Surface effects and phenomena on ablative materials

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## Acknowledgments

Dr. Francesco Panerai (University of Kentucky/NASA Ames)

Paul Zhang (University of Kentucky)  
Martin Weng (University of Kentucky)  
Raghava Davuluri (University of Kentucky)  
Ali Omidy (University of Kentucky)  

Nima Nouri (University of Kentucky)  
Rick Fu (University of Kentucky)  
Joseph Ferguson (University of Kentucky)  
Mark Miller (Princeton University)  

Dr. Jean Lachaud (UC Santa Cruz/NASA Ames)  
Dr. Michael Wright (NASA Ames)  

Dr. Sean Bailey (University of Kentucky)  
Dr. Nagi Mansour (NASA Ames)
Introduction
MSL predictions

- MSL TPS was a success: performed remarkably well
- The heat shield was instrumented for TPS performance
- Predictions do not match arc-jet test (under-prediction)
- Predictions do not match flight data (over-prediction)

Charring ablators

- Charring ablators are made by impregnation of phenolic resin on preform matrix.
- The material has two “phase”, consisting of a network of carbon fibers and a very porous phenolic matrix dispersed on and in between the fibers.
- The highly porous structure makes it a low-density material (ablator).

Micrographs of PICA at different magnifications. (Agrawal et al., 2013)

Charring ablators

- At first, when the material is subjected to heat, the phenolic pyrolyzes, while the carbon fibers stay (essentially) intact
- After a while, the surface starts to recess, as the matrix ablates
- The charring phenomenon enhanced the effectiveness of the TPS in two distinct ways:
  - **Mitigates the problem**, by absorbing the heat inside the TPS (endothermic pyrolysis reactions, char cooling)
  - **Circumvents the problem**, by attenuating the heat flux before it reaches the TPS (blowing gas in the outer flow, transport property in the boundary layer)

KATS Modeling Framework

- **General**
  - written in C++
  - reads 3D Unstructured grid in CGNS format

- **Parallelization**
  - ParMETIS for domain decomposition
  - MPI for inter-processors communications
  - PETSC Krylov subspace method as linear solver for iteration

- **Spatial discretization**
  - Cell-centered finite volume method
  - Second-order central differencing

- **Time integration**
  - Fully implicit
  - First-order backward Euler time integration

- **Inviscid fluxes scheme**
  - Steger–Warming flux-vector splitting, AUSM+up, Roe, etc.

- **Numerical flux Jacobian and analytical source Jacobian**
3D Conservation equations

\[ \frac{\partial Q}{\partial t} + \nabla \cdot (F - F_d) = S \]

Weak form after integrating over a finite volume \( V \)

\[ \int_V \frac{\partial Q}{\partial t} \, dV = \int_V \nabla \cdot (F_d - F) \, dV + \int_V S \, dV. \]

Apply Gauss theorem

\[ \int_V \frac{\partial Q}{\partial t} = \int_F (F_d - F) \cdot n + \int_V S \]

Implicit backward Euler time integration; Primitive variables is introduced

\[ V_c l \frac{\partial Q}{\partial t} = \sum_{face} (F_d - F)_j \cdot n_j A_j + SV_{cel} \equiv R^{n+1} = R^n + \frac{\partial R^n}{\partial P} \Delta P \]

Update of primitive variables comes from

\[ \left[ \frac{V}{\Delta t} \frac{\partial Q}{\partial P} - \frac{\partial R}{\partial P} \right] \Delta P = R, \]
Fluid Governing Equation (low speed)

\[
Q = \begin{pmatrix}
\rho_1 \\
\vdots \\
\rho_{ngs} \\
\rho_g u \\
\rho_g v \\
\rho_g w \\
E
\end{pmatrix}, \quad P = \begin{pmatrix}
\rho_1 \\
\vdots \\
\rho_{ngs} \\
u \\
v \\
w \\
T
\end{pmatrix}, \quad S = \begin{pmatrix}
\omega_1 \\
\vdots \\
\omega_{ngs} \\
0 \\
0 \\
0 \\
0
\end{pmatrix},
\]

\[
F = \begin{pmatrix}
\rho_1 u & \rho_1 v & \rho_1 w \\
\vdots & \vdots & \vdots \\
\rho_{ngs} u & \rho_{ngs} v & \rho_{ngs} w \\
\rho_g u^2 + p & \rho_g vu & \rho_g wu \\
\rho_g vw & \rho_g v^2 + p & \rho_g wv \\
\rho_g ww & \rho_g vw & \rho_g w^2 + p \\
(E+p)u & (E+p)v & (E+p)w
\end{pmatrix}, \quad F_d = \begin{pmatrix}
-\mathbf{J}_1 \\
\vdots \\
-\mathbf{J}_{ngs} \\
\tau_{xx} & \tau_{xy} & \tau_{xz} \\
\tau_{yx} & \tau_{yy} & \tau_{yz} \\
\tau_{zx} & \tau_{zy} & \tau_{zz} \\
\tau u - q - \sum_{i=1}^{ngs} (\mathbf{J}_i h_i)
\end{pmatrix}.
\]
Material Response Governing Equation

\[
\mathbf{Q} = \begin{pmatrix}
\phi \rho g_1 \\
\vdots \\
\phi \rho g_{n_{gs}} \\
\rho_{s_1} \\
\vdots \\
\rho_{s_{n_{gs}}} \\
\phi \rho g u \\
\phi \rho g v \\
\phi \rho g w \\
\phi E_g + E_s
\end{pmatrix}, \quad \mathbf{P} = \begin{pmatrix}
\phi \rho g_1 \\
\vdots \\
\phi \rho g_{n_{gs}} \\
\rho_{s_1} \\
\vdots \\
\rho_{s_{n_{gs}}} \\
u \\
v \\
w \\
T
\end{pmatrix}, \quad \mathbf{S} = \begin{pmatrix}
\dot{\omega}_g_1 \\
\vdots \\
\dot{\omega}_g_{n_{gs}} \\
\dot{\omega}_{s_1} \\
\vdots \\
\dot{\omega}_{s_{n_{gs}}} \\
D_x \\
D_y \\
D_z \\
S_D
\end{pmatrix},
\]

\[
\mathbf{F} = \begin{pmatrix}
\phi \rho g_1 u & \phi \rho g_1 v & \phi \rho g_1 w \\
\vdots & \vdots & \vdots \\
\phi \rho g_{n_{gs}} u & \phi \rho g_{n_{gs}} v & \phi \rho g_{n_{gs}} w \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0 \\
\phi \rho g u^2 + p & \phi \rho g u v & \phi \rho g w v \\
\phi \rho g u v & \phi \rho g v^2 + p & \phi \rho g w v \\
\phi \rho g u w & \phi \rho g v w & \phi \rho g w^2 + p \\
\phi \rho g u H & \phi \rho g v H & \phi \rho g w H
\end{pmatrix}, \quad \mathbf{F}_d = \begin{pmatrix}
-J_1 \\
\vdots \\
-J_{n_{gs}}
\end{pmatrix}, \quad \mathbf{F}_{\text{cond}} = \begin{pmatrix}
0 \\
0
\end{pmatrix}.
\]
• Porous medium flow model
  • Gas momentum is solved as distinct momentum equations
  • Diffusive effect of porous media is treated as source term,
    \[ D_x, D_y, \text{ and } D_z \]
    \[
    \begin{pmatrix}
      K_{xx} & K_{xy} & K_{xz} \\
      K_{yx} & K_{yy} & K_{yz} \\
      K_{zx} & K_{zy} & K_{zz}
    \end{pmatrix}
    \begin{pmatrix}
      D_x \\
      D_y \\
      D_z
    \end{pmatrix}
    = -\phi \mu
    \begin{pmatrix}
      u \\
      v \\
      w
    \end{pmatrix}
    \]

• If transverse isotropy is assumed
  \[
  \begin{pmatrix}
    K_{xx} \\
    K_{yy} \\
    K_{zz}
  \end{pmatrix}
  \begin{pmatrix}
    D_x \\
    D_y \\
    D_z
  \end{pmatrix}
  = -\phi \mu
  \begin{pmatrix}
    u \\
    v \\
    w
  \end{pmatrix}
  \Rightarrow
  D_x = -\frac{\phi \mu}{K_{xx}} u, \quad D_y = -\frac{\phi \mu}{K_{yy}} v, \quad D_z = -\frac{\phi \mu}{K_{zz}} w.
  \]

• Conductive heat transfer model
  • Similarly, if the material is transverse isotropic
    \[ F_{\text{cond},x} = k_{xx} \frac{\partial T}{\partial x}, \quad F_{\text{cond},y} = k_{yy} \frac{\partial T}{\partial y}, \quad F_{\text{cond},z} = k_{zz} \frac{\partial T}{\partial z}. \]
Coupling strategy

- Two meshes carefully aligned at the interface

- Resulting interface values are taken as boundary conditions for both solver

6th Ablation Workshop, April 10-11 2014, Champaign IL
Test-case: Flow tube experiment

- Flow in a tube, then in a porous sample
- Laminar flow (Re = 2.3)
- “Free” flow using KATS-CFD, porous media using KATS-MR
- Both code integrated using flux coupling
Filled cylinder ablator

Figure 3. Photograph of virgin (left) and oxidized (right) FiberForm samples.

In Fig. 5 the surface temperature measured with the pyrometer is plotted as a function of time for sample a7, tested at a furnace temperature of 1300 K. During the heating phase, with He flow, the temperature of the sample gradually increases to the target value. Enough time is given for the temperature to stabilize to the set value. As the gas flow is switched from He to air and the oxidation phase is started, a jump in surface temperature is observed (a magnified view is shown on the right plot of Fig. 5). As predicted, the jump is due to the exothermic nature of oxidation reactions, causing the surface temperature to increase. This is also confirmed by the numerical predictions presented later in the paper. Values of $T = T_w$, where $T_w$ is the temperature of the surface and $T$ the target furnace temperature, are found to be between 9 and 13 K.

Percent mass loss and recession are plotted in Fig. 6. As expected, mass loss is higher at higher temperature. Similarly to what was found in previous experiments, the mass loss rate seems to slow at temperatures between 900 and 1100 K, and then increases again at higher temperatures. This behavior shall be further investigated in the future with dedicated tests.
The relation to mean pore diameter is discussed in [9], presenting Knudsen number (mean free path transport conditions within the porous material, as shown in Fig. 4. Below 220 mm of the upstream extension tube.

The test conditions are detailed in Table 1. The experiments are performed at temperatures from 700 to 1300 K, using steps of 100 K, and pressures of 1.6, 10, and 60 kPa, maintained for a total of 1 h of oxidation time during each run. Gas properties are calculated using the Chemical Equilibrium with Applications code [16] from the NASA Glenn Research Center. The Reynolds number confirms that the flow regime is different from the incoming gas regime.

Experimental procedures for a laminar flow in a pipe of diameter 6 mm, entrance length for the highest value (60 kPa). Mass flow ratio) regimes from continuum to rarefied, well predicted from the entrance length

\[ \frac{L_e}{D} \approx 0.06 \frac{Re}{\mu} \]

\[ \lambda \approx 0.0022 \frac{D}{L} \]

The three pressure levels are selected to cover three different transition regimes, respectively, within the pores of the material. The characteristic scale of the flow regime at the fiber scale is different than the transition regimes, respectively, within the pores of the material. The characteristic scale of the flow regime at the fiber scale is different than the transition regimes, respectively, within the pores of the material.

Experiments at 1.6, 10, and 60 kPa cover continuum, slip, and transition regimes, respectively, within the pores of the material. The characteristic scale of the flow regime at the fiber scale is different than the transition regimes, respectively, within the pores of the material. The characteristic scale of the flow regime at the fiber scale is different than the transition regimes, respectively, within the pores of the material.

The oxidation reaction occurred during the transient heating phase. Once the target temperature condition. The supply of He ensured that no oxidation in the test section below 220 mm of the upstream extension tube.

The transient phase to the target pressure is monitored by adjusting the suction rate of the mechanical pump downstream to have a duration of 5 min for the lowest pressure condition, approximately 1 min. For the test conditions, the entrance length can be estimated from

\[ L_e \approx \frac{D}{5} \]

Temperature changes in length, inner diameter, and outer diameter with an uncertainty of

\[ L \approx \frac{D}{5} \]

Density changes for all specimens are documented in Sec. III.

To determine the exact volume recession due to oxidation for each sample, a suitable posttest method is implemented to cope with the brittleness of the carbon preform specimens. The oxidized samples are found to easily crumble into pieces in any attempt of manual extraction from the glass holder. Therefore, the specimen/holder assembly is impregnated in epoxy resin, by means of an encapsulation system (the pore diameter) is much smaller than that of the assembly and oven-cured for 5 min. For a laminar flow

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\[ \lambda \approx 0.0022 \frac{D}{L} \]

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The encapsulated resin/hardener mixture (CaldoFix, Struers A/S, Ballerup, Denmark) is poured into a plastic mold hosting the assembly and oven-cured for 5 min. The entrance length can be estimated from

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\[ L_e \approx \frac{D}{5} \]

Density changes for all specimens are documented in Sec. III.
Pyrolysis gas transport
Why we need 3D modeling?

- Side-wall heating on small samples
- Gas transport inside the material
- Anisotropic material properties
Iso-Q geometrical blowing effects

Temperature

Pressure

Strong blowing through the sides

Solid density

Mass flux
• The TACOT (Theoretical Ablative Composite for Open Testing) is used — similar to PICA
• Only charring ablation is modeled: no surface recession allowed to occur
• Four geometries with different aspect ratio H/R are chosen

Geometries

Heat flux

Sample A
Sample B
Sample C
Sample D
Iso-Q geometrical blowing effects

Sample A

Sample B

Sample C

Sample D
2) Cylinder — permeable side wall

Table 2: Geometric specifications for Case 2.1 to 2.4

<table>
<thead>
<tr>
<th>Sample-holder location</th>
<th>Case #</th>
<th>Sample</th>
<th>(d), c m</th>
<th>(h), c m ((x_1, z_1)) to ((x_2, z_2)), c m</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2.1</td>
<td>A</td>
<td>2.5</td>
<td>(0.75, -6) to (1.25, -4)</td>
</tr>
<tr>
<td></td>
<td>2.2</td>
<td>B</td>
<td>5</td>
<td>(1.5, -6) to (2.5, -4)</td>
</tr>
<tr>
<td></td>
<td>2.3</td>
<td>C</td>
<td>10</td>
<td>(0, -6) to (3, -5.5)</td>
</tr>
<tr>
<td></td>
<td>2.4</td>
<td>D</td>
<td>10</td>
<td>(0, -3) to (3, -2.5)</td>
</tr>
</tbody>
</table>

Figure 4: Sample geometry for sample A- to D-

The initial and boundary condition of the two sets are identical, and are adopted from the arc-jet experiments of Ref. [13]. These conditions are summarized in Table 3. Note that, along the iso-Q sample surface, the pressure
Iso-Q geometrical blowing effects

Figure 28: Gas streamlines for Case 2.1, at various time

Figure 29: Gas mass flow rate through the surface of iso-Q sample

A- \( \cdot \) various time; symbols are results of a 4 cm thick sample

Figure 34: Gas mass flow rate through the surface of iso-Q sample

B- \( \cdot \) various time; symbols are results of a 4 cm thick sample

Figure 39: Gas mass flow rate through the surface of iso-Q sample

C- \( \cdot \), at various time

Figure 44: Gas mass flow rate through the surface of iso-Q sample

The pyrolysis gas moving patterns are somewhat similar to Case 1.4, as depicted in Figs. 42 and 43. A region with high \( \dot{\theta} m \) is observed at the lower right of the sample, where streamlines all point toward outside of the material. This indicates that a huge amount of gases flows through the bottom corner of the testing sample. Figure 44 shows the same trend: the surface blowing rate is huge at the bottom of the sample side-wall. In addition, Fig. 44 (Case 2.4) is very similar to Fig. 24 (Case 1.4), which suggests that the sample-holder does not change the surface mass flow rate much.

5.3. Comparison of mass flow rate at the stagnation point

Table 4 shows the pyrolysis gas blowing rate at the stagnation point of the iso-Q samples. For comparison, the table also displays the mass flow rate of a 1D model that uses the exact same condition. It is seen from the table that, when 1) the diameter of the sample is increased, or 2) the thickness of the sample is decreased, the stagnation blowing rate is increased. Nevertheless, the blowing rate is less than what is predicted by the 1D assumption.

Table 4: Gas mass flow rate through the stagnation point (arc length = 0 m)

<table>
<thead>
<tr>
<th>Sample blowing rate ( \dot{\theta} m ), kg/m(^2)s</th>
<th>( t ), sec</th>
<th>1D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 sec A-</td>
<td>5.30E-02</td>
<td>4.64E-03</td>
</tr>
<tr>
<td>10 sec A-</td>
<td>2.33E-02</td>
<td>1.61E-03</td>
</tr>
<tr>
<td>20 sec A-</td>
<td>1.76E-02</td>
<td>4.99E-04</td>
</tr>
<tr>
<td>30 sec A-</td>
<td>1.49E-02</td>
<td>2.33E-04</td>
</tr>
<tr>
<td>Sample B-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 sec B-</td>
<td>4.37E-03</td>
<td>6.51E-03</td>
</tr>
<tr>
<td>10 sec B-</td>
<td>1.60E-03</td>
<td>2.07E-03</td>
</tr>
<tr>
<td>20 sec B-</td>
<td>4.30E-04</td>
<td>5.78E-04</td>
</tr>
<tr>
<td>30 sec B-</td>
<td>1.05E-04</td>
<td>6.55E-04</td>
</tr>
<tr>
<td>Sample C-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 sec C-</td>
<td>9.78E-03</td>
<td>1.30E-02</td>
</tr>
<tr>
<td>10 sec C-</td>
<td>3.73E-03</td>
<td>5.63E-03</td>
</tr>
<tr>
<td>20 sec C-</td>
<td>1.07E-03</td>
<td>2.49E-03</td>
</tr>
<tr>
<td>30 sec C-</td>
<td>6.01E-03</td>
<td>1.08E-03</td>
</tr>
<tr>
<td>Sample D-</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 sec D-</td>
<td>1.30E-02</td>
<td>6.51E-03</td>
</tr>
<tr>
<td>10 sec D-</td>
<td>5.63E-03</td>
<td>2.07E-03</td>
</tr>
<tr>
<td>20 sec D-</td>
<td>2.49E-03</td>
<td>5.78E-04</td>
</tr>
<tr>
<td>30 sec D-</td>
<td>6.01E-03</td>
<td>1.08E-03</td>
</tr>
</tbody>
</table>
### Stagnation point blowing rates for all samples

<table>
<thead>
<tr>
<th>t, sec</th>
<th>1D</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>A-</th>
<th>B-</th>
<th>C-</th>
<th>D-</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>3.01E-02</td>
<td>4.64E-03</td>
<td>6.76E-03</td>
<td>9.65E-03</td>
<td>1.19E-02</td>
<td>4.37E-03</td>
<td>6.51E-03</td>
<td>9.78E-03</td>
<td>1.30E-02</td>
</tr>
<tr>
<td>10</td>
<td>2.33E-02</td>
<td>1.61E-03</td>
<td>2.25E-03</td>
<td>3.56E-03</td>
<td>4.66E-03</td>
<td>1.60E-03</td>
<td>2.07E-03</td>
<td>3.73E-03</td>
<td>5.63E-03</td>
</tr>
<tr>
<td>20</td>
<td>1.76E-02</td>
<td>4.99E-04</td>
<td>6.31E-04</td>
<td>9.52E-04</td>
<td>1.27E-03</td>
<td>4.30E-04</td>
<td>5.78E-04</td>
<td>1.07E-03</td>
<td>2.49E-03</td>
</tr>
<tr>
<td>30</td>
<td>1.49E-02</td>
<td>2.33E-04</td>
<td>6.46E-04</td>
<td>9.62E-04</td>
<td>1.79E-03</td>
<td>1.05E-04</td>
<td>6.55E-04</td>
<td>1.08E-03</td>
<td>6.01E-03</td>
</tr>
</tbody>
</table>

- Could be several order of magnitude of difference when compared to the 1D model
Why we need 3D modeling?

• Side-wall heating on small samples
• Gas transport inside the material
• Anisotropic material properties

NASA's MSL entry capsule

Courtesy: NASA Ames Arc-Jet facility
Multi-scale approach
Micro-scale approach

- Light weight charring ablators (such as PICA) are composed of a fiber matrix impregnated by a resin
- Only very recently has the capability to access real microstructure become possible both experimentally and computationally
- To understand the behavior of the material at the macro-scale, the micro-scale effects are taken into account

The artificial material misses several features!
Fiber-scale features are accurately resolved
Orthotropic geometry and thermophysical properties are confirmed for preform composites
Analysis of the tomographs allows accurate computations of important properties for material response modeling (tortuosity, permeability, porosity) etc.
Reconstruction of porous carbon materials
Spallation
Spallation

- Mechanical erosion of the material
- Accelerates material failure
- Undesirable because hard to predict (and model...)

Can be caused by

- Fracture from high pyrolysis gas pressure
- Soot formation (coking)
- Volumetric fiber erosion and detachment
- Fracture from high thermal stress
- Shear stress on fibers

Agrawal et al., 2013
Thermo-Mechanical Response

- Most specimens failed between 600 and 900 kPa
- The charred PICA samples made from arc-jet articles showed similar behavior and tensile strength as the furnace char.

- 10 sec of constant heat flux
- High stress region does not correspond to high temperature region
- When combine with volumetric fiber ablation, could results in mechanical erosion
Spalled particles in arc-jet environment

Mach 5 High-enthalpy Argon flow

- One way coupling of CFD and Lagrangian particle code
- Surface kinetics on particle
- Inverse-problem approach for parameter identification

Concluding remarks

• Development of models to capture
  • multi-scale effects
  • coupling effects
• Detailed experiments aimed at
  • understanding near surface properties
  • calculating micro-scale parameters
Questions?