad \text{for} \quad i = 1, N_c$$

- $\dot{m}_{i,c}$ is the mass flux of the $i^{th}$ species produced or consumed by heterogeneous surface reactions between the solid char and the combustion gases.
- $y_{i,g}$ is the chemical composition (mass fractions) of the pyrolysis gas.
**Surface Mass Balance (SMB)**

- **Overall SMB:**

\[
(\rho v)_w = \dot{m}_g + \dot{m}_c = \dot{m}
\]

\(\dot{m}_c\) is the **char** mass flux

\(\dot{m}_g\) is the **pyrolysis** gas mass flux

\(\dot{m}\) is the **total** ablation mass flux

\[
\rho D_{im} \frac{\partial y_i}{\partial \eta} \bigg|_w + \dot{m}_g y_{i,g} + \dot{m}_{i,c} = (\rho v)_w y_{iw} \quad i = 1, N_c
\]

\(\dot{m}_{i,c}\) is the mass flux of the \(i^{th}\) species produced or consumed by heterogeneous surface reactions between the solid char and the combustion gases

\(y_{i,g}\) is the chemical composition (mass fractions) of the pyrolysis gas
Surface energy balance (SEB)

- **Overall SEB:**

\[
\left( k \frac{\partial T}{\partial \eta} \right)_{w} + \sum_{i=1}^{N_c} h_{iw} \rho_D \frac{\partial y_i}{\partial \eta} \bigg|_{w} + m_g h_{gw} + m_c h_{cw} = m h_w + \dot{q}^{ss}_{cond}
\]

The conduction term \(\dot{q}^{ss}_{cond}\) is represented by a closed expression available at steady state.
**Surface energy balance (SEB)**

- **Steady-state ablation approximation:**

  By integrating the *in-depth energy equation* between the material back surface (virgin state) and the gas-solid interface and assuming the steady-state solution yields:

  \[
  \dot{q}_{\text{cond}}^{ss} = \dot{m}_c h_{cw} + \dot{m}_g h_{gw} - (\dot{m}_c + \dot{m}_g) h_{vin}
  \]

  In the steady-state condition the pyrolysis gas mass flow rate becomes a *known fraction*, \(\phi\), of the char mass flow rate:

  \[
  \phi = \frac{\dot{m}_g}{\dot{m}_c} = \left( \frac{\rho_v}{\rho_c} - 1 \right)
  \]

  \(\rho_v = \text{“virgin” density}\)

  \(\rho_c = \text{“char” density}\)
Ablation model based on the multiple oxidizing species (MOS) reaction mechanisms

The rate of erosion (kg/m²s) of carbon by an oxidizing species can be expressed as:

\[
\dot{m}_i = p_i^n \cdot A_i T_w^b \exp\left(-\frac{E_i}{RT_w}\right)
\]

<table>
<thead>
<tr>
<th>Surface reaction</th>
<th>(A_i)</th>
<th>(E_i,) kcal/mol</th>
<th>(b)</th>
<th>(n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Cs + H_2O \rightarrow CO + H_2)</td>
<td>(4.8 \times 10^5)</td>
<td>68.8</td>
<td>0.0</td>
<td>0.5</td>
</tr>
<tr>
<td>(Cs + CO_2 \rightarrow 2CO)</td>
<td>(9.0 \times 10^3)</td>
<td>68.1</td>
<td>0.0</td>
<td>0.5</td>
</tr>
<tr>
<td>(Cs + OH \rightarrow CO + H)</td>
<td>(3.61 \times 10^2)</td>
<td>0.0</td>
<td>-0.5</td>
<td>1.0</td>
</tr>
</tbody>
</table>

The total erosion rate of carbon due to the surface heterogeneous reactions is:

\[
\dot{m}_c = \dot{m}_{H_2O} + \dot{m}_{CO_2} + \dot{m}_{OH} = \rho_c \dot{s} \quad (\text{kg/m}^2\text{s})
\]

The surface mass balance is solved for all the species without the need of any control procedure to switch from diffusion-limited to kinetic-limited erosion.
The pyrolysis gas composition injected into the main flow is considered to be in **chemical equilibrium** at the wall temperature and pressure.

- Pyrolysis gas composition is calculated by a chemical equilibrium code at different values of pressure and temperature and stored in a database.
- The elemental composition of the phenolic resin, to be used in the chemical equilibrium code, is calculated starting from a simple phenol molecule ($C_6H_6O$).
RSRM Subscale Nozzle Test Case: Input Data

Simulations address an experimental work carried out at the NASA JPL to study nozzle materials for the Space Shuttle Reusable SRM using the Ballistic Test and Evaluation System sub-scale motor (BATES)

Characteristics

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>RSRM subscale nozzle</th>
</tr>
</thead>
<tbody>
<tr>
<td>Throat Diameter (cm)</td>
<td>5.588</td>
</tr>
<tr>
<td>TPS Material</td>
<td>carbon-phenolic (FM-5055)</td>
</tr>
</tbody>
</table>

- Orthogonal structured grid
- Grid stretched in axial and radial directions

- Numerical investigation has addressed some of the tests that uses the FM-5055 carbon-phenolic material*:

<table>
<thead>
<tr>
<th>Test no</th>
<th>Prop.</th>
<th>$t_b$ (s)</th>
<th>$\bar{p}_c$ (MPa)</th>
<th>AI%</th>
<th>$H_2O$</th>
<th>$CO_2$</th>
<th>$OH$</th>
<th>$\rho_v$ (g/cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>#22</td>
<td>MOD. 8</td>
<td>11.52</td>
<td>4.73</td>
<td>16</td>
<td>0.1125</td>
<td>0.0298</td>
<td>0.0098</td>
<td>1.51</td>
</tr>
<tr>
<td>#1</td>
<td>MOD. 8</td>
<td>11.28</td>
<td>4.93</td>
<td>16</td>
<td>0.1125</td>
<td>0.0298</td>
<td>0.0098</td>
<td>1.50</td>
</tr>
<tr>
<td>#8</td>
<td>JPL-612</td>
<td>12.03</td>
<td>4.86</td>
<td>18</td>
<td>0.0643</td>
<td>0.0151</td>
<td>0.0035</td>
<td>1.50</td>
</tr>
<tr>
<td>#29</td>
<td>JPL-612</td>
<td>12.10</td>
<td>4.82</td>
<td>18</td>
<td>0.0643</td>
<td>0.0151</td>
<td>0.0035</td>
<td>1.51</td>
</tr>
</tbody>
</table>

RSRM Subscale Nozzle Test Case: Results* (1/2)

- Steady-state simulations at mean chamber pressure have been conducted
- Different $\phi$ values have been used because of the uncertainty of the char density (highest and lowest $\phi$ values found in literature for the FM-5055)


- Increasing the $\phi$ ratio produces an increase of the pyrolysis mass flow rate and a decrease of the char mass flow rate (due to the blowing effect of the pyrolysis gas injection)
RSRM Subscale Nozzle Test Case: Results* (2/2)

- A single steady-state simulation at mean chamber pressure provides the mean erosion rate

![Graph showing erosion rate vs. nozzle radial coordinate and nozzle axial coordinate for different φ values: φ=0 (no pyrolysis), φ=0.145, φ=0.383, and experimental data.]

- Although the char mass flow rate is decreasing with φ, the erosion rate is yet increasing with increasing φ due to the decrease of the char density
- The growth of the erosion rate due to the increasing of the φ value produces a lowering in surface temperature

ZEFIRO 23 & ZEFIRO 9A NOZZLES

Data provided by AVIO Group S.p.A. have been used to study the complete nozzle erosion of Zefiro 23 and 9A

- The two motors share the same architecture for the nozzle thermal protection system:
  - CARBON-CARBON ablative liner for the throat/entrance and the after–throat divergent
  - CARBON-PHENOLIC ablative liner for the 1st forward divergent and 2nd forward divergent

<table>
<thead>
<tr>
<th>Material</th>
<th>Density $\rho$</th>
<th>$\phi$ ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>carbon-carbon</td>
<td>$\approx 1.9$ g/cm$^3$</td>
<td></td>
</tr>
<tr>
<td>carbon-phenolic</td>
<td>$\approx 1.5$ g/cm$^3$</td>
<td>0.12</td>
</tr>
</tbody>
</table>

![Diagram of Zefiro 23 nozzle erosion](image1)

![Diagram of Zefiro 9A nozzle erosion](image2)
Zefiro 23 & Zefiro 9A: Results*

Pyrolysis gas injection in the boundary layer for Zefiro 23

- The species $C_2H_2$ (acetylene) is only present in the pyrolysis gas, so it represents a tracer species which can be used to visualize the pyrolysis gas diffusion in the boundary layer.

- The pyrolysis gas is mainly composed of $CO$ and $H_2$, with a minor amount of $C_2H_2$ and $H$ and its injection in the boundary layer blows the oxidizing species away from the surface (this effect, however, is minimal due to the small $\phi$ ratio).

Zefiro 23 & Zefiro 9A: Results

Pressure, temperature and mass blowing rates (total, char, pyrolysis) distributions for Zefiro 23

- Surface pressure is unaffected by the pyrolysis gas injection
- Surface temperature shows a drop corresponding to the material change
- Total mass blowing rate shows a step increase corresponding to the material change due to pyrolysis gas injection
- Char blowing rate is essentially unaffected by pyrolysis gas injection (pyrolysis blowing effect is minimal due to small $\phi$ ratio)
ZEFIRO 23 & ZEFIRO 9A: RESULTS

Erosion rate distribution for Zefiro 23 and Zefiro 9A

- Due to different material densities (higher for carbon-carbon and lower for carbon-phenolic), the step increase in terms of recession rate is larger than the one in terms of mass blowing rate.

- The step is larger for Zefiro 23 because the material change occurs at a section with a lower expansion ratio than for Zefiro 9A.

- The difference in recession rate corresponding to the material change is $\approx 0.025 \text{ mm/s}$ for Zefiro 23 and $\approx 0.015 \text{ mm/s}$ for Zefiro 9A. Such a difference can generate a step between the two materials of few millimeters at the end of the firing.
ZEFIRO 23 & ZEFIRO 9A: RESULTS

Comparison between predicted and measured nozzle profile after motor firing

- Experimental measurements are available for each ablative liner
- Final nozzle shapes have been predicted considering the effect of **nozzle shape change** and of **variable chamber pressure**
**ZEFIRO 23 & ZEFIRO 9A: RESULTS**

Comparison between predicted and measured nozzle profile after motor firing

- Experimental measurements are available for each ablative liner

- Erosion prediction shows a good agreement with the experimental data for the measuring points closer to the throat, but departs from the experimental profile for the remaining measuring points

![Graphs showing comparison between predicted and measured nozzle profile for ZEFIRO 23 and ZEFIRO 9A](image-url)
ZEFIRO 23 & ZEFIRO 9A: RESULTS

Comparison between predicted and measured nozzle profile after motor firing

- Experimental measurements are available for each ablative liner

- Results show a good reproduction of the eroded profile for the carbon-phenolic forward divergent, provided that the measuring points are sufficiently far from the material change
Conclusions

• Integration of CST in CFD code permits to bypass equilibrium thermochemical tables and semi-empirical coefficients for the evaluation of the ablation rate in case of steady-state ablation.

• Steady-state CFD simulation with ablative boundary conditions based on GSI modeling can be used for the evaluation of the erosion rate for carbon-based material.

• A model able to describe the erosion behavior of pyrolyzing and non-pyrolyzing carbon-based materials for solid rocket nozzle applications has been developed and validated showing good results.

• Time has come to integrate more tightly CFD and material thermal response code. We are looking forward to put aside the steady-state ablation approximation... Who is going to take the challenge?