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A FINITE ELEMENT METHOD FOR MULTI-DIMENSIONAL ABLATION PROBLEMS

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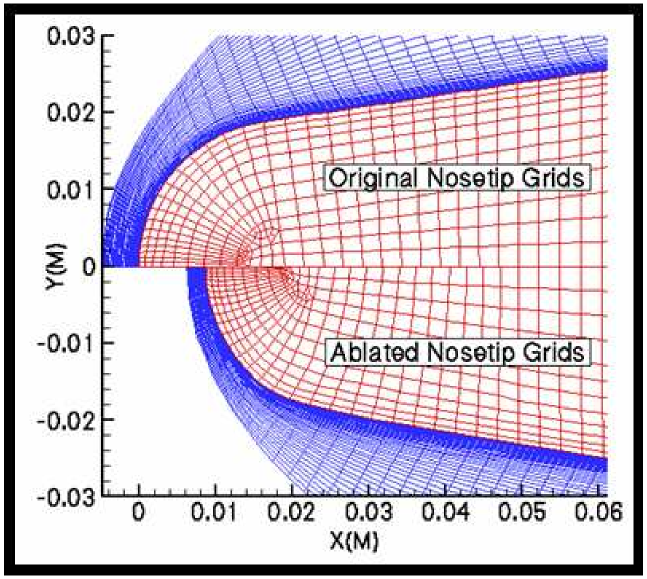
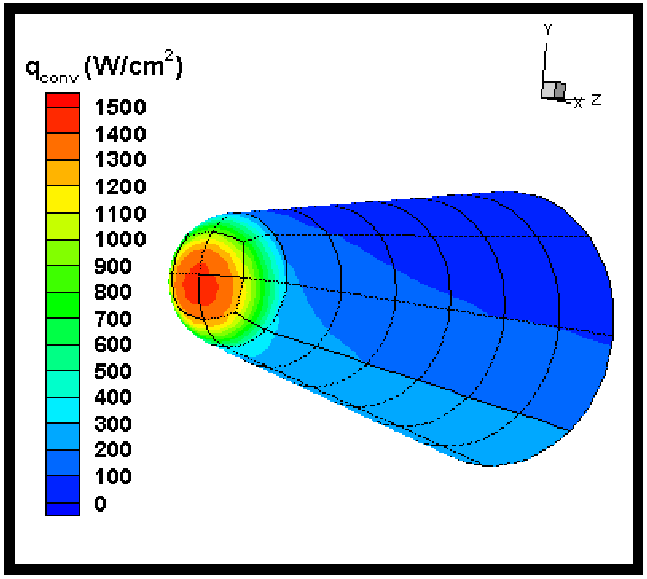
General Motivation - Multidimensional Ablation

- **Primarily interested in the thermal analysis of re-entry bodies**
- **Material thermal response involving aerodynamic heating and ablation is critical for a variety of aerospace applications**
  - **Vehicle nosetip analysis over various trajectories**
  - **Flight test analyses for captive carry configurations**
  - **Ablating fins on ballistic reentry vehicle**
- **Newer, more complex configurations demand more than one-dimensional simulation methods**
- **Interest in other types decomposing porous materials,** *e.g.* **foams**

Example of Ablation without Decomposition
Original Coupled Code

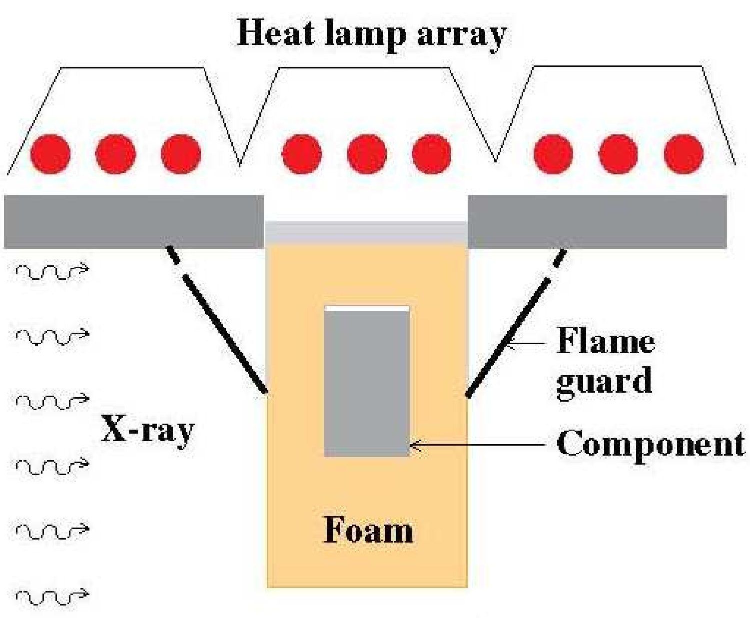




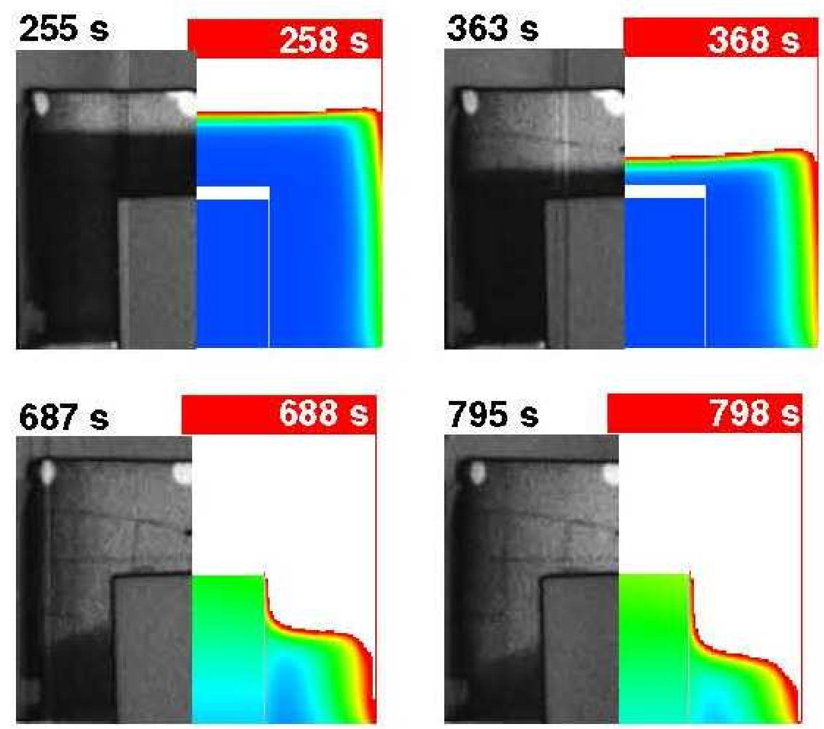
Mesh Motion **Temperature**

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

Experiment



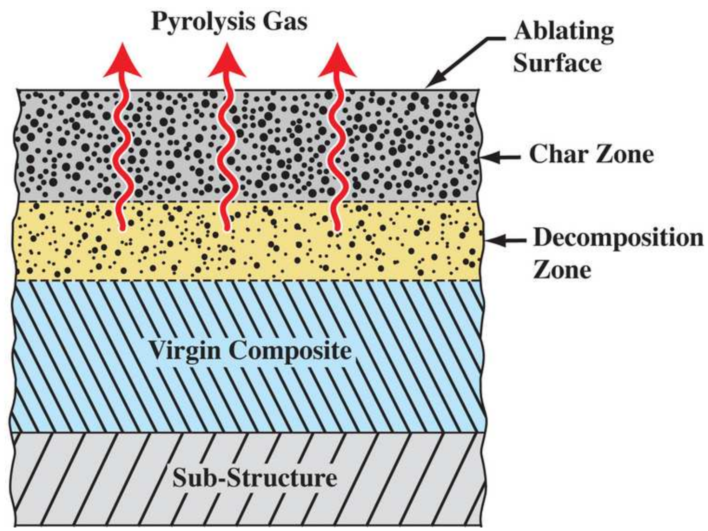
Comparison



Element death used to simulate foam decomposition

No pyrolysis included

Specific Problem : Ablation in Non-decomposing and Decomposing Materials



- **Non-decomposing materials are characterized by ablation 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 ablation and pyrolysis in depth; pyrolysis gas flow in porous matrix (char) is thermally important (*e.g.*, phenolic carbon, phenolic silica)**

Computational Mechanics Applied to Ablation

- 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
- 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

Current Objectives & 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**
  - **Ablation boundary conditions; coupling with simplified flow codes**
  - **Add elastic, deforming mesh capability**
  - **Add remeshing in parallel**
  - **Coupling with hypersonic CFD code**

Assumptions for Ablation 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
- Pyrolysis gas is nonreactive with an ideal gas EOS
- Darcy's law is an adequate description of porous flow, bouyancy neglected
- Standard Galerkin FEM for discretization; fully coupled FEM solution using implicit time integration

Development of Ablation Model - Gas Flow Eqn (1)

The decomposing material bulk density is represented by

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

where ϕ is the porosity.

Solid Continuity

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

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

Fluid Continuity

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

Development of Ablation Model - Gas Flow Eqn (2)

Fluid Momentum (Darcy Law)

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

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

Equation of State

$$\rho_g = M P_g / Z \mathcal{R} T_g$$

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.

Development of Ablation Model - Gas Flow Eqn (3)

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

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

The gas velocity is recovered from Darcy's law.

Development of Ablation Model - Energy Eqn (1)

Solid Energy

$$\frac{\partial(1-\phi)\rho_s h_s}{\partial t} - \nabla \cdot (1-\phi)\lambda_s \nabla T_s = Q_s$$

and

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

where the chemical source and reaction rates are defined by

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

and the kinetic coefficients and species are

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

Development of Ablation Model - Energy Eqn (2)

Fluid Energy

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

Adding the Solid and Fluid Energy equations and assuming thermal equilibrium ($T_s = T_g = T$) 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 Ablation Model - Energy Eqn (3)

Combined Energy

$$(\rho C_P)_e \frac{\partial T}{\partial t} + \rho_g C_{P_g} \mathbf{u} \cdot \nabla T - \nabla \cdot \lambda_e \nabla T = H \frac{\partial (1-\phi)\rho_s}{\partial t}$$

where

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

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

$$H = h_g - h_s - Q$$

Development of Ablation Model - Reaction Kinetics (1)

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

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

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

$\rho_1, \rho_2 =$ resin components

$\rho_3 =$ reinforcement component

$\Gamma =$ volume fraction resin

Development of Ablation Model - Reaction Kinetics (2)

Assuming Arrhenius kinetics then

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

with

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

$\rho_c =$ **density char**

$\rho_v =$ **density virgin resin**

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

Development of Ablation Model - Reaction Kinetics (3)

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

$$\omega_i = \frac{(\rho_i - \rho_{r_i})}{\rho_{r_0}} \quad for \quad i = 1, 2, 3$$

The rate equations for the three components are then

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

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

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

Boundary Conditions for Ablation Model (1)

The overall flux boundary condition is

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

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.

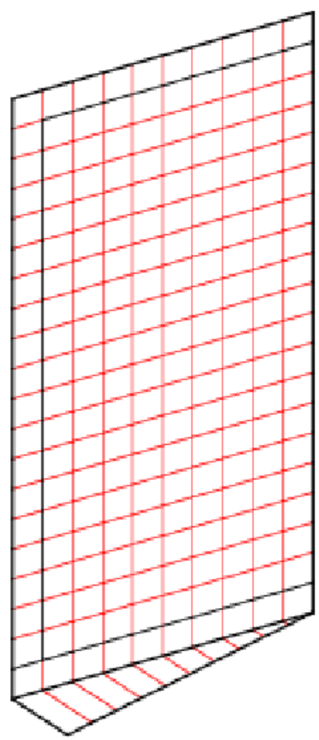
Boundary Conditions for Ablation Model (2)

- **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**

Boundary Conditions for Ablation Model (3)

- Q Star Ablation Boundary Condition
  - Heat of formation type boundary condition; heat is removed from surface at fixed temperature
  - $q_{abl} = \dot{m} Q^*$ where $\dot{m} =$ mass flux, $Q^* =$ heat of ablation (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 Ablation Boundary Condition
  - Uses tabulated data
  - $q_{abl} = \dot{m}(h_w - h_c)$ with $h_c =$ enthalpy of ablating material, $\dot{m} = \rho_e u_e C_M B_c$ and $C_M =$ mass transfer Stanton number
  - Recession rate computed from surface flux balance

Test Problem - Decomposition



- Carbon Phenolic Decomposition
- TGA Type Numerical Experiment
- 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}: $536K$ for Carbon Phenolic
- Variable properties
- Predictor, multiple corrector integration
- Stiff ODE solver for chemistry
- Comparison with 1D CVFEM Code

Carbon Phenolic Decomposition Time Histories

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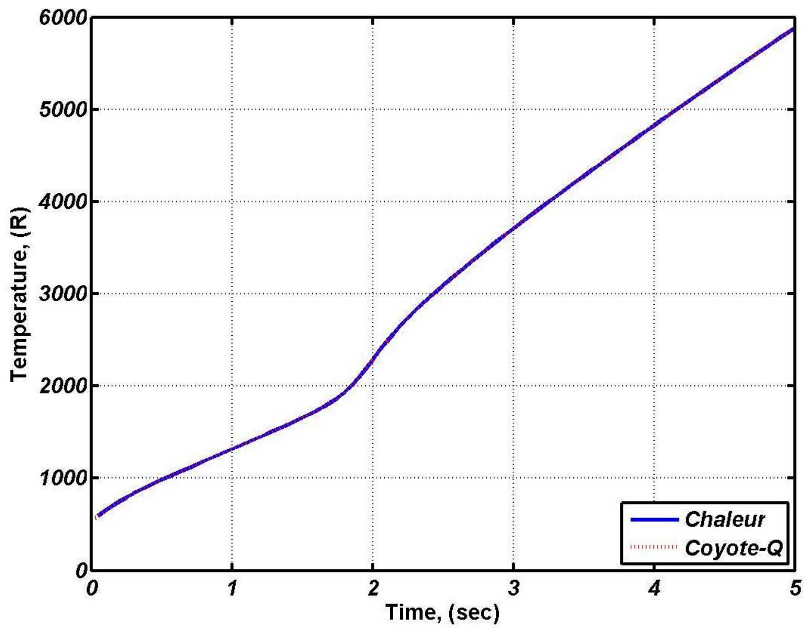
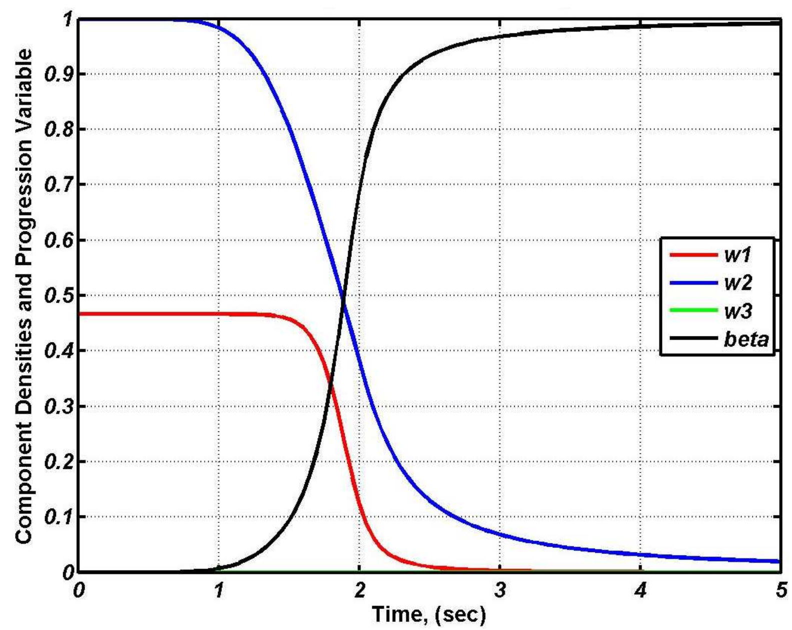
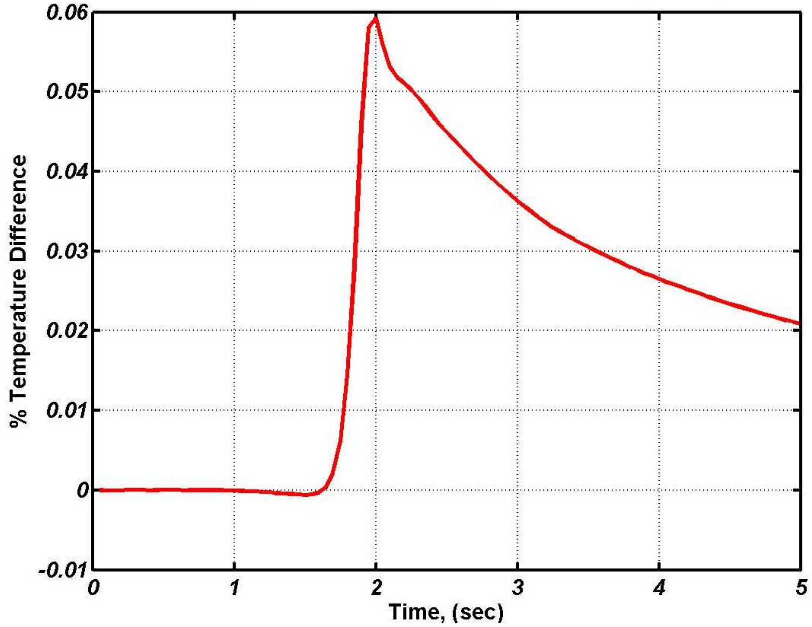


Temperature

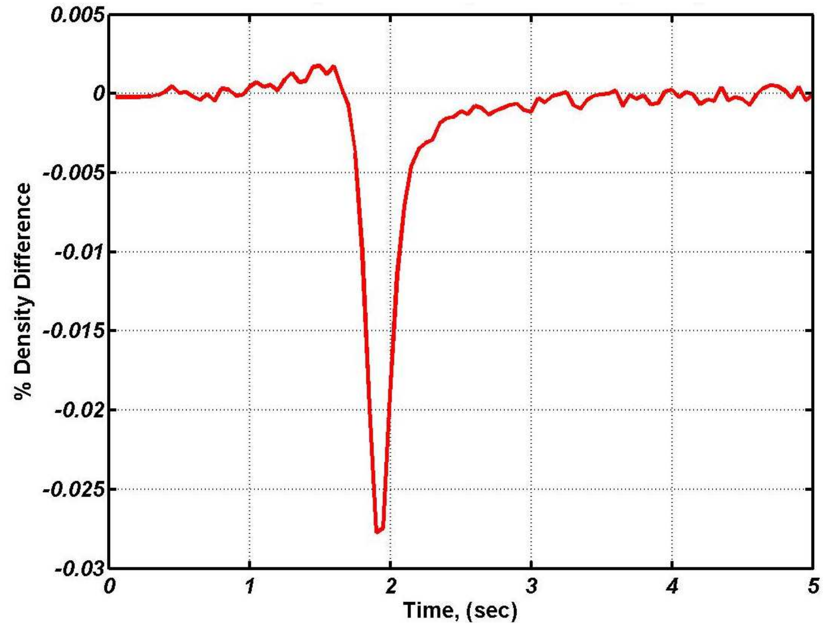


Species

Carbon Phenolic Decomposition
Code Comparison

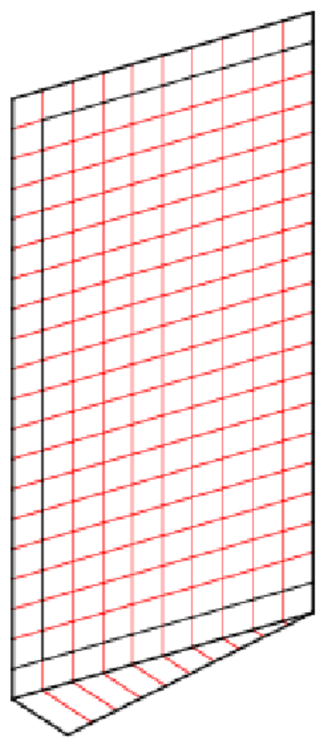


Temperature



Density

Test for Ablation, Decomposition & Gas Flow



- Carbon Phenolic Decomposition
- Aero Heating at Surface
- Q^* Ablation Boundary Condition
- 3D Wedge Geometry
- 4 Species, 2 Reactions
- W_1= Resin A, W_2=Resin B
- W_3=Binder, β=Extent of Reaction
- T_{init}: $536K$ for Carbon Phenolic
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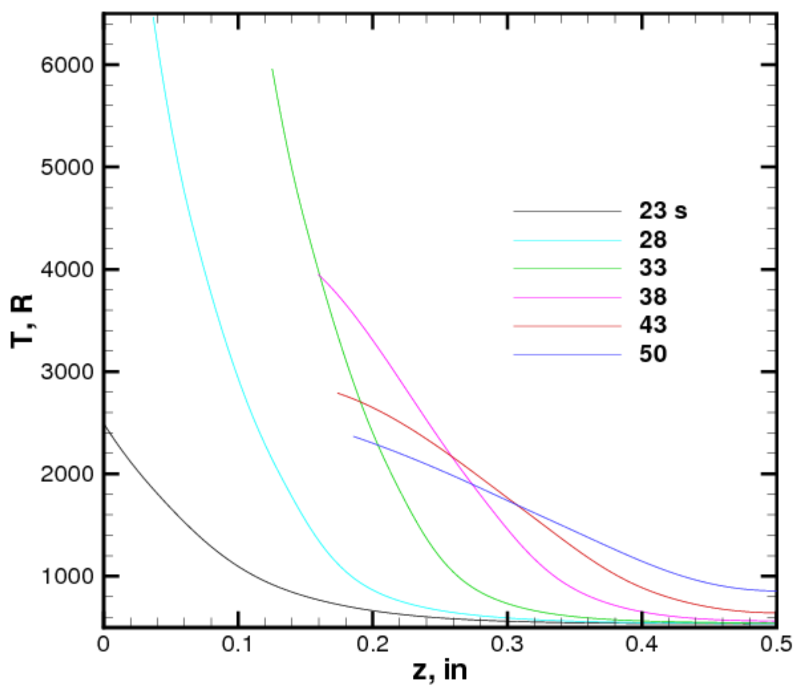
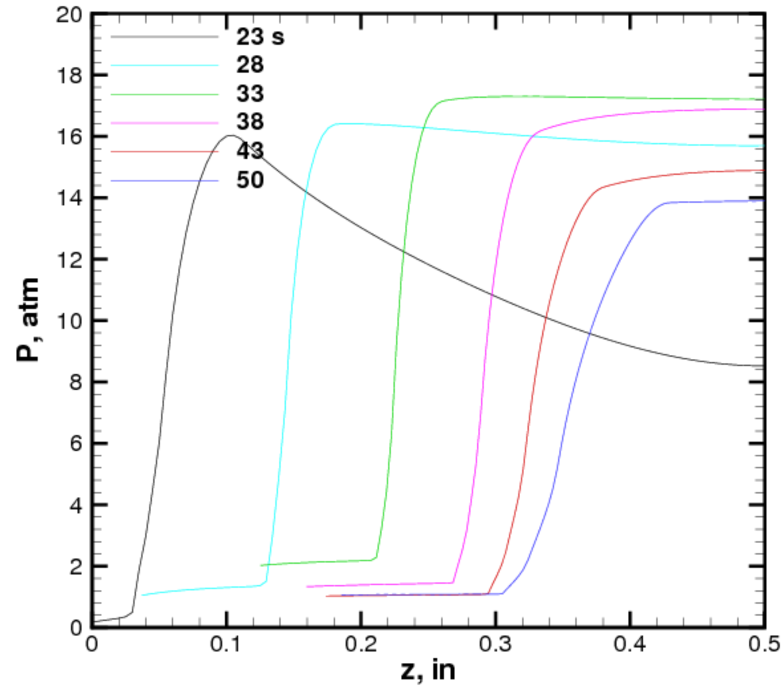
Carbon Phenolic Decomposition
Chaleur Code Results (1)

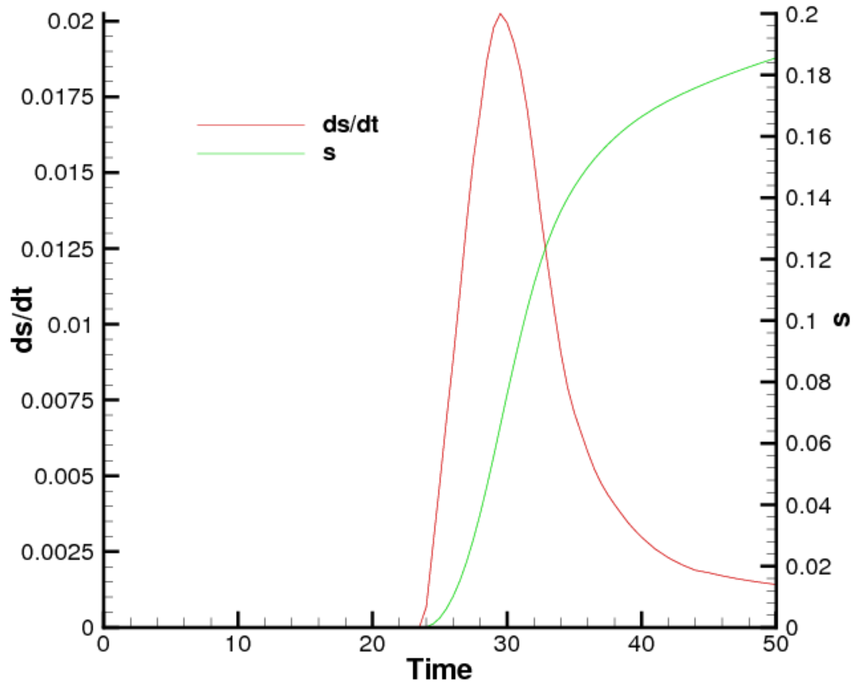


Temperature

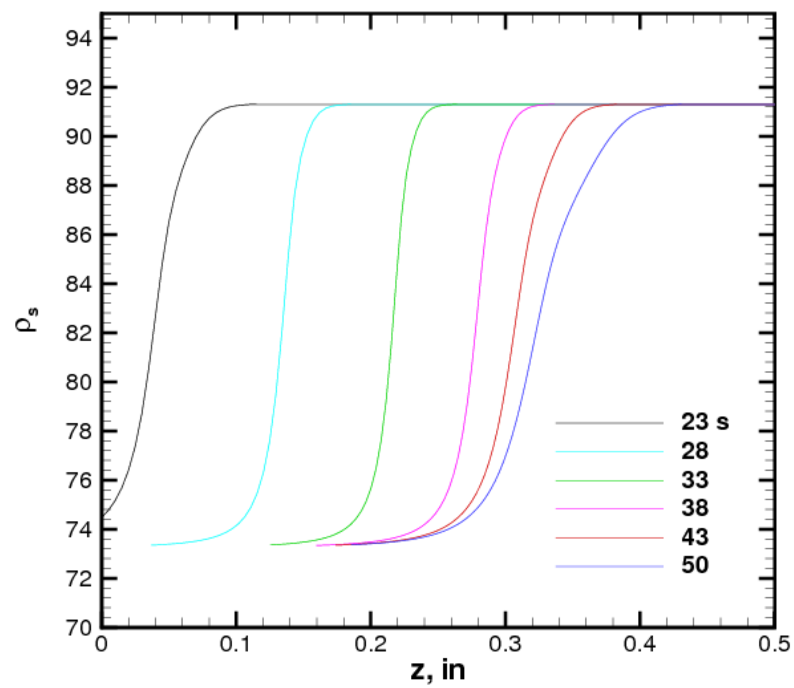


Pressure

Carbon Phenolic Decomposition
Chaleur Code Results (2)



Recession & Rate



Gas Generation

Concluding Remarks

- Formulated an initial/boundary value problem for multidimensional ablation including in-depth decomposition
- Developed standard FEM for coupled equations describing ablation
- Demonstrated viable method for standard (CMA) decomposition chemical kinetics

- Continue testing for gas generation and porous flow
- Continue implementation of mesh motion and remeshing
- Evaluate proposed methods for foam decomposition problems