Prediction of TACOT Decomposition Using the Chaleur Code

5th Ablation Workshop
February 28, 2012

Ben Blackwell
Blackwell Consulting/Sandia National Laboratories

Micah Howard
Aerosciences Department/Sandia National Laboratories
Chaleur

- 1-D control volume finite element discretization on contracting grid
- Full Newton iteration scheme
- 2\textsuperscript{nd} order spatial discretization
- 1\textsuperscript{st} and 2\textsuperscript{nd} order time integrator
- Updated thermal properties within iteration loop
- Segregated solution of energy (T) and gas phase continuity (\(\rho_g\)) on same grid
- Semi-analytical integration of decomposition kinetics
TACOT Case 1 – Temperature History

Test Case 2.1
Thermocouple Data

- TC₁ (0 mm)
- TC₂ (1 mm)
- TC₃ (2 mm)
- TC₄ (4 mm)
- TC₅ (8 mm)
- TC₆ (12 mm)
- TC₇ (16 mm)
- TC₈ (24 mm)
- TC₉ (50 mm)

Solid Lines = PATO
Squares = Chaleur

T [K] vs Time [s]
TACOT Case 1 – Blowing Rate, Pyrolysis Zones, Recession

![Test Case 2.1](image)

**Test Case 2.1**

Blowing Rates, Pyrolysis Zone, Recession

- Mass Flux [Kg/m²s]
- Depth [m]

Legend:
- Solid Lines = PATO
- Squares = Chaleur

**Variables:**
- *m_dot_g*
- *m_dot_c*
- *virgin 98*
- *char 2*
- *wall recession*
TACOT Case 2 – Temperature History

Test Case 2.2
Thermocouple Data

Solid Lines = PATO
Squares = Chaleur

T [K]

0  20  40  60  80  100  120
Time [s]
TACOT Case 2 – Blowing Rate, Pyrolysis Zones, Recession

![Graph showing Mass Flux vs. Time and Depth with various lines representing different data sets with legends indicating Solid Lines = PATO and Squares = Chaleur.](image)
TACOT Case 3 – Temperature History

![Graph showing temperature history with various thermocouples labeled TC1 to TC9]

- TC1 (0 mm)
- TC2 (1 mm)
- TC3 (2 mm)
- TC4 (4 mm)
- TC5 (8 mm)
- TC6 (12 mm)
- TC7 (16 mm)
- TC8 (24 mm)
- TC9 (50 mm)

Solid Lines = PATO
Squares = Chaleur
TACOT Case 3 – Blowing Rate, Pyrolysis Zones, Recession
EST

- Element potential based equilibrium surface thermochemistry solver
- Currently being developed for solving ablation thermochemistry problems
- Can be used in two modes
  - Stand-alone to generate B’ tables
  - Coupled with Chaleur to generate B’ on-the-fly
$B'_c$ for TACOT in Air – Mutation vs. EST

Considering 25 specie reduced set
TACOT Case 4 – Temperature History

Test Case 2.3
Thermocouple Data

Solid Lines = PATO
Squares = Chaleur+EST/CEA (tabular)
TACOT Case 4 – Blowing Rate, Pyrolysis Zones, Recession

Test Case 2.3
Blowing Rates, Pyrolysis Zones, Recession

Mass Flux [Kg/m2/s]

Time [s]

Solid Lines = PATO
Squares = Chaleur+EST/CEA (tabular)

Depth [m]
TACOT Case 4 – Temperature History

Test Case 2.3
Thermocouple Data

- TC_0 (0 mm)
- TC_1 (1 mm)
- TC_2 (2 mm)
- TC_3 (4 mm)
- TC_4 (8 mm)
- TC_5 (12 mm)
- TC_6 (16 mm)
- TC_7 (24 mm)
- TC_8 (50 mm)

Solid = Chaleur+EST/CEA (tabular)
SQRS = Chaleur+EST/CEA (on-the-fly)
TACOT Case 4 – Blowing Rate, Pyrolysis Zones, Recession

Test Case 2.3
Blowing Rates, Pyrolysis Zones, Recession

- mass flux [kg/m²/s]
- depth [m]
- time [s]

Solid = Chaleur+EST/CEA (tabular)
Squre = Chaleur+EST/CEA (on-the-fly)
TACOT Case 4 – Temperature History

Test Case 2.3
Thermocouple Data

- TC_a (0 mm)
- TC_b (1 mm)
- TC_c (2 mm)
- TC_d (4 mm)
- TC_e (8 mm)
- TC_f (12 mm)
- TC_g (16 mm)
- TC_h (24 mm)
- TC_i (50 mm)

Solid = Chaleur+EST/CEA (tabular)
Sqr = Chaleur+EST/JANAF (on-the-fly)
TACOT Case 4 – Wall Data History

Case 2.3 - Surface Response

TACOT in Air

Solid Line = EST (CEA data)
Dashed Line+Squares = ACE (JANAF/ACE data)
TACOT Case 4 – Blowing Rate, Pyrolysis Zones, Recession

Test Case 2.3
Blowing Rates, Pyrolysis Zone, Recession

- $m_{dot,g}$
- $m_{dot,c}$
- Virgin 98
- Char 2
- Wall recession

Solid = Chaleur+EST/CEA (tabular)
Squrs = Chaleur+EST/JANAF (on-the-fly)
Questions?