Modeling Pyrolyzing Ablative Materials with COMSOL Multiphysics®

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Outline

• Definition and Applications
• General Pyrolyzing Ablator Problem
• Solution Example Using Finite Element Model
• Summary and Conclusions
Definitions

• **Ablation** is removal of material from the surface of an object by melting, vaporization, chipping, or other erosive processes.

• **Pyrolysis** is the decomposition of a material brought about by high temperatures.

• **Pyrolyzing Ablator** is a material that undergoes sub-surface decomposition when heated and when becomes sufficiently hot, loses surface mass loss through melting or vaporization.
Applications of Pyrolyzing Ablator Modeling

- Reentry Heat Shields
- Laser Machining
- Rocket Nozzles
- Plasma Heating
- Wood Combustion
Heated Pyrolyzing Ablator

From Başkaya, A. O. “CFD Analysis of The Cork-Phenolic Heat Shield Of A Reentry Cubesat In Arc-Jet Conditions Including Ablation And Pyrolysis”, 15th International Planetary Probe Workshop
General Problem Illustration

- Radiation In
- Radiation Out
- Convection In
- Chemical Species Diffusion
- Ablation Products
- External Flow
- Pyrolysis Zone
- Char or Residue
- In-Depth Conduction
- Pyrolysis Gas
- Virgin Material
- Backface
- Frontface

Virgin Material
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)
Decomposition Model

• 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
In-Depth 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)
    \[ \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \left( \frac{\partial \dot{m}_gh_g}{\partial y} \right) + \dot{s} \left( \frac{\partial \rho h_s}{\partial y} \right) = 0 \]
  - Transient energy balance (1-D transformed coordinate)
    \[ \rho C_p \left( \frac{\partial T}{\partial t} \right)_y = \frac{1}{A} \frac{\partial}{\partial y} \left( kA \frac{\partial T}{\partial y} \right)_t - \bar{h}(T) \left( \frac{\partial \rho}{\partial t} \right)_y + \dot{s} \rho C_p \left( \frac{\partial T}{\partial y} \right)_t + \frac{1}{A} \left( \frac{\partial \dot{m}_gh_gA}{\partial y} \right)_t \]
  - Transient Energy Balance (1- and 2-D fixed coordinate)
    \[ \rho C_p \left( \frac{\partial T}{\partial t} \right) = \frac{1}{A} \nabla (kA \nabla T) - \bar{h}(T) \left( \frac{\partial \rho}{\partial t} \right) + \frac{1}{A} \nabla \cdot (\dot{m}_gh_gA) \]
Surface Energy Balance and Pyrolysis Gas Flow

\[ \alpha I + \rho_e u_e C_H (h_r - h_w) + F \sigma \varepsilon (T_w^4 - T_\infty^4) + \dot{m}_w h_w = 0 \]

\[ \nabla^2 \Phi = \frac{\partial \rho}{\partial t} \]

\[ \dot{m}_g = \nabla \Phi \]
Surface thermochemistry conditions computed from equilibrium thermochemistry in terms of normalized mass fluxes.

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

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

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

In-Depth Conduction and Surface Energy Balance
Decomposition Reactions
In-Depth Pyrolysis Gas Flow
Surface Thermochemistry
Moving Boundary
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

\[ I = I_o \cdot \exp(-C (r/r_o)^2) \]
\[ I_o = 1 \times 10^7 \text{ W/m}^2 : C = 5 \]
2-D Problem Animation

Time=0.00 Total Density, kg/m³

Time=0.00 Temperature, K

Animation is twice actual speed
Original and Deformed Mesh

Time=0 s Mesh

Time=30 s Mesh
Summary

- COMSOL 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
- COMSOL allows for modifications to model to be made quickly and easily
- Solution algorithms are efficient and stable
- Integrated environment provides a very user friendly and powerful system for modeling
- Multiphysical modeling capability allows for structural and external flow to be incorporated into analysis (in progress)
For Additional Information

QUESTIONS?
Final Recession Profile at 30 s

Height, m

Radius, m

2-D
1-D
Quasi 1-D
Example Problems

• Look at four examples solved with COMSOL
  – 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/min
- 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

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

- COMSOL
- Runge-Kutta
- Difference

Temperature, K

Density, kg/m$^3$
TGA Results - II

\[ \beta = 10 \text{ K/min} \]

\[ \text{Decomposition Rate, kg/m}^3\text{s} \]

\[ \text{Temperature, K} \]

\[ \text{Difference} \]

\[ \begin{align*}
0.000 & \quad 0.005 & \quad 0.010 & \quad 0.015 & \quad 0.020 & \quad 0.025 & \quad 0.030 & \quad 0.035 & \quad 0.040 \\
300 & \quad 400 & \quad 500 & \quad 600 & \quad 700 & \quad 800 & \quad 900 & \quad 1000 & \quad 1100 & \quad 1200
\end{align*} \]
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
• Specified surface temperature (3000 K) and steady recession rate ($1 \times 10^{-4}$ m/s)
• 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 Density Profile Comparison

Graph showing the comparison of finite difference and COMSOL solutions for density profile. The graph includes a label indicating a velocity of $1 \times 10^{-4}$ m/s.
FIAT Temperature Profile Comparison

Temperature, K vs. Distance, m

- FIAT
- COMSOL SS
- Difference

Relative Difference

1×10^-4 m/s
FIAT Density Profile Comparison

- Density, kg/m³
- Distance, m
- Relative Difference

- 1 × 10^{-4} m/s

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

• Problem is for a planar, finite width slab heated on one surface
• Frontface free stream enthalpy of 40 MJ/kg, a heat transfer coefficient of 0.1 kg/m$^2$-s, and reradiation
• Backface is adiabatic
• Full surface thermochemistry
• Thermocouples located at 0.001, 0.002, 0.004, 0.008, 0.016, 0.024, and 0.050 m
• COMSOL Multiphysics® results compared to FIAT results
FIAT Surface Temperature Comparison

Time, s

Temperature, K

Relative Difference

- COMSOL
- FIAT
- Difference

0.0%
0.5%
1.0%
1.5%
2.0%
Char and Pyrolysis Surface Mass Loss Rates

![Graph showing mass loss rates and relative differences over time.](image-url)
FIAT In-Depth Temperature Comparison

![Graph showing temperature comparison between COMSOL and FIAT surfaces and their respective depth points over time.](image)
FIAT Temperature Profile Comparison after 60 s

Temperature, K vs. Distance, m

- COMSOL
- FIAT
- Difference

Relative Difference (%)

- 2.0%
- 1.5%
- 1.0%
- 0.5%
- 0.0%
- -0.5%
FIAT Density Profile Comparison after 60 s
Two-Dimensional Transient Example
BACKUP
Density Comparison 1-D vs 2-D

1-D

Time=30 Total Density, kg/m³

2-D

Time=30 Surface: Density 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
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.

\[ B'_c = \frac{\dot{m}_c}{\rho_e u_e C_M} \]
\[ B'_g = \frac{\dot{m}_g}{\rho_e u_e C_M} \]

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

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

\[ h_w = h_w(p, B'_g, T_s) \]
COMSOL Multiphysics® User Interface
Example Uses of Pyrolyzing Ablator
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
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