Definition of Ablation Test-case series #3

6th Ablation Workshop, Urbana-Champaign, Illinois
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Introduction

Motivation: Why did we start this? -> pure curiosity
• How do codes compare? – if same model.
• How do models compare? – if different physics implemented.

Goal
• propose problems of increasing complexity until it is agreed that the most-elaborated well-defined problem is formulated

Method to design a test case
1. census on problems of interest
2. census on code capabilities
3. draft a proposition of test case (necessarily a compromise)
4. iterate with the community until the test-case definition is clear and complete

We try our best to propose SOFT test-cases
• Simple, Open, Focused, Trouble-free.
Introduction

Elemental composition

- Reinforcement: ex-cellulose carbon fibers, heat treated at 2000 K, density 1600 kg/m$^3$, length: 1 mm, diameter: 10 microns.
- Matrix: ex-novolac/formaldehyde polymer, virgin density 1200 kg/m$^3$

Architecture

- Random fiber distribution and orientation
- Fiber volume fraction: 10%
- Fiber-coating matrix
- Matrix volume fraction: 10%
- Initial porosity: 80%

Properties

- Inspired from open literature data - when available for similar materials conductivity, heat capacity, pyrolysis gases (composition, decomposition, finite-rate chemistry)
- Derived/computed - when not found in the literature formation enthalpy of the solid, thermodynamic properties of the pyrolysis gases at equilibrium, viscosity, permeability, tortuosity, B’ table for air.
Introduction

Previous Test-cases

- **0 – TACOT**: Theoretical Ablative Composite for Open Testing created from literature data. It is a low-density carbon/phenolic.

- **1st test-case (2011)**: 15 participants / 25 codes in the open literature. Mostly a simple heat transfer problem chosen for its simplicity

- **2nd test-case series (2012)** – progress: convective boundary condition & recession
  - 2.1 - bridge between 1st and 2.2 (non-physical but useful for code developers)
  - 2.2 - 1D state-of-the-art design level – low heat-flux
  - 2.3 - 1D state-of-the-art design level – high heat-flux
  - 2.4 - Comparison of methods to compute recession rates (e.g. B’ tables)

- **3rd test-case series:**
  - Initial version (2012): 5th Ablation Workshop, Lexington, KY.
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Material properties

The TACOT material created in series #1/#2 is being re-used.
- Only minimal changes (imposed by the test-case)

Unchanged properties w.r.t. TACOT_2.2:
- Conductivity
- Capacity/Enthalpy
- Arrhenius Law
- Chemistry

Differences w.r.t. TACOT_2.2:
- Extension of pressure and $B_g$ range for gas and wall properties
  - Enthalpy, $B_c$, dynamic viscosity, density,…
- Orthotropic conductivity ($\alpha_1 = 1.0$, $\alpha_2 = 2.0$)

TACOT 3.0 ([TACOT_3.0.xls](http://ablation2014.engineering.uky.edu/?p=148)) data can be downloaded from:
http://ablation2014.engineering.uky.edu/?p=148
Material properties

TARGET (Thermochemical Ablation Routine for the Generation of Equilibrium Tables) is a tool able to generate thermochemical ablation tables for any atmospheric environment based on the CEA equilibrium routines and thermochemical database.

- Thermochemical tables are relating surface temperature, pressure and pyrolysis gas injection to a dimensionless surface mass flux owing to ablation \( F(T,P,B'_c, B'_g)=0 \).

- The shape of the \( B'_c \) curves depend on the material and atmospheric composition and on the choice of surface and gas species.

- Experience, insight, and experimental data are all important ingredients in the development of suitable thermochemical tables for a selected TPS material.
Material properties

The advantages are:

- The possibility to calculate tables **on-the-fly**, as a subroutine of a material thermal response code
- The calculation of equilibrium using the **minimization of free energy** instead of the equilibrium constants approach of the ACE (Aerotherm Chemical Equilibrium)
- The use of **modular routines** based on CEA code which are more computational efficient and easier to modify
- The use of the more up to date **thermochemical database from CEA** instead of the obsolete JANNAF database used by the ACE code (TARGET can use both)
- The **pyrolysis gas** composition can be temperature-dependent
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Test-case series #3

Goal of the test-case:
- Extend test-case series #2 to 3D
- Test 3D aspects of the codes
- Add complexity in a progressive fashion

Geometry derived from an “Iso-q” geometry, with modifications:
- Cylinder with elliptic arc as outer surface, in order to
- Reduce heat flux peak at the shoulder in order to reduce/eliminate flow-structure interaction

Definition document (AblationTestCaseSeries#3) can be downloaded from: http://ablation2014.engineering.uky.edu/?p=146
Flow calculation

- To avoid structure-flow interaction:
- Heat flux level was found to limit the ablation
- Flow conditions were found for the heat flux level

The heat transfer coefficient and pressure profiles over the ellipsoid geometry have been estimated using:

- a non-equilibrium aero-thermodynamic hypersonic CFD code.
- The free stream conditions used in this calculation are for air at
  - a temperature of 225 K,
  - at a density of $2.3 \times 10^{-3}$ kg/m$^3$,
  - traveling at 7000 m/s.
- A super-catalytic wall is used, at a temperature of 225 K.
- Pressure at stagnation point equals 0.1 atm.

- The pressure distribution necessitated a re-calculation of the gas and wall properties for TACOT.
Test-case series #3

KATS
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
Test-case series #3

Mach 5 Argon flow

Graph showing the variation of $q_w / q_w(0)$ and $p_w / p_w(0)$ with arc length $S$ [m].

Thermodynamic properties at different Mach numbers:

- Temperature $T$ in range 1000 to 16000 K
- Pressure $p$ in range 1000 to 45000 Pa

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Boundary conditions:

- Re-radiation with the environment
  
  \[ q = \alpha \epsilon \left( T^4 - T_w^4 \right) \]

- Enthalpy form boundary condition
  
  \[ q = \rho_e u_e C_h (h_e - h_w) + \rho_e u_e C_h \left[ B_c (h_c - h_w) + B_g (h_g - h_w) \right] \]

- Blowing correction
  
  \[ \frac{C_h}{C_{h_0}} = \frac{2 \lambda B_0'}{e^{2 \lambda B_0} - 1} \quad \lambda = 0.5 \]

- Wall, gas, virgin and char enthalpy are defined (TACOT_3.0).
- Total enthalpy \( (h_e) \) is given
- Mass flow rate and pressure are given as a function of time and position

### Time variation at stagnation point

<table>
<thead>
<tr>
<th>time (s)</th>
<th>( \rho_e u_e C_h(0) ) (kg·m(^{-2})·s(^{-1}))</th>
<th>( h_e ) (J·kg(^{-1}))</th>
<th>( p_w(0,t) ) (Pa)</th>
<th>( p_w(11.17,t) ) (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>( 0.1 \cdot 10^{-2} )</td>
<td>0</td>
<td>405.3</td>
<td>405.3</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1</td>
<td>( 2.5 \cdot 10^7 )</td>
<td>10132.5</td>
<td>405.3</td>
</tr>
<tr>
<td>40</td>
<td>0.1</td>
<td>( 2.5 \cdot 10^7 )</td>
<td>10132.5</td>
<td>405.3</td>
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<tr>
<td>40.1</td>
<td>( 0.1 \cdot 10^{-2} )</td>
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<td>405.3</td>
</tr>
<tr>
<td>120</td>
<td>( 0.1 \cdot 10^{-2} )</td>
<td>0</td>
<td>405.3</td>
<td>405.3</td>
</tr>
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</table>

- Spatial variation of the flow rate \( (q_w/q_w(0)) \).
- Spatial variation of pressure \( (p_w/p_w(0)) \), initial pressure \( p_w(s) = \text{constant} \).
Test-case series #3

Test-case definition

- Test 3.0:
  - Isotropic TACOT
  - Zero ablation $Bc’=0$
- Test 3.1:
  - Isotropic TACOT
  - Non-zero ablation $Bc’(T,P,Bg’)$

- Test 3.2
  - Orthotropic TACOT ($\alpha_1 = 1.0, \alpha_2 = 2.0$)
  - TTT-direction aligned with the axis of axisymmetry (axisymmetric test-case)
- Test 3.3
  - Orthotropic TACOT ($\alpha_1 = 1.0, \alpha_2 = 2.0$)
  - TTT-direction $30^\circ$ rotated (counter-clockwise) w.r.t. axis of axisymmetry (3D test-case)

Model: Test 3.0/3.1/3.2

$$\begin{vmatrix}
\lambda_{TTT} & 0 \\
0 & \lambda_{IP}
\end{vmatrix} =
\begin{vmatrix}
\alpha_1 & 0 \\
0 & \alpha_2
\end{vmatrix} \lambda_{isotropic}$$

Model: Test 3.3
Test-case series #3

Results at generated for Test-case 3.1, 3.2 and 3.3

- With SAMCEF Amaryllis

- At time $t = 40$ s.
  - Temperature [K]
  - Density [kg/m$^3$]
  - Pressure [N/m$^2$]
Test-case series #3

Gas-mass flow [kg/(m^2.s)]
- Modulus along the outer surface

- At time t = 0.8 s
Test-case series #3

Comparison of results
- Temporal evolution at 10 thermo-couple positions and at the stagnation point

<table>
<thead>
<tr>
<th>TC</th>
<th>Y-coordinate [cm]</th>
<th>Z-coordinate [cm]</th>
<th>TC</th>
<th>Y-coordinate [cm]</th>
<th>Z-coordinate [cm]</th>
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</thead>
<tbody>
<tr>
<td>1</td>
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<td>6</td>
<td>0.00</td>
<td>2.286</td>
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<td>2.540</td>
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<td>0.00</td>
<td>3.048</td>
<td>10</td>
<td>4.445</td>
<td>3.048</td>
</tr>
</tbody>
</table>

- Result files
  - Results every 0.1 second
  - File names:
    - Temperature: CodeName_Energy_TestCase_3-i.txt
    - Pressure: CodeName_Pressure_TestCase_3-i.txt
    - Density: CodeName_Density_TestCase_3-i.txt

Test-case series #3

Test-case 3.1 thermo-couple results
Test-case series #3

Test-case 3.2 thermo-couple results
Test-case series #3

Test-case 3.3 thermo-couple results
Test-case series #3

Questions/Remarks?