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A FINITE ELEMENT METHOD FOR DECOMPOSING POROUS MEDIA PROBLEMS

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Motivation – Simulation of Multi-dimensional Material Decomposition & Deposition

General interest in a wide spectrum of problems with material removal or addition during thermal processing

- Decomposing porous materials (*e.g.*, foams) have been a continuing area of interest
- Rapid prototyping provided a material addition problem area
- Currently interested in better methods for thermal analysis of atmospheric re-entry bodies (thermal decomposition)
  - Vehicle nosetip analysis over various trajectories
  - Thermal protection of surfaces on atmospheric re-entry vehicles
  - New configurations may require full three-dimensional analysis

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Computational Methods – Material Surface Motion

- Focus on thermal problems involving conduction, radiation and chemically reactive materials
- All methods are finite element based
- Consider two methods for tracking material addition/removal
- Element Birth/Death
  - Not a PDE based method; algorithmic construction
  - Requires careful code implementation
  - Allows arbitrarily large surface deformations; modest to poor surface resolution
  - Computationally fast
- Moving Mesh
  - PDE based method using an elastic mesh motion
  - Requires coupling with thermal field solution; ALE methods
  - Large surface deformations are problematic
  - Computationally complex

Computational Method – Element Birth and Death

- The following computational features must be considered for a general finite element addition or removal process
- Criteria for element removal or addition (e.g., temperature or chemical species level, time) and evaluation location within the element
- Accounting for residual mass and energy within a deleted element may be required; dynamic, zero-dimensional, bulk nodes may be needed
- Boundary condition inheritance is essential for both element removal and addition
- Dynamic topologies imply complexities for enclosure radiation and view factor updating
- Dynamic topologies complicate interface to matrix solvers

Computational Examples – Element Birth and Death

The following demonstrate use of element removal and addition

- Foam Decomposition
- Laser Sintering

Foam Decomposition – Physical Description

- Thermal environment produces chemical reaction in contained material
- Decomposition reaction causes pyrolysis gas generation, surface recession and flow through char
- Geometry change in reactive material region; radiation enclosures and open flow areas develop

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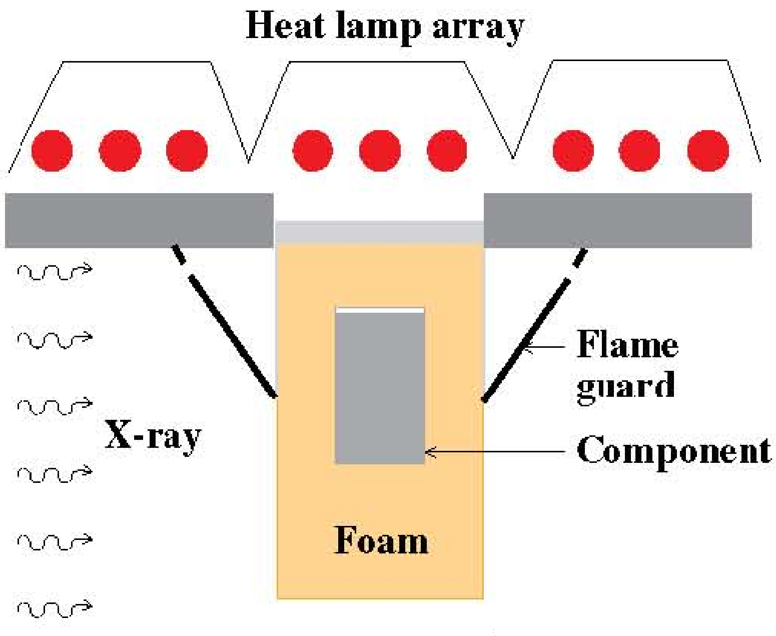
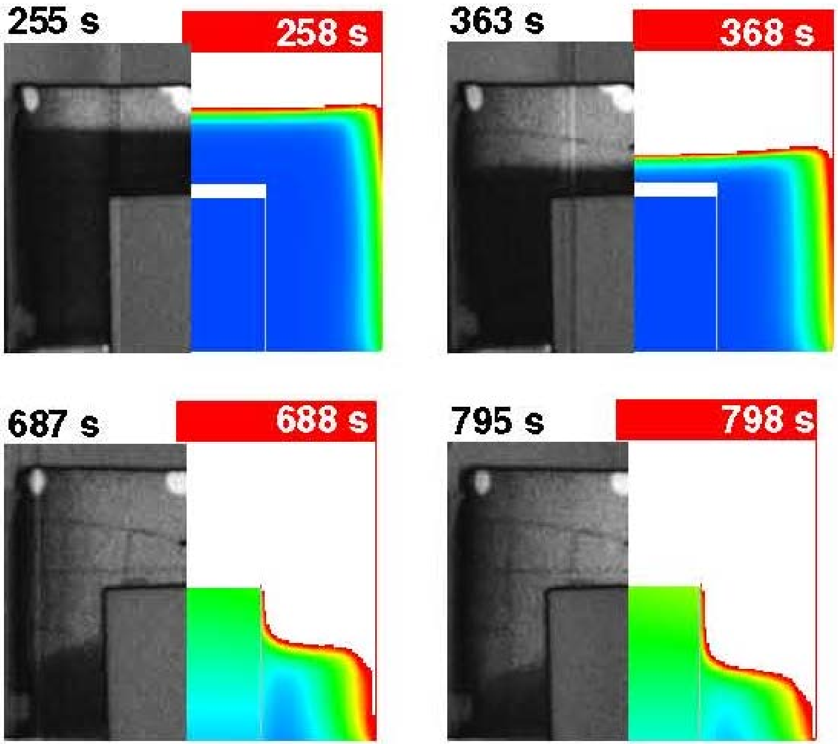
Foam Decomposition – Test & Computation





- Element death used to simulate foam decomposition
- No pyrolysis included

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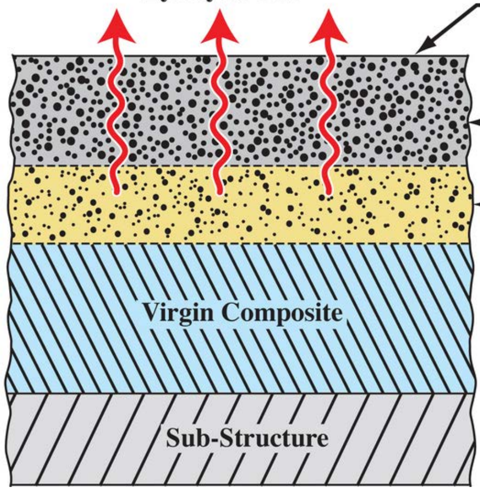
Specific Problem : Material Response in Non-decomposing & Decomposing Materials

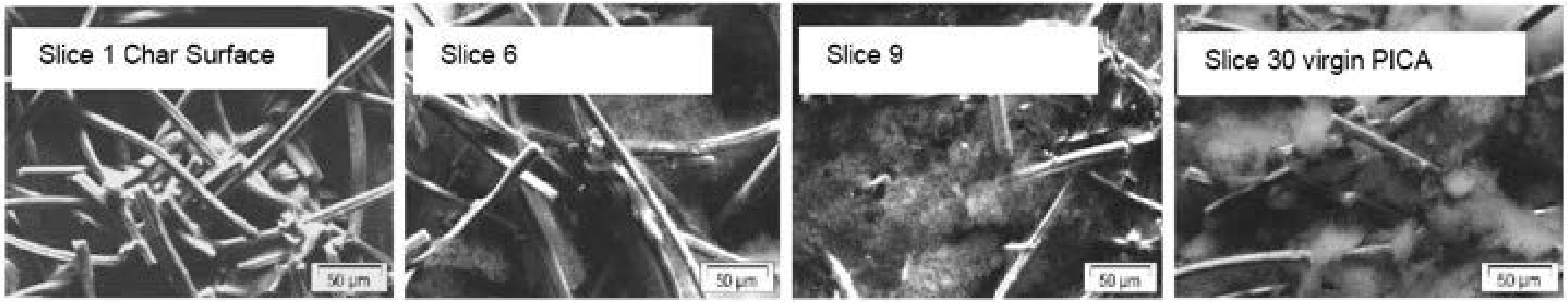


- Non-decomposing materials are characterized by material removal phenomena limited to the material surface; no chemical or phase changes occur in depth (*e.g.*, Teflon, carbon-carbon)

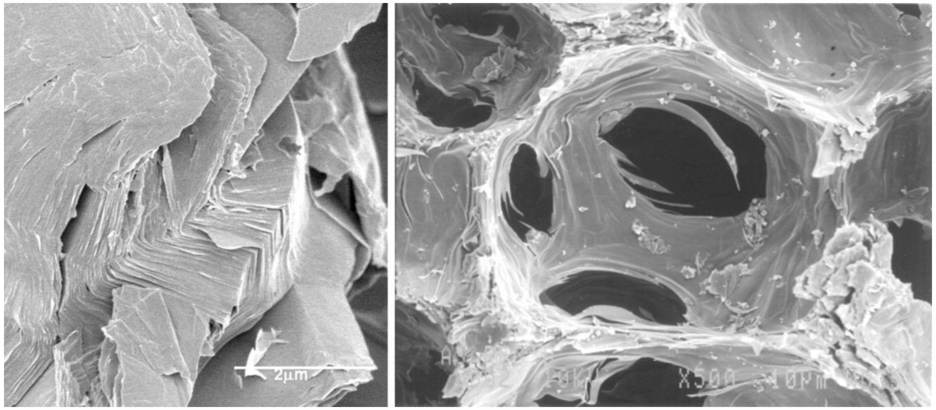
- Decomposing materials are characterized by surface removal of material and pyrolysis in depth; pyrolysis gas flow in porous matrix (char) is thermally important (*e.g*., quartz phenolic, PICA)

Typical Thermal Protection Materials

Phenolic Impregnated Carbon Ablator (PICA)[1]



Carbon Foam[2]



[1] M. Stackpoole, *et al*, AIAA 2008-1202

[2] A. Roy, WPAFB

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Material Decomposition Mechanics – Aerospace Application

Material decomposition is a multidimensional, multiple time scale, coupled thermal, fluid/structure interaction problem

- Varying hypersonic external flow, real gas
- Thermal protection materials can be complex, heterogeneous composites
- Thermal decomposition results in material loss and surface recession, changing domain
- High heat fluxes, pyrolysis reactions and complex chemistry
- Pyrolysis gas flow through char layer, evolving porosity
- Substructure may involve geometrically complex, coupled conduction/radiation domain
- Time scales vary between fluid, thermal and chemical processes

Computational Mechanics Applied to Material Decomposition (1)

Long history of numerical simulation for ablation, mainly one-dimensional and non-decomposing

- Moyer & Rindall (1968), CMA (Charring Materials Ablation) code has been an industry standard; 1D finite difference, node-dropping scheme
- Hogge & Gerrekens (1982, 1985); 1D and 2D finite element, deforming mesh with spines
- Blackwell & Hogan (1994, 1996); 1D and 2D CVFEM with Lynch & O'Neill elastic mesh motion
- Chen & Milos (1997, 2006); 1D CV - Fully Implicit Ablation and Thermal (FIAT) Code, grid compression, pyrolysis gas

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Computational Mechanics Applied to Material Decomposition (2)

- Kuntz, Hassan & Potter (2001); 2D/3D FEM with elastic mesh motion coupled with FV hypersonic CFD code
- Amar, Blackwell & Edwards (2006); 1D CVFEM with contracting mesh scheme and pyrolysis gas flow
- Lachaud, *et al* (2008, 2009); 3D ALE-FVM using OPENFOAM code; pyrolysis gas flow, multiscale modeling at the fiber scale
- Dec & Braun (2009); 3D GFEM with elastic mesh motion and pyrolysis gas flow
- Amar, Calvert & Kirk (2011); 3D Galerkin FEM with pyrolysis gas flow
- Gartling & Hogan (2001); 3D Galerkin FEM with element death for foam decomposition

Overview of Sandia Analysis Capabilities for Decomposing Materials

- CMA (Charring Materials Ablation) code
- Chaleur – 1-D non-isothermal, reacting porous media with moving mesh and surface recession
- Coyote_q – multi-D non-isothermal, reacting porous media with moving mesh, surface recession, and enclosure radiation
- EST – equilibrium surface thermochemistry
- Other specialized or simplified analysis codes

Computational Approach

- Extend existing Thermal Analysis Finite Element software (conduction, chemical reaction and radiation) to accommodate ablation problems with material decomposition
- Map CMA type chemistry models to existing general chemical kinetics methods
- Add porous flow capability for compressible pyrolysis gases; variable porosity
- Mixture energy equation
- Surface recession boundary conditions; coupling with simplified flow codes
- Add elastic, deforming mesh capability
- Add remeshing in parallel
- Coupling with hypersonic CFD code

Assumptions/Methods for Material Decomposition Model

- Two component system assumed with a solid and gas; constant volume process
- Solid and gas are in thermal equilibrium
- Chemical reaction converts virgin solid to char plus gas; porosity in solid (char) evolves with reaction
- Chemical kinetics are solved at element integration points using an operator split and stiff ODE solver
- Pyrolysis gas is nonreactive with an ideal gas EOS
- Darcy's law is an adequate description of porous flow
- Standard Galerkin FEM for discretization; fully coupled FEM solution using implicit time integration for energy and flow
- Segregated solution for mesh motion; surface recession rate derived from surface energy balance

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Development of Material Decomposition Model – Gas Flow Equation (1)

The decomposing material bulk density is represented by

$$\rho_b = \phi \rho_g + \left(1 - \phi\right) \rho_s$$

where ϕ is the porosity.

Solid Continuity

$$\frac{\partial \left(1 - \phi\right) \rho_s}{\partial t} = \dot{R}_s$$

where $\dot{R}_s$ is the solid decomposition rate and by assumption is equal in magnitude to the gas generation rate.

Fluid Continuity

$$\frac{\partial \phi \rho_g}{\partial t} + \nabla \bullet \rho_g \mathbf{u}_g = \dot{R}_g = -\dot{R}_s = -\frac{\partial \left(1 - \phi\right) \rho_s}{\partial t}$$

Development of Material Decomposition Model – Gas Flow Equation (2)

Fluid Momentum (Darcy Law)

$$\mathbf{u}_g = -\frac{\Lambda}{\mu}\nabla P_g$$

where Λ is the permeability tensor and μ is the gas viscosity

Equation of State

$$\rho_g = MP_g / ZRT_g$$

and also

$$\frac{\partial \rho_g}{\partial t} = -\rho_g \beta \frac{\partial T_g}{\partial t} + \rho_g \kappa \frac{\partial P_g}{\partial t}$$

where β and κ are expansion coefficients.

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Development of Material Decomposition Model – Gas Flow Equation (3)

Combining the continuity, momentum and EOS equations produces a pressure equation for flow in a decomposing porous material.

$$\phi\rho_g\kappa\frac{\partial P_g}{\partial t} - \phi\rho_g\beta\frac{\partial T_g}{\partial t} - \nabla\bullet\left(\frac{\rho_g\Lambda}{\mu}\nabla P_g\right) = -\rho_g\frac{\partial\phi}{\partial t} - \frac{\partial\left(1-\phi\right)\rho_s}{\partial t}$$

The gas velocity is recovered from Darcy's law.

Development of Material Decomposition Model – Energy Equation (1)

Solid Energy

$$\frac{\partial (1-\phi)\rho_s h_s}{\partial t} + \nabla \bullet (1-\phi)\rho_s h_s \mathbf{u}_m - \nabla \bullet (1-\phi)\lambda_s \nabla T_s = Q_s$$

and

$$Q_s = Q\dot{R}_g = -Q\frac{\partial (1-\phi)\rho_s}{\partial t}$$

where the chemical source and reaction rates are defined by

$$Q = \sum_{j=1}^{J} q_j^* r_j \qquad\qquad r_j = k(T)\prod_{i=1}^{I}[N_i]^{\mu_{ij}}$$

and the kinetic coefficients and species are

$$K_j(T) = T^{\beta_j} A_j \exp(-E_j/RT) \qquad\qquad \frac{d}{dt}[N_i] = \sum_{j=1}^{J} \nu_{ij} r_j$$

Development of Material Decomposition Model – Energy Equation (2)

Fluid Energy

$$\frac{\partial \phi \rho_g h_g}{\partial t} + \nabla \bullet \rho_g \mathbf{u}_r h_g - \nabla \bullet \phi \lambda_g \nabla T_g = Q_g = 0$$

Adding the Solid and Fluid Energy equations and assuming thermal equilibrium $\left(T_s = T_g = T\right)$ leads to a combined (bulk) energy equation. The combined equation is simplified using continuity and defining some effective properties for the solid/fluid system.

Development of Material Decomposition Model – Energy Equation (3)

Combined Energy

$$\left(\rho C_P\right)_e \frac{\partial T}{\partial t} + \rho_g C_{P_g} \mathbf{u}_r \bullet \nabla T + \left(1-\phi\right)\rho_s C_{P_s} \mathbf{u}_m \bullet \nabla T - \nabla \bullet \lambda_e \nabla T$$

$$= H \frac{\partial\left(1-\phi\right)\rho_s}{\partial t} + Q_s$$

where

$$\left(\rho C_P\right)_e = \phi \rho_g C_{P_g} + \left(1-\phi\right)\rho_s C_{P_s}$$

$$\lambda_e = \phi \lambda_g + \left(1-\phi\right)\lambda_s$$

$$H = h_g - h_s$$

$$\mathbf{u}_r = \mathbf{u}_g - \mathbf{u}_m$$

Development of Material Decomposition Model – Reaction Kinetics (1)

The gas generation rate is required for the source terms in the pressure and temperature equations.

$$\dot{R}_g = -\dot{R}_g = -\frac{\partial(1-\phi)\rho_s}{\partial t}$$

The chemistry model for ablators usually consists of three components; two reacting resin components and a non-reactive reinforcement component. The two resin components decompose over different temperature ranges. The solid density is defined by

$$\rho_s = \Gamma(\rho_1 + \rho_2) + (1-\Gamma)\rho_3$$

where

ρ_1, ρ_2 = resin components

ρ_3 = binder component

Γ = volume fraction resin

Development of Material Decomposition Model – Reaction Kinetics (2)

Assuming Arrhenius kinetics then

$$\dot{R}_s = -\frac{\partial\left(1-\phi\right)\rho_s}{\partial t} = -\Delta\left[\frac{\left(1-\phi\right)\rho_s - \left(1-\phi_c\right)\rho_c}{\Delta}\right]^m A\exp\left(-E/RT\right)$$

with

$$\Delta = \left(1-\phi_v\right)\rho_v - \left(1-\phi_c\right)\rho_c$$

ρ_c = density char

ρ_v = density virgin resin

This form has been used in many previous 1D methods.

Development of Material Decomposition Model – Reaction Kinetics (3)

To use the standard chemical kinetics package that integrates the species rate equations define

$$\omega_i = \frac{\left(\rho_i - \rho_{i_r}\right)}{\rho_{i_o}} \quad \text{for} \quad i = 1,\ 2,\ 3$$

and the subscripts denote residual (*r*) and original (*o*) values. The rate equations for the three components are then

$$\frac{d\omega_1}{dt} = -r_1 = -k_1\omega_1^3 = -\omega_1^3 A_1 \exp\left(-E_1/RT\right)$$

$$\frac{d\omega_2}{dt} = -r_2 = -k_2\omega_2^3 = -\omega_2^3 A_2 \exp\left(-E_2/RT\right)$$

$$\frac{d\omega_3}{dt} = 0$$

Boundary Conditions for Material Decomposition Model (1)

The overall flux boundary condition is

$$q_{cond} = -k\frac{\partial T}{\partial t} = q_{conv} + q_{rad} + q_{abl}$$

Two convective heating boundary conditions specifications are usually encountered for the energy equation and are dependent on the source of the heating information.

Two types of ablation boundary condition specifications are also standard.

Boundary Conditions for Material Decomposition Model (2)

- Aeroheating Boundary Condition
  - Standard tabular forms of heating produced from a number of legacy flow codes
  - Data produced at specific body locations with time (trajectory) as dependent variable
  - Heating data is for a fixed, cold wall temperature; hot wall corrections needed
  - $q_{aero} = \rho_e u_e C_H (h_r - h_w)$ where C_H = Stanton number, h_r = free stream recovery enthalpy and h_w= gas enthalpy at wall temperature
- Navier-Stokes Boundary Condition
  - Computed convective heat transfer $q_{aero} = q_{conv}$ from CFD code

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Boundary Conditions for Material Decomposition Model (3)

- Q Star Surface Recession Boundary Condition
  - Heat of formation type boundary condition; heat is removed from surface at fixed temperature
  - $q_{abl} = \dot{m}Q^*$ where $\dot{m}$ is the mass flux, and Q^* is the heat of decomposition (fixed property)
  - Solve flux balance at surface to find q_{abl} from which local mass flux is found and recession rate is computed from $\dot{s} = \dot{m}/\rho$
- Thermochemical Material Decomposition Boundary Condition
  - Uses tabulated data (B-prime tables)
  - $q_{abl} = \dot{m}\left(h_w - h_c\right)$ where h_c is the enthalpy of ablating material, $\dot{m} = \rho_e u_e C_M B_c$ and C_M is the mass transfer Stanton number
  - Recession rate computed from the surface flux balance

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Mesh Motion for Material Decomposition

The recession rate $\dot{s}$ is used to set displacement boundary conditions on the ablating surface for the current time step

$$\mathbf{d}_{abl\_surf} = \dot{s}\,\Delta t\,\hat{\mathbf{n}}$$

where $\hat{\mathbf{n}}$ is the normal to the surface.

The mesh is moved according to the solution of the boundary value problem described by the equations (Kanchi & Masud, IJNMF 2007)

$$\nabla \bullet \left[\left(1 + \tau \right) \nabla \right] \mathbf{d} = \mathbf{0}$$

where τ is a spatially varying weighting parameter that controls mesh distortion.

In a FE implementation, the local element weighting is $\tau_{elem} = \dfrac{1 - V_{\min}/V_{\max}}{V_{elem}/V_{\max}}$
where V are element volumes.

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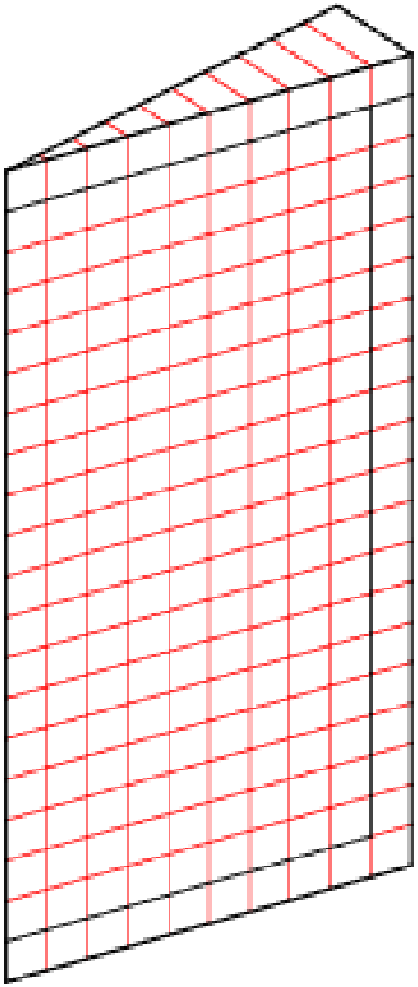
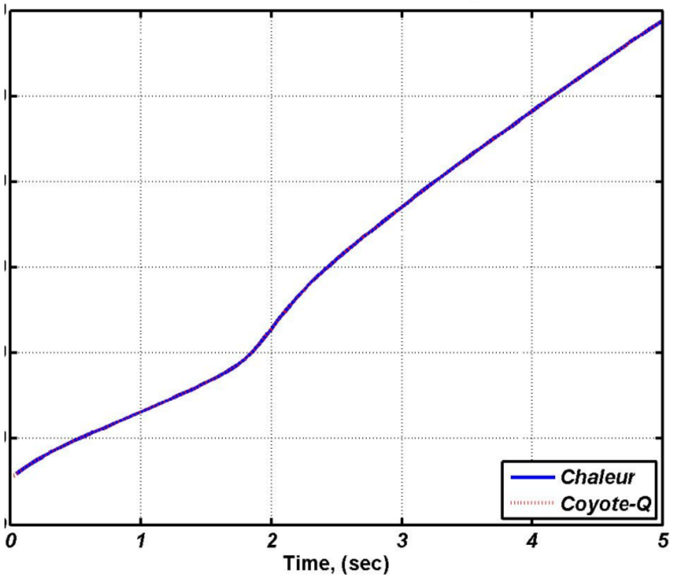
Test Problem - TGA Numerical Experiment

- Decomposition Kinetics
- Material with In-depth Decomposition
- Constant Volume Heating of Material
- 3D Wedge Geometry
- 4 Species, 2 Reactions
- W_1 = Resin A, W_2 = Resin B
- W_3 = Binder, β = Extent of Reaction
- T_{init} = 536 K
- Variable properties
- Predictor, multiple corrector integration
- Stiff ODE solver for chemistry
- Comparison with 1D CVFEM Code

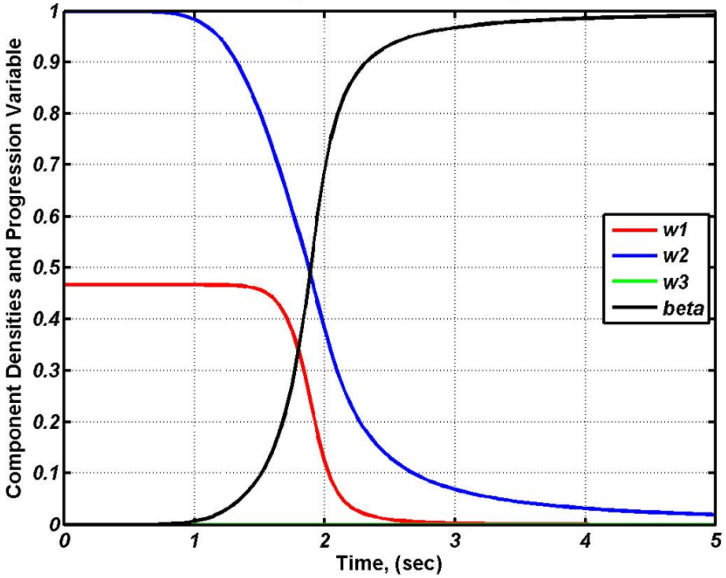


Material with In-depth Decomposition – Time Histories

Temperature

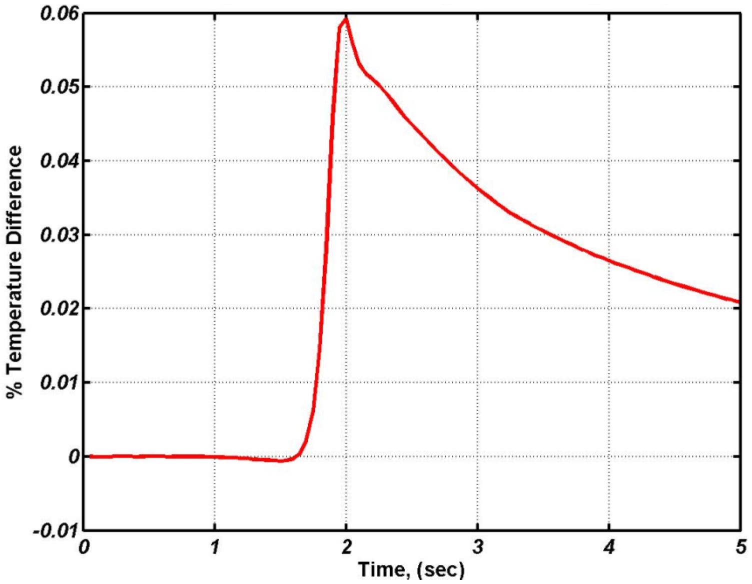


Species

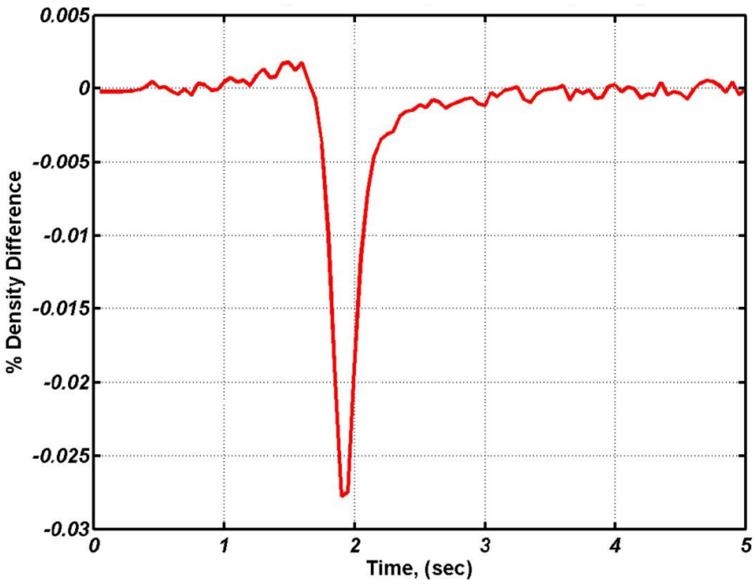


Material with In-depth Decomposition – Code Comparison

Temperature

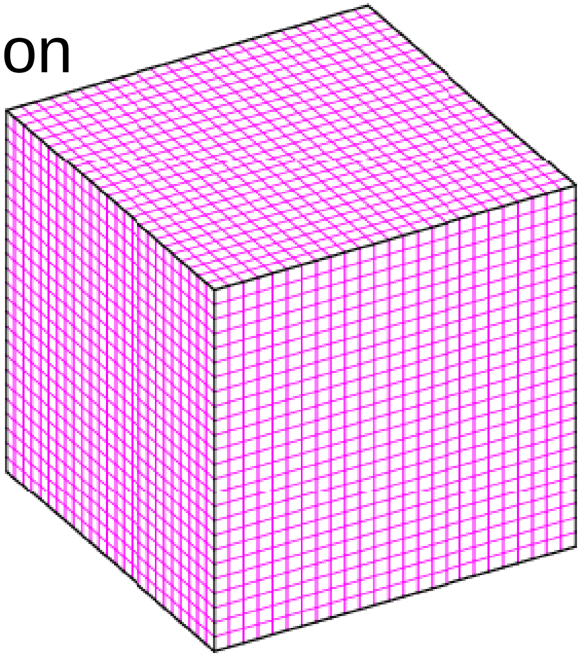


Density

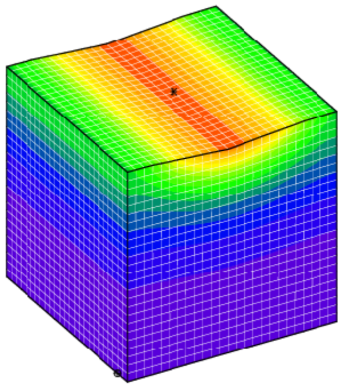


Test Problem – Material Decomposition of a Block

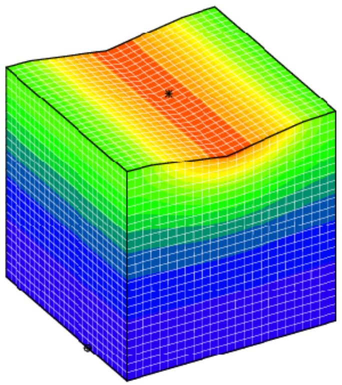
- Carbon-Carbon Surface Decomposition
- 3D Block Geometry
- Material decomposition on top surface with spatially varying heat transfer coefficient
- BC's:
  - Aerodynamic Heating Decks
  - Constant Pressure & Radiation
- Predictor-corrector integration with autostep



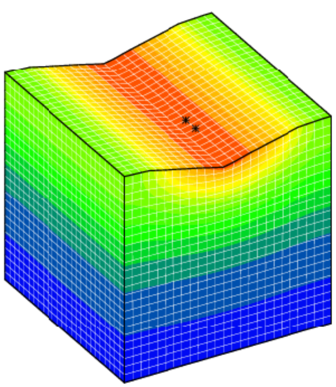
Material Decomposition on a Block – Spanwise Variation in Heating



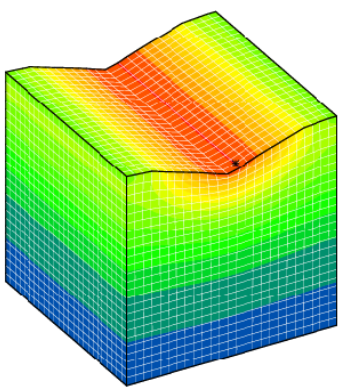
t = 100 sec



t = 200 sec

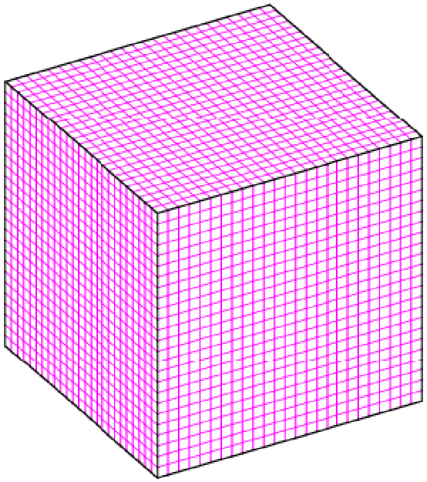


t = 300 sec



t = 400 sec

5th NASA Ablation Workshop Test Case – Code Comparisons for a Fictitious Material



- Fictitious material used for comparisons
  - TACOT (Theoretical Ablative Composite for Open Testing ~ similar to PICA)
- Problem definition
  - one-dimensional, 5cm thick
  - T_{init} = 300K, P_{atm} = 1 atm
  - Transient front-face boundary condition
    - Convective heating boundary condition for one minute
    - Cooled by radiation to surroundings
  - Adiabatic and impermeable on back-face
  - Tabular material data
  - In-depth chemistry and pyrolysis gas flow
  - Analyzed with and without surface recession

5^{th} NASA Ablation Workshop Comparison Problem 2.x

- Multiple cases were considered with differing convective heating rates
  - Cases 1 & 2 with lower heating rate
    - targeted surface temp ~1600K
  - Case 3 with higher heat rate
    - targeted surface temp ~3000K

Time (s)	*$\rho_e u_e C_H$ (kg/m²-s)*	*h_e (J/kg) Cases 1&2*	*h_e (J/kg) Case 3*
0	**0.3**	**0**	**0**
0.1	**0.3**	**1.5×10^{-6}**	**2.5×10^{-7}**
60.0	**0.3**	**1.5×10^{-6}**	**2.5×10^{-7}**
60.1	**0.0**	**0**	**0**
120	**0.0**	**0**	**0**

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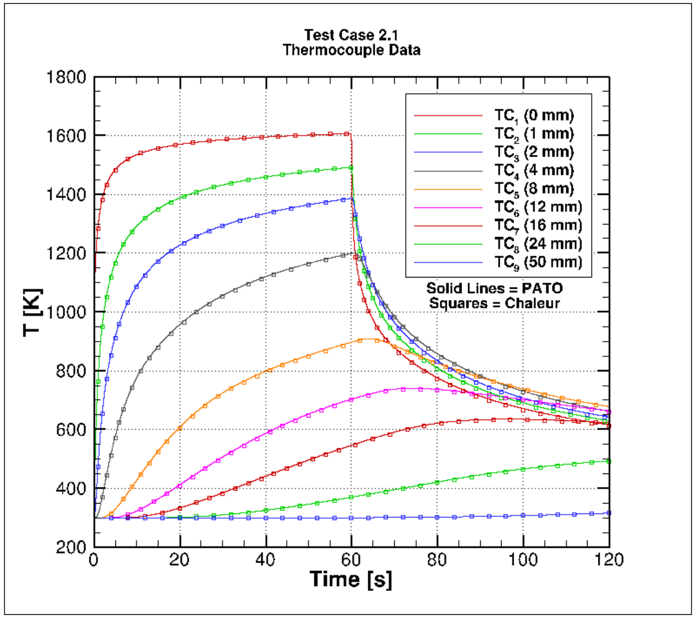
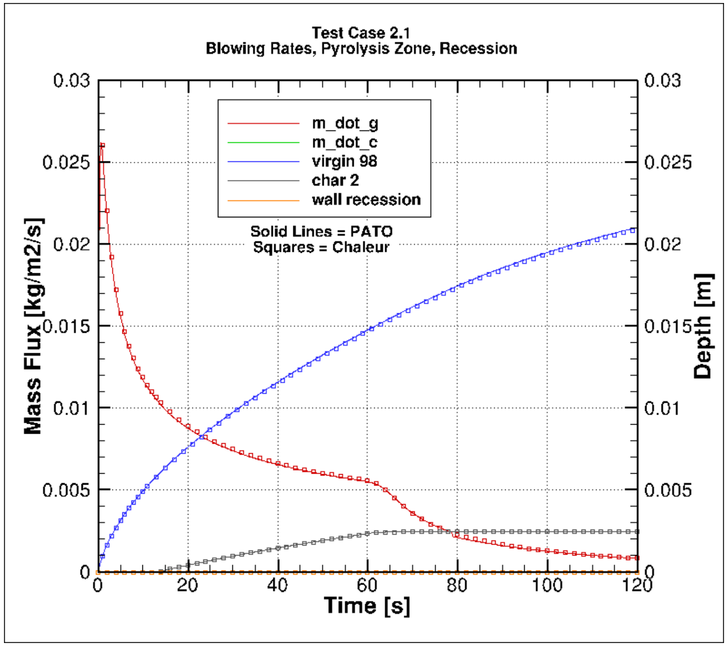
Thermochemical Response without Surface Recession for Lower Heat Rate (charing)

In-depth temperature response

Mass loss rates and surface response





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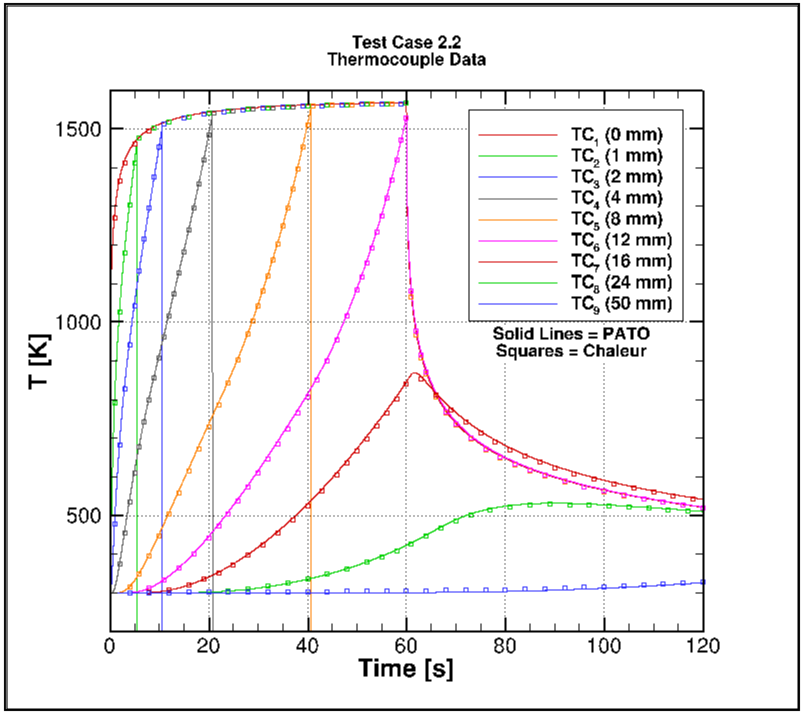
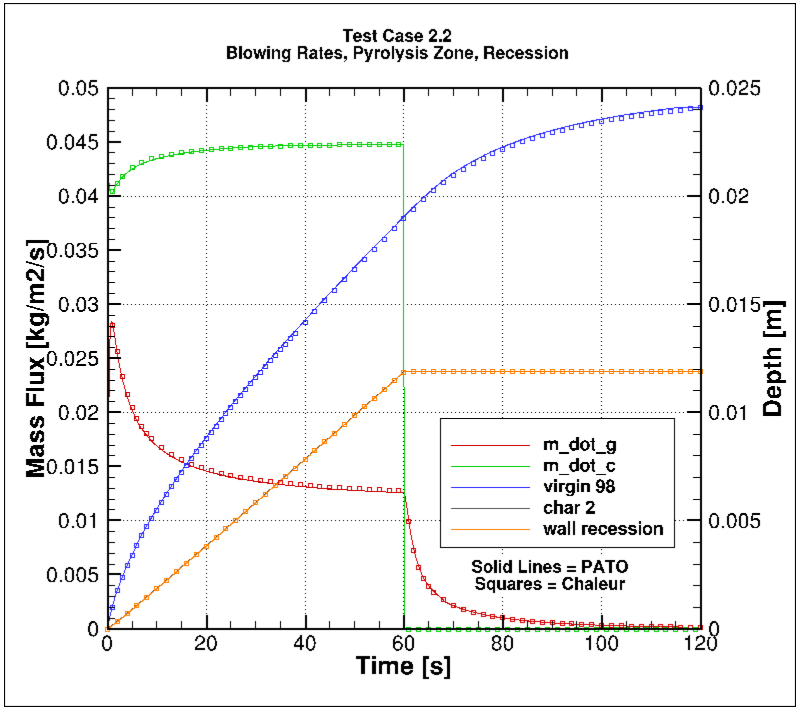
Thermochemical Response with Surface Recession for Lower Heat Rate

In-depth temperature response



Mass loss rates and surface response



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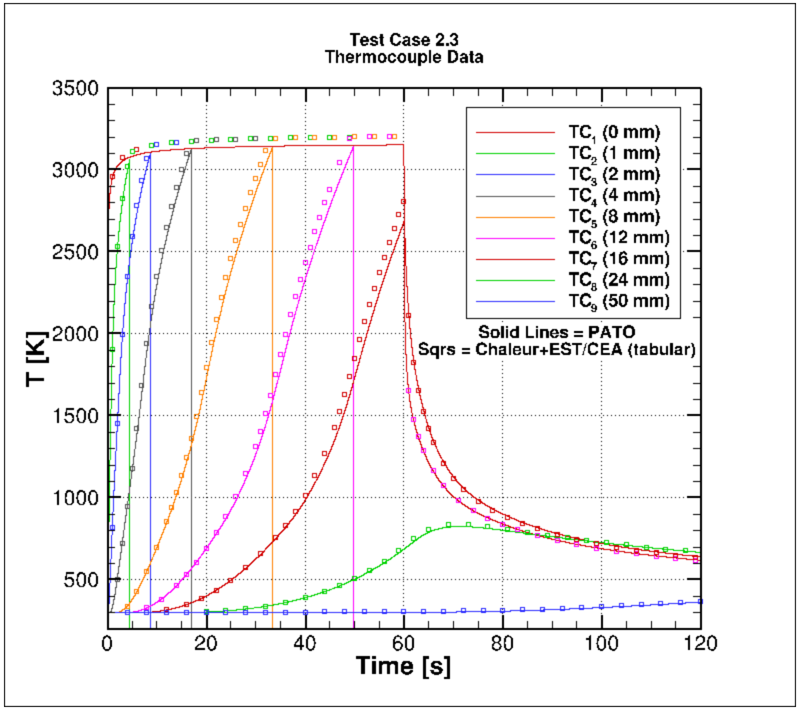
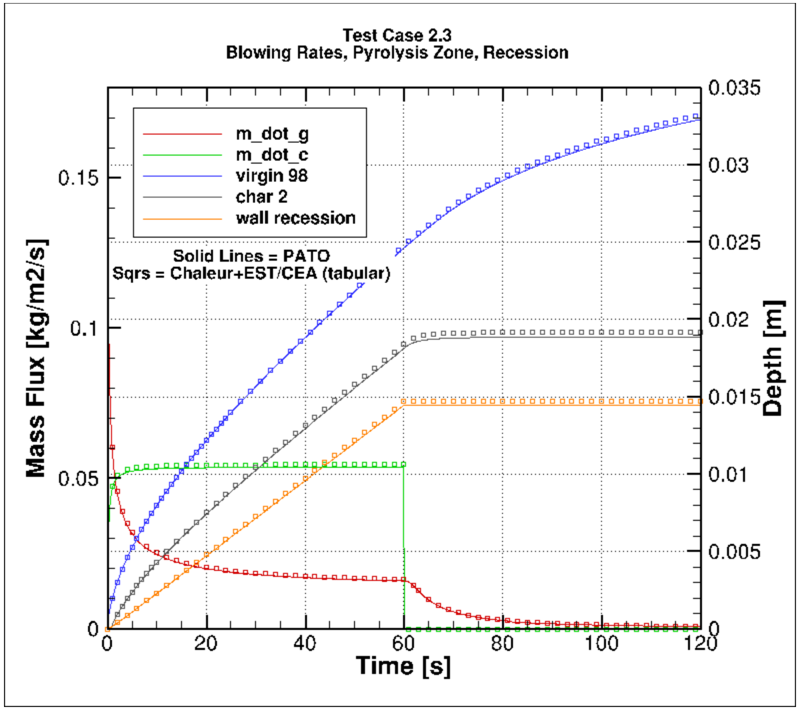
Thermochemical Response with Surface Recession for Higher Heat Rate

In-depth temperature response

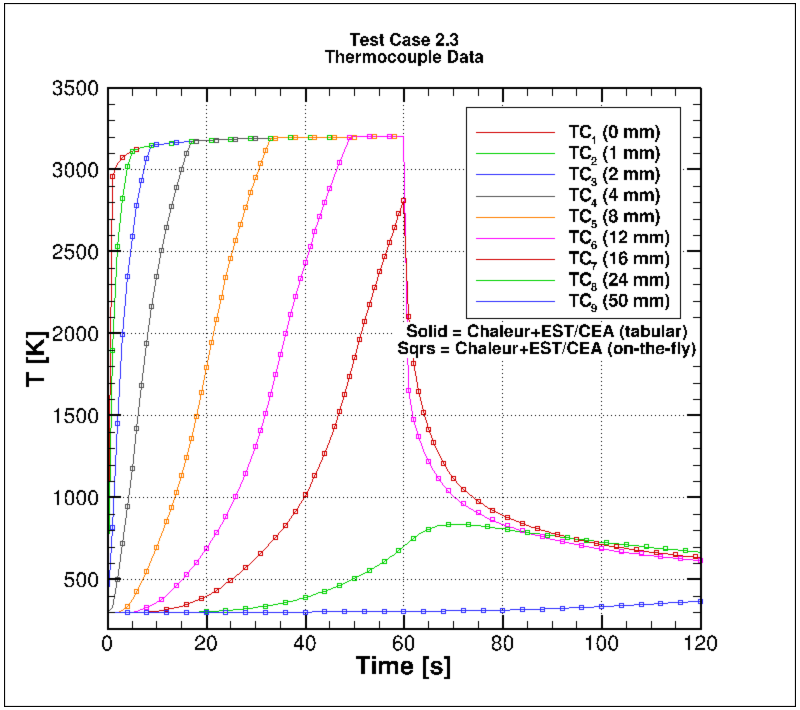


Mass loss rates and surface response

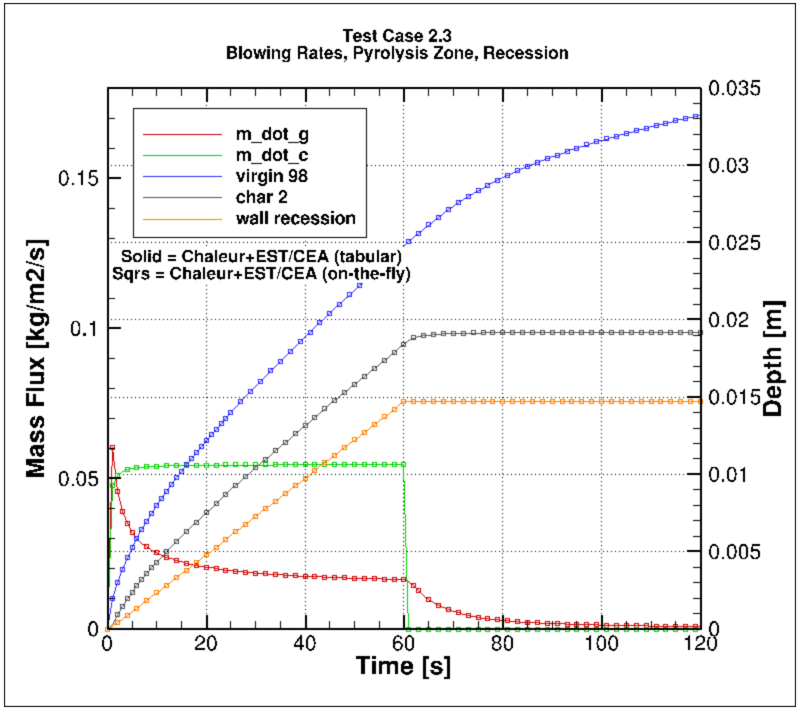


Comparison of EST Subroutine and B-prime Table Lookup for Higher Heating Rate

In-depth temperature response



Mass loss rates and surface response



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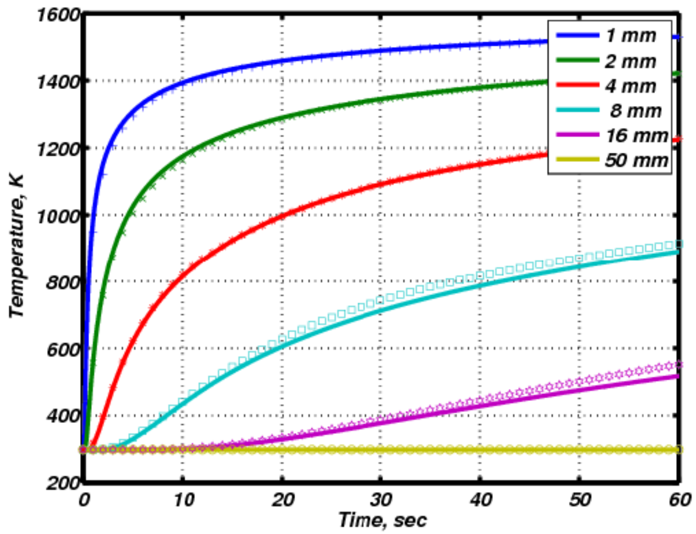
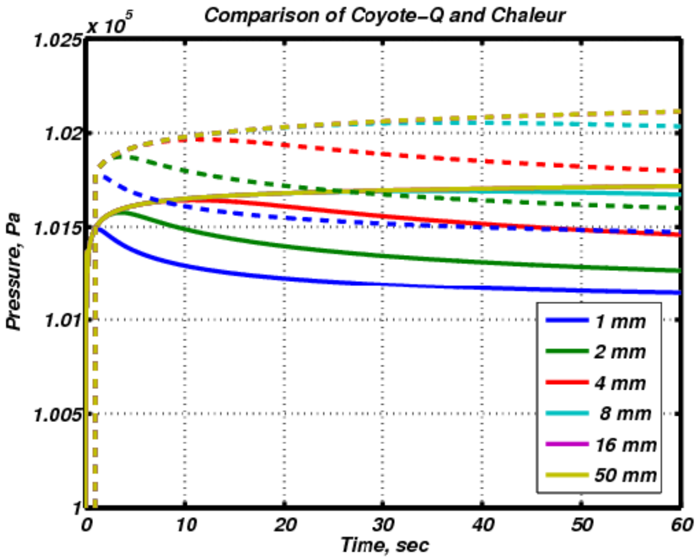
TACOT Predictions
CMA Type Model

Temperature



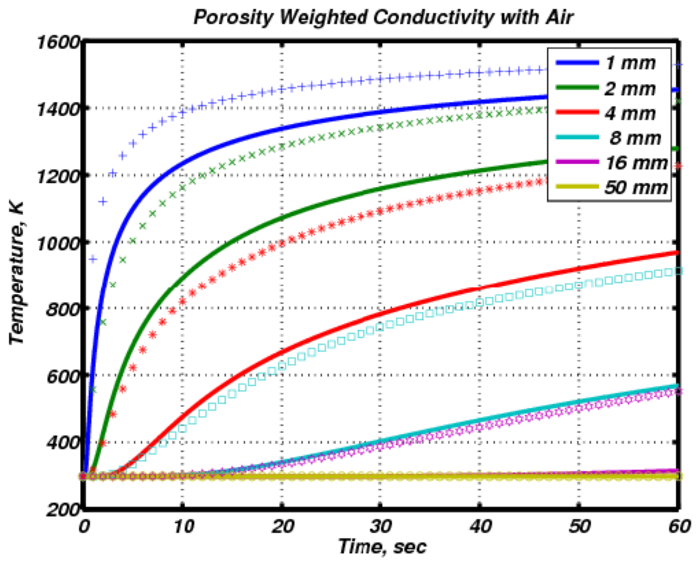
Pressure



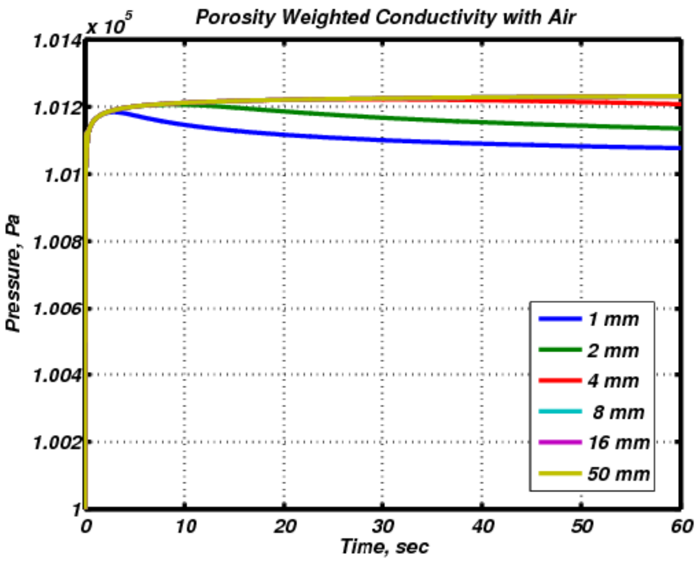
- Temperature comparison with FIAT Code
- Pressure comparison with Chaleur Code
- Model neglects pyrolysis gas thermal conductivity

TACOT Predictions
Porous Media Type Model

Temperature

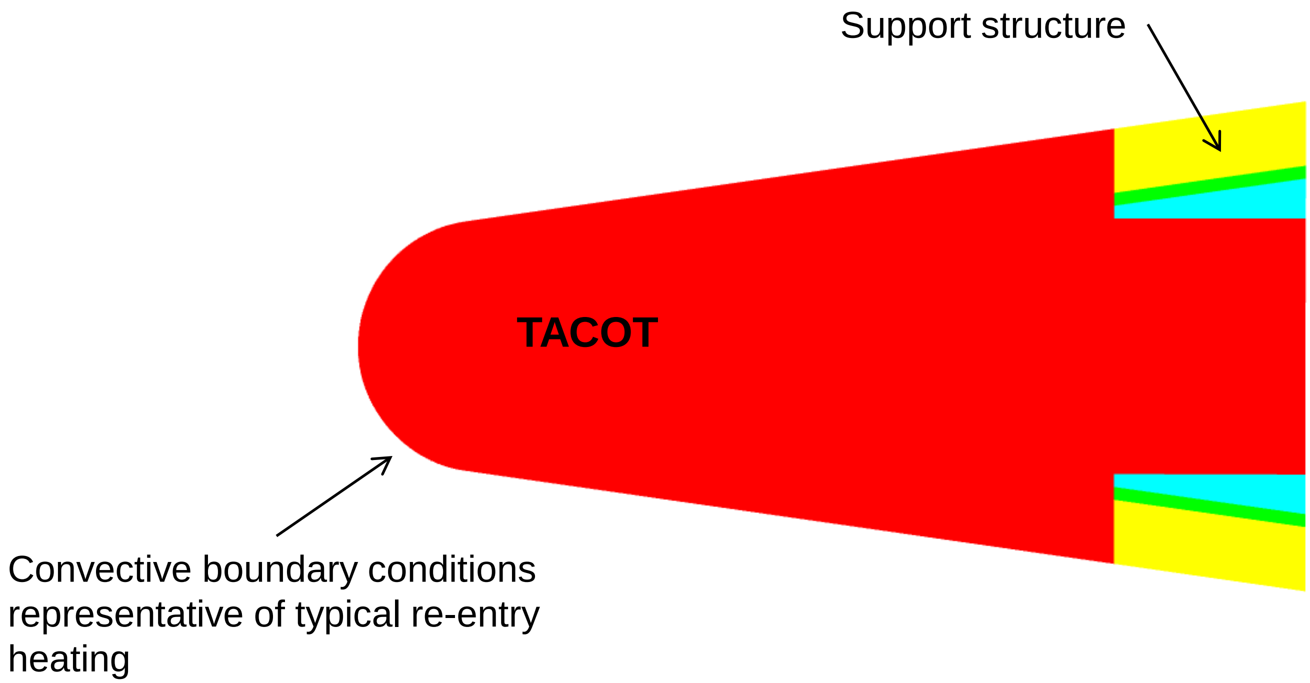


Pressure

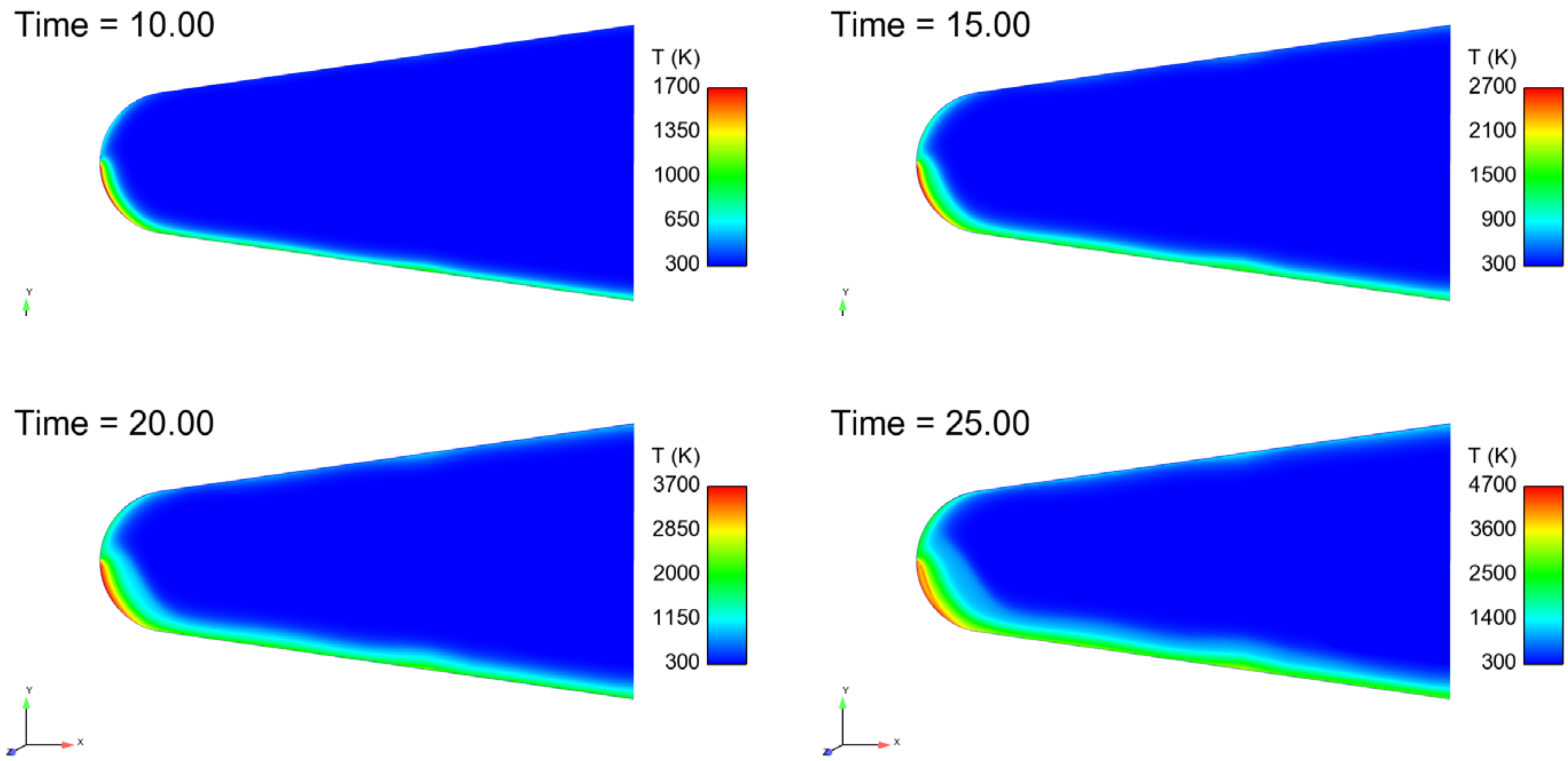


- Model includes pyrolysis gas thermal conductivity

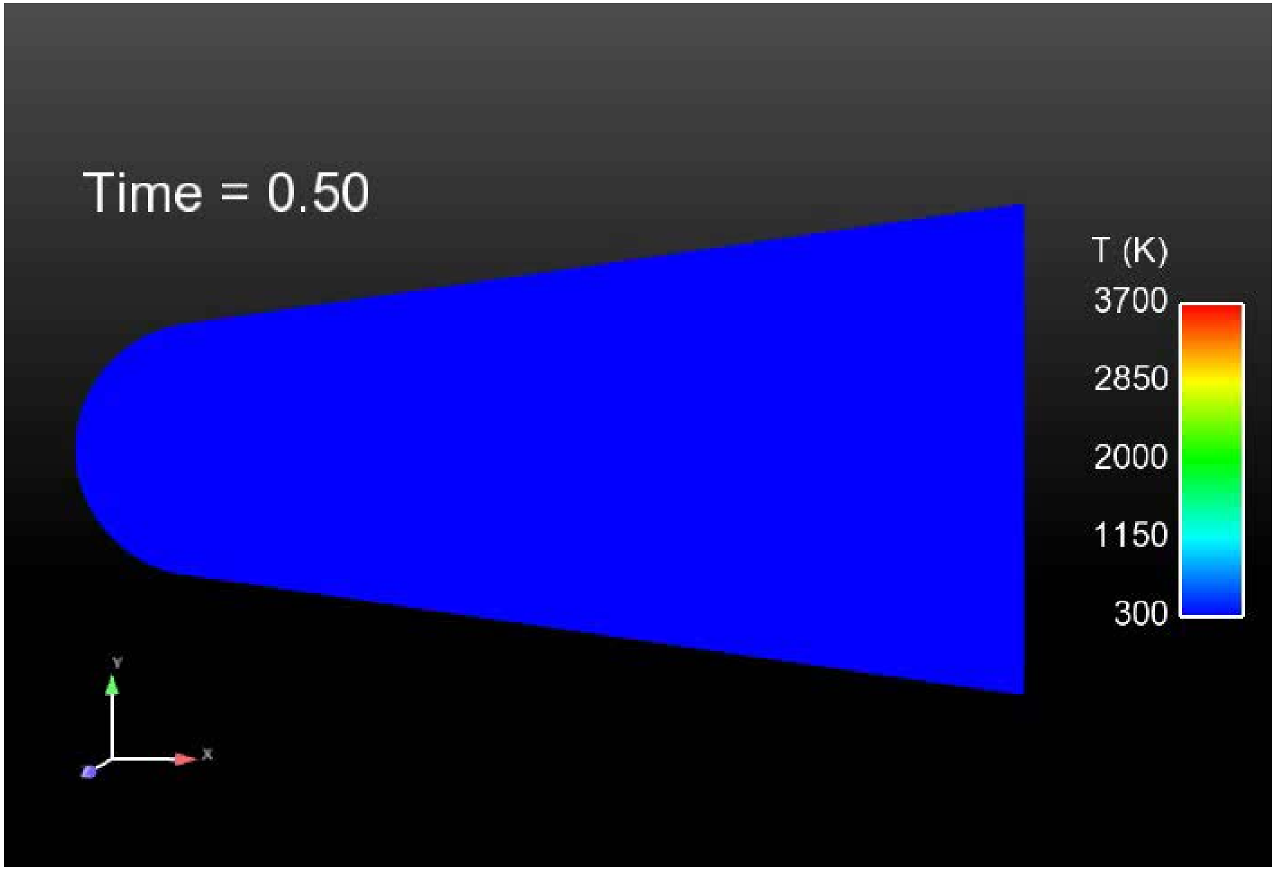
Example of 2-D Planar Problem with In-depth Decomposition of TACOT



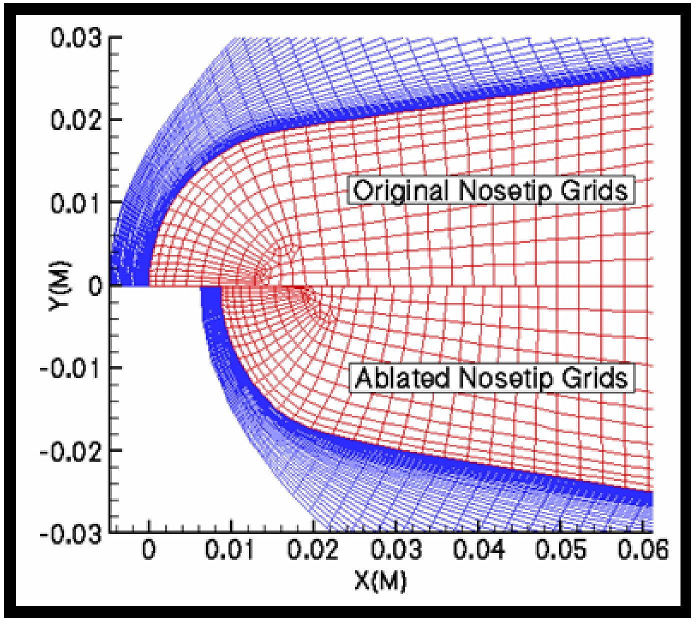
Thermal Response for 2-D Aeroheating with In-Depth Material Decomposition

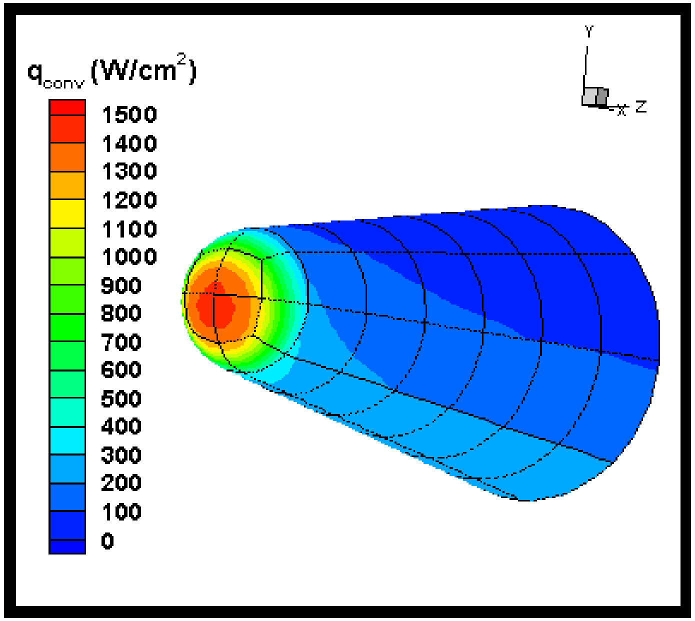


Note different temperature ranges


Time = 0.50
T (K)
3700
2850
2000
1150
300
Y
X

Example of Surface Recession without Decomposition – Coupled Codes





Mesh Motion

Temperature

- Iterative coupling of hypersonic CFD code with material response code
- Trajectory : 25 seconds duration with *Ma* = 22 to 12
- Carbon/carbon nosetip material

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Concluding Remarks

- Demonstrated the use of finite element birth/death for material decomposition and addition problems
- Formulated an initial/boundary value problem for multidimensional material decomposition including in-depth decomposition
- Developed standard FEM for coupled equations describing material removal processes
- Demonstrated viable method for standard (CMA) decomposition chemical kinetics
- Continue testing for gas generation and porous flow
- Continue testing of mesh motion and remeshing

Thank you