Verification of a Finite Element Model for Pyrolyzing Ablative Materials

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Outline

• Objective
• General Pyrolyzing Ablator Problem
• Solution Examples Using Finite Element Model
  – Thermogravimetric Analysis (TGA)
  – One-Dimensional Steady-State Profile
  – One-Dimensional Transient
  – Two-Dimensional Transient
• Summary and Conclusions
Objective

- NASA primarily relies on custom written codes to analyze ablation and design TPS systems
- The basic modeling methodology was developed 50 years ago
- Through the years, CFD, thermal, and structural mechanics calculations have migrated from custom, user-written programs to commercial software packages
- Objective is to determine that a commercial finite element code can accurately and efficiently solve pyrolyzing ablation problems
Advantages of Commercial Codes

• Usability (e.g. GUI)
• Built-in pre- and post-processing
• Built-in grid generation
• Efficient solution algorithms
• Multi-dimensional capability (planar, cylindrical, 1-D, 2-D, & 3-D)
• Built in function capability (predefined, analytic, and tabular)
• Validated by a wide user base
• Reduced life cycle cost
• Regular upgrades and maintenance
• Modeling flexibility
• Better documentation
Finite-Element Program Choice

• COMSOL Multiphysics® chosen as simulation platform
• General-purpose software platform
  – Developed to handle wide variety of modeling physics
  – Allows arbitrarily inclusions of differential and algebraic modeling equations in domains, along boundaries, and at points
• Solvers based on advanced numerical methods
• Arbitrary Lagrangian-Eulerian (ALE) capability (moving boundary)
• Dynamic grid reallocation
• Flexible solution algorithms (fully coupled and sequential)
• Provides coupling between physical phenomena
• Incorporates automation and optimization capabilities
• Unified user interface (formulation, gridding, plotting, animation, & reporting)
Example Uses of Pyrolyzing Ablator
General Problem Illustration

External Flow

Chemical Species Diffusion

Radiation Out

Convection In

Radiation In

Ablation Products

Char or Residue

Pyrolysis Gas

Pyrolysis Zone

In-Depth Conduction

Virgin Material

Backface

Frontface
Modeling Requirements for Pyrolyzing Ablators

- Non-linear heat conduction in solids
- Non-linear, thermal boundary conditions
- Moving boundaries
- Non-linear, time-dependent quasi-solid in-depth reactions
- Transport and thermal properties as a function of material state as well as temperature
- Inclusion of the thermal effects of gas flow within the solid material
- In-depth pore pressure due to pyrolysis gas transport (not always employed)
Material consists of three constituents (although the number could be increased)

\[ \rho = \Gamma (\rho_A + \rho_B) + (1 - \Gamma) \rho_C \]

Components A and B decompose according to:

\[ \left( \frac{\partial \rho_i}{\partial t} \right)_y = -A_i \exp \left( -\frac{E_i}{RT} \right) \rho_{o,i} \left( \frac{\rho_i - \rho_{r,i}}{\rho_{o,i}} \right) \psi_i \]

Material properties are a function not only of temperature, but also material state
Temperature History

• In-depth temperature time history can come from:
  – Thermogravimetric Analysis (TGA)
    \[ T = \beta t + T_0 \]
  – Steady-State energy balance (1-D transformed coordinate)
    \[ \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \left( \frac{\partial \dot{m}_g h_g}{\partial y} \right) + \dot{s} \left( \frac{\partial \rho h_s}{\partial y} \right) = 0 \]
  – Transient energy balance (1-D transformed coordinate)
    \[ \rho C_p \left( \frac{\partial T}{\partial t} \right)_y = \frac{1}{A} \frac{\partial}{\partial y} \left( k A \frac{\partial T}{\partial y} \right)_t - \bar{h}(T) \left( \frac{\partial \rho}{\partial t} \right)_y + \dot{s} \rho C_p \left( \frac{\partial T}{\partial y} \right)_t + \frac{1}{A} \left( \frac{\partial \dot{m}_g h_g A}{\partial y} \right)_t \]
  – Transient Energy Balance (2-D fixed coordinate)
    \[ \rho C_p \left( \frac{\partial T}{\partial t} \right) = \frac{1}{A} \nabla (k A \nabla T) - \bar{h}(T) \left( \frac{\partial \rho}{\partial t} \right) + \frac{1}{A} \nabla \cdot (\dot{m}_g h_g A) \]
Material Selection

• For comparisons, utilize Theoretical Ablative Composite for Open Testing (TACOT) Material Properties

• Open, simulated pyrolyzing ablator that has been used a baseline test case for modeling ablation and comparing various predictive models

• Properties Required
  – Solid virgin and char specific heat, enthalpy, thermal conductivity, absorptivity and emissivity
  – Pyrolysis gas enthalpy
  – Surface thermochemistry mass loss and gas phase enthalpy
Thermophysical properties defined separately for virgin and char constituents. Composite properties determined by mixing rule based on mass.

\[ k = x k_v + (1 - x) k_c \]
\[ C_p = x C_{p,v} + (1 - x) C_{p,c} \]
\[ x = \frac{\rho_v}{\rho_v - \rho_c} \left( 1 - \frac{\rho_c}{\rho} \right) \]
Virgin and char enthalpies computed from integration of specific heats.

\[
h = \int_{T_0}^{T} C_p \, dT + h_0
\]

\[
h = x h_v + (1 - x) h_c
\]
Pyrolysis gas enthalpy computed from equilibrium thermochemistry as a function of temperature and pressure.

\[ h_{pg} = h_{pg}(p, T) \]
Surface thermochemistry conditions computed from equilibrium thermochemistry in terms of normalized mass fluxes.

\[ B'_c = \frac{m_c}{\rho_e u_e C_M} \]

\[ B'_g = \frac{m_g}{\rho_e u_e C_M} \]

\[ B'_c = B'_c(p, B'_g, T_s) \]
Surface Thermochemistry – Gas Phase Enthalpy

Enthalpy of gases at the wall computed similarly from equilibrium thermochemistry.

\[ h_w = h_w(p, B'_g, T_s) \]

Graph showing how enthalpy changes with temperature and \( B'_g \) for different values of \( B'_g \) at a constant pressure of 1 atm.
Example Problems

• Look at four examples
  – Thermogravimetric Analysis (TGA)
  – Steady-state one-dimensional thermal and density profile
  – One-dimensional transient temperature and recession history
  – Two-dimensional transient temperature and recession history
Thermogravimetric Analysis (TGA) Example
Thermogravimetric Analysis (TGA) Example

• Three component TACOT model
• Linear ramp increase in temperature at 10 K/s
• First-order time integration, not a spatial problem
• Results provide density and reaction rate for three components as a function of time
• COMSOL Multiphysics® results compared to independent fourth-order Runge-Kutta calculation
TGA Results - I

$\beta = 10 \text{ K/s}$

**Density, kg/m$^3$**

- COMSOL
- Runge-Kutta
- Difference
TGA Results - II

\[ \beta = 10 \text{ K/s} \]
Steady-State Profile Example
Steady-State Profile Example

• After long times in an infinite sample with a fixed surface temperature and recession, temperature and density profile will reach a steady state
• Problem solution becomes independent of time
• For this problem, specified surface temperature (3000 K) and recession rate ($1\times10^{-4}$ m/s) was used
• COMSOL Multiphysics® results compared to independent second order finite difference calculation and results from the Fully Implicit Ablation and Thermal Analysis Program (FIAT)
Finite Difference Temperature Profile Comparison

![Graph showing temperature profile comparison between Finite Difference and COMSOL solutions](image)

- Finite Difference
- COMSOL
- Solution Difference
Finite Difference Density Profile Comparison

Finite Difference

COMSOL

Solution Difference

Density, kg/m³

Distance, m

Relative Difference

220

230

240

250

260

270

280

290

0

0.02

0.04

0.06

0.08

0.1

0

0.02

0.04

0.06

0.08

0.1

-0.14%

-0.12%

-0.10%

-0.08%

-0.06%

-0.04%

-0.02%

0.00%

0.02%

0.04%

0.06%

0.08%

0.10%

0.12%

0.14%
FIAT Density Profile Comparison

Density, kg/m³

Distance, m

Relative Difference

-2.5%
-2.0%
-1.5%
-1.0%
-0.5%
0.0%
-0.5%
-1.0%
-1.5%
-2.0%
-2.5%

FIAT
COMSOL SS
Difference
One-Dimensional Transient Example
One-Dimensional Transient Example

• Problem is for a planar, finite width slab heated on one surface
• Full surface thermochemistry
• COMSOL Multiphysics® results compared to FIAT results
Char and Pyrolysis Surface Mass Loss Rates

![Graph showing mass loss rates over time for COMSOL mc, COMSOL mg, FIAT mc, and FIAT mg. The graph also shows the difference between COMSOL mc and mg, and FIAT mc and mg.](image-url)
FIAT In-Depth Temperature Comparison

Temperature, K

Time, s

FIAT Surface
FIAT TC1 - 0.001 m
FIAT TC2 - 0.002 m
FIAT TC3 - 0.004 m
FIAT TC4 - 0.008 m
FIAT TC5 - 0.016 m
FIAT TC6 - 0.024 m
FIAT TC7 - 0.050 m

COMSOL Surface
COMSOL TC1 - 0.001 m
COMSOL TC2 - 0.002 m
COMSOL TC3 - 0.004 m
COMSOL TC4 - 0.008 m
COMSOL TC5 - 0.016 m
COMSOL TC6 - 0.024 m
COMSOL TC7 - 0.050 m
**FIAT Temperature Profile Comparison after 60 s**

The graph compares the temperature profiles for COMSOL and FIAT over distance. The x-axis represents distance in meters, ranging from 0 to 0.05 m, while the y-axis shows temperature in Kelvin (K), ranging from 0 to 3000 K. The black line represents the COMSOL profile, the red squares indicate the FIAT profile, and the black dashed line shows the percentage difference between the two profiles. The percentage difference is color-coded with red for positive deviations and blue for negative deviations, with values ranging from 0.5% to -2.5%.
Two-Dimensional Transient Example
Two-Dimensional Transient Example

- Problem is for a two-dimensional, axisymmetric puck
- Top of puck heated with Gaussian flux profile
- Pyrolysis gas flow calculated from potential flow
- Full surface thermochemistry with recession
- 2-D COMSOL Multiphysics® results compared to a series of 1-D results
2-D Problem Animation

Animation is twice actual speed
Original and Deformed Mesh
Pyrolysis Gas Flowrate

Time=5.0 Pyrolysis Gas Flow, kg/m²-s

Time=10 Pyrolysis Gas Flow, kg/m²-s

Time=20 Pyrolysis Gas Flow, kg/m²-s

Time=30 Pyrolysis Gas Flow, kg/m²-s
Final Recession Profile at 30 s
Summary

• This work has demonstrated that a commercial finite element code is a suitable tool for modeling pyrolyzing ablative materials

• General capabilities of COMSOL Multiphysics® allow for a wide variety of geometries and problems to modeled

• Code allows for modifications to model to be made quickly and easily

• Advanced solution algorithms are efficient and stable

• Integrated environment provides a very user friendly and powerful system for modeling

• Multiphysical modeling capability allows for structural end external flow to be incorporated into analysis (in progress)