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Phenomena and Material Property Requirements for a Combined Structural and Thermal Ablation Model

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Logan, Utah

Overview

Applications

Phenomena

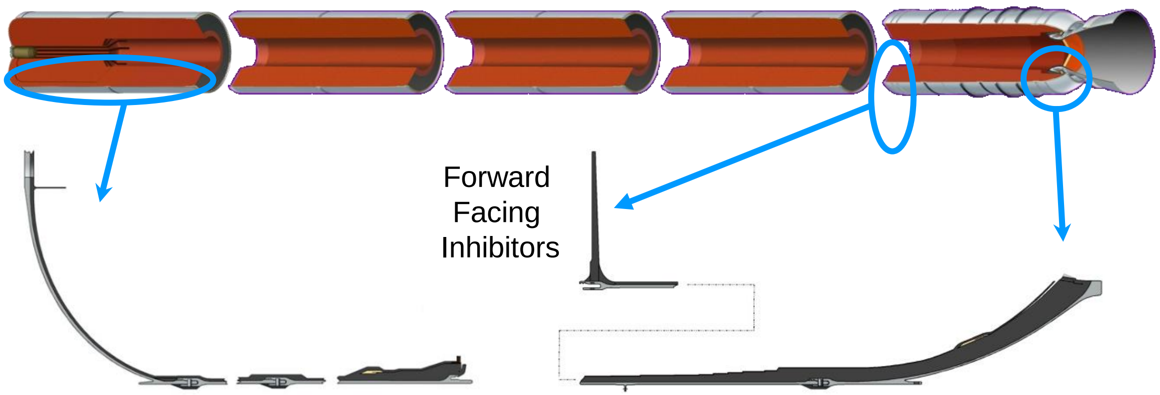
Mathematical models

ATK code development (ITRAC and Hero)

Thermal property requirements

Structural considerations

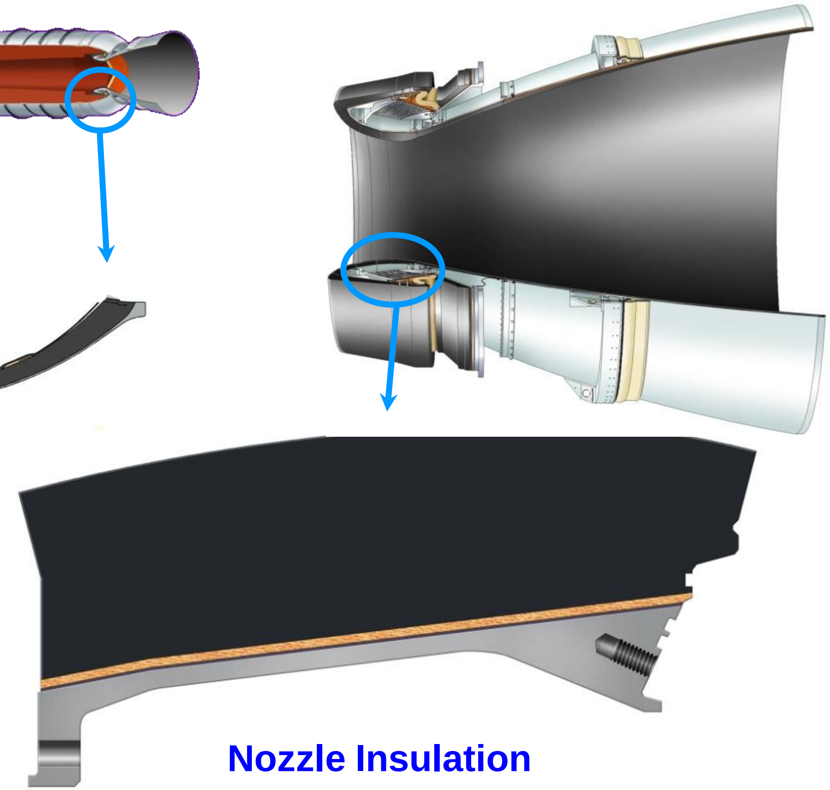
On-going work



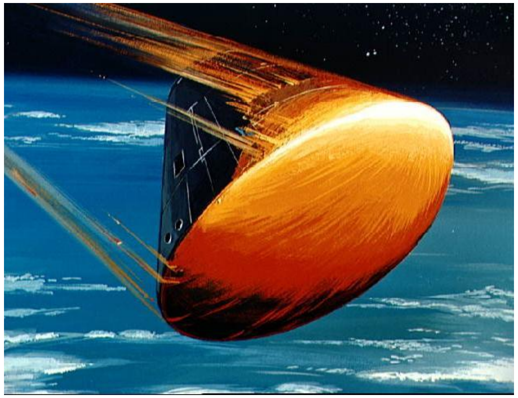
Segment Insulation

Aft Segment Insulation

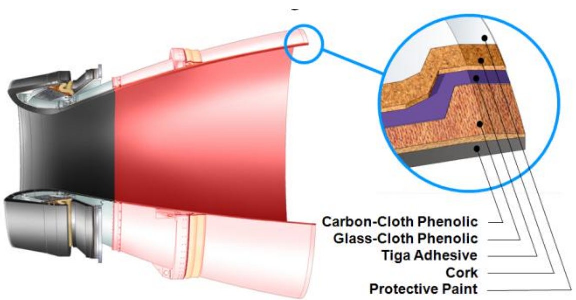
Internal Insulation



Nozzle Insulation



Re-entry Thermal Protection Systems



External Insulation

Phenomena

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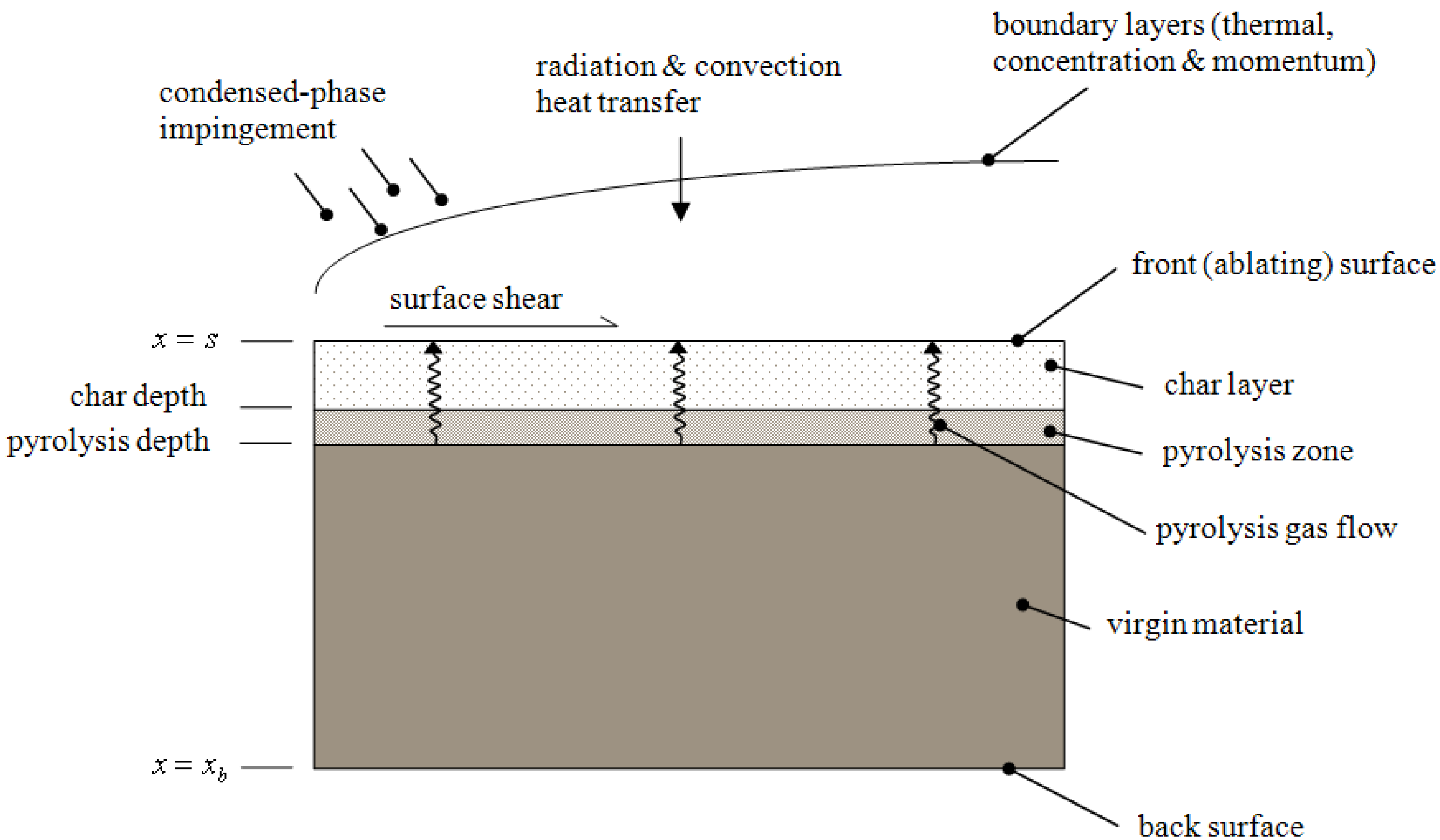
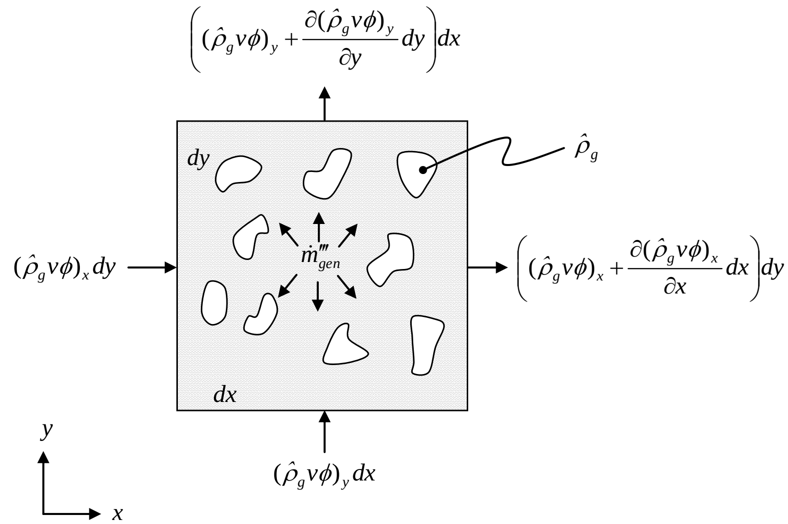
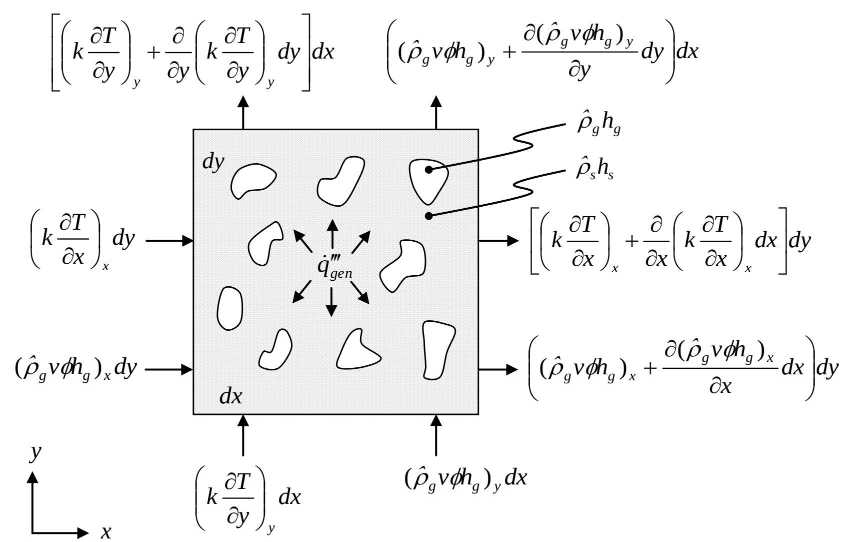


- **Mass balance (gas phase)**
  - Solid to gas conversion (pyrolysis)
  - Gas advection (permeation)
  - Storage (in the internal pores)
- **Momentum balance**
  - Balances friction with pressure gradient (Darcy's model)
- **Energy balance**
  - Conduction (in solid phase)
  - Storage (in solid and gas phases)
  - Pyrolysis energy
  - Advected energy (heat exchange with pyrolysis gases)



Control-volume for mass balance



Control-volume for energy balance

In-Depth Modeling

- **Pyrolysis**

$$\frac{\partial \rho_s}{\partial t} = -(\rho_v - \rho_c)\frac{\partial \alpha}{\partial t}$$

rate of solid density change

$$\alpha = \frac{\sum_i x_i \alpha_i}{\sum_i x_i}$$

overall versus component extent-of-reaction

$$\frac{\partial \alpha}{\partial t} = \frac{\sum_i x_i \frac{\partial \alpha_i}{\partial t}}{\sum_i x_i}$$

overall pyrolysis rate

$$\frac{d\alpha_i}{dt} = A_i e^{\left(-\frac{E_{a,i}}{RT}\right)}(1-\alpha_i)^{m_i}$$

Arrhenius model for component extent-of-reaction

- **Mass/Momentum Equation**

$$(\rho_v - \rho_c)\frac{\partial \alpha}{\partial t} + \nabla \cdot \left(\frac{\hat{\rho}_g}{\mu_g}\mathbf{\Gamma}\nabla P\right) - \hat{\rho}_g(\phi_c - \phi_v)\frac{\partial \alpha}{\partial t} - \frac{\phi \hat{\rho}_g}{k_g}\frac{\partial P}{\partial t} + \phi \beta_g \hat{\rho}_g \frac{\partial T}{\partial t} = 0$$

generation — advection (permeation) — storage

  - Neglected storage (quasi-steady)

$$(\rho_v - \rho_c)\frac{\partial \alpha}{\partial t} + \nabla \cdot \left(\frac{\hat{\rho}_g}{\mu_g}\mathbf{\Gamma}\nabla P\right) = 0$$

generation — advection (permeation)

  - 1-D simplification (with neglected storage)

$$\dot{m}''_g(x_p) = -\frac{1}{A}\int_{x_p}^{x_b} A \frac{\partial \rho_s}{\partial t} dx$$

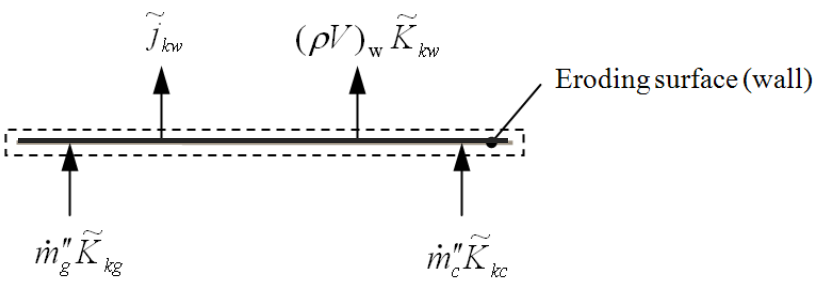
Solution of M/M equation primarily needed for solution of energy equation. Analyst can choose level of fidelity.

- **Energy Equation**

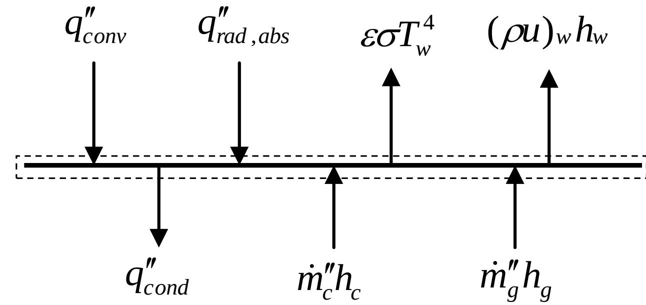
$$(Q_s - h_s + h_g)(\rho_v - \rho_c)\frac{\partial \alpha}{\partial t} + \hat{\rho}_g \phi \frac{\partial h_g}{\partial t} + \rho_s \frac{\partial h_s}{\partial t} + \hat{\rho}_g \mathbf{v}_D \cdot \nabla h_g - \nabla \cdot \mathbf{K}\nabla T = 0$$

pyrolysis energy — storage — advection — conduction

Surface Modeling



Control-surface for elemental balance



Control-surface for energy balance

- **Unity Lewis number**

$$q''_{cond} = \rho_e u_e C_H [H_r - (1+B')h_w + B'_c h_c + B'_g h_g] + \alpha_w q''_{rad,inc} - \varepsilon\sigma T_w^4$$

- **Unequal diffusion coefficients**

$$q''_{cond} = \rho_e u_e C_H (H_r - h_w)_{f.e.g} + \rho_e u_e C_M \left[\left(\sum_i K_{ie} - \sum_i K_{iw} \right) h_i^{T_w} + B'_c h_c + B'_g h_g - B' h_w \right] + \alpha_w q''_{rad,inc} - \varepsilon\sigma T_w^4$$

- **Equal diffusion coefficients**

$$q''_{cond} = \rho_e u_e C_H (H_r - h_w)_{f.e.g} + \rho_e u_e C_M \left[\left(\sum_i Z^*_{ie} - \sum_i Z^*_{iw} \right) h_i^{T_w} + B'_c h_c + B'_g h_g - B' h_w \right] + \alpha_w q''_{rad,inc} - \varepsilon\sigma T_w^4$$

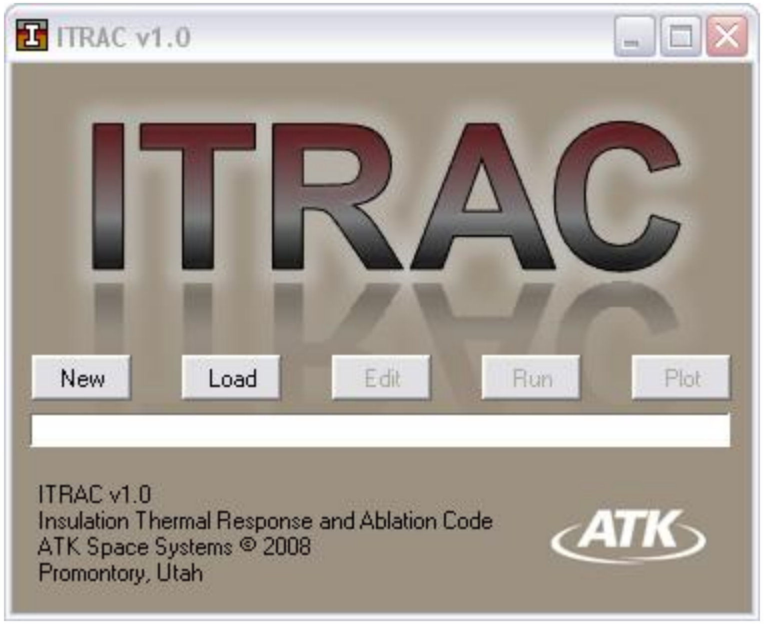
- **Surface ablation rate**

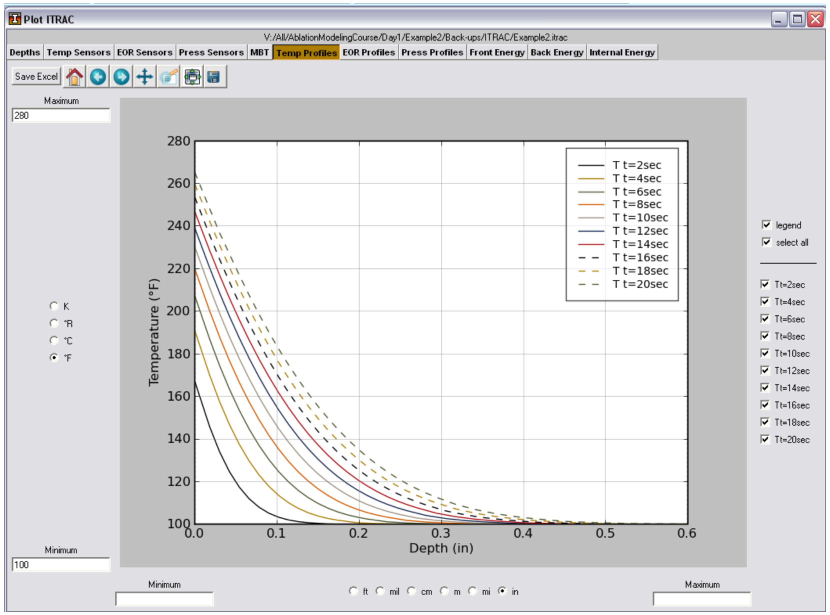
$$\dot{s}_{chem} = \frac{\dot{m}''_c}{\rho_c} = \frac{B'_c \rho_e u_e C_M}{\rho_c}$$

Thermochemistry ("b-prime") tables from ACE code

ITRAC

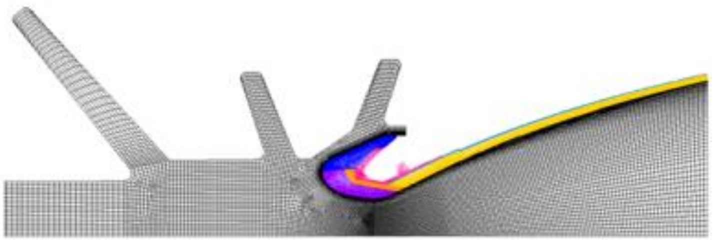
- 1-D (planar, cylindrical, and spherical)
- Variable-grid finite-volume method
- Heat transfer, material pyrolysis, pore pressure, thermochemical ablation
- Various mechanical erosion models
- User-defined dynamic link libraries (DLLs)
- Ignition model

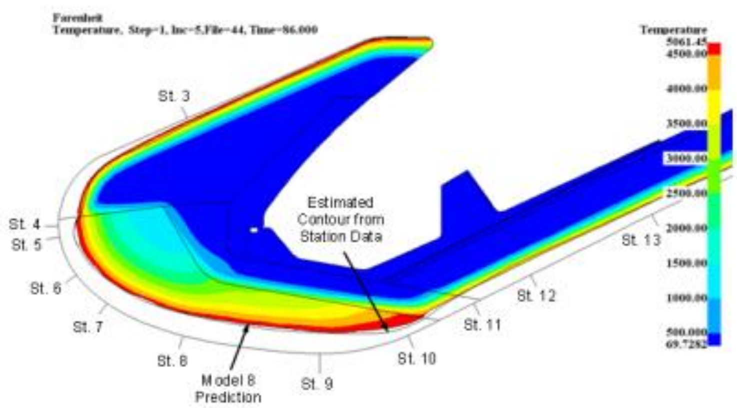




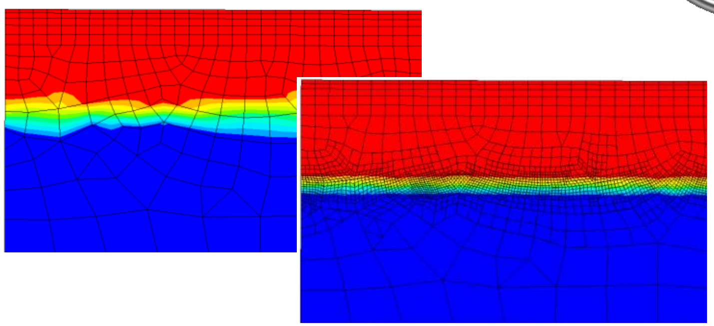
Hero (Heat Transfer and Erosion Analysis Program) ATK

- Multi-D
- Variable-grid finite-element (hierarchical) method
- Heat transfer, material pyrolysis, pore pressure, thermochemical ablation, radiosity, structural
- Fluid-thermal-structural interaction (FTSI) capabilities (FEM Builder)
- Adaptive refinement
- Parallel processing

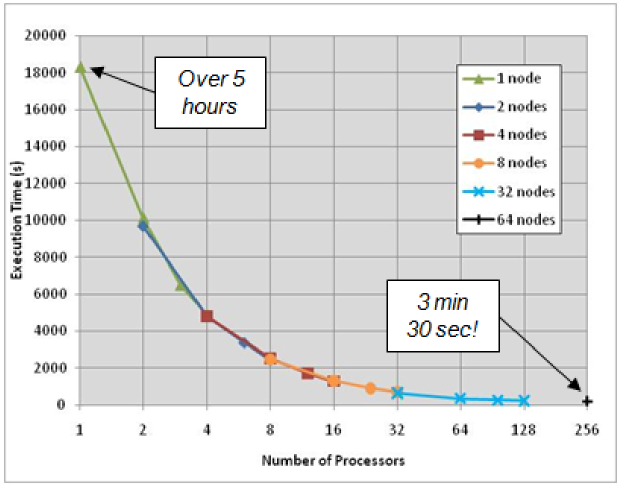




FTI Nozzle Analysis



Hero Adaptive Refinement



Run-Time Improvement with Parallel Processing

Hero (Heat Transfer and Erosion Analysis Program)

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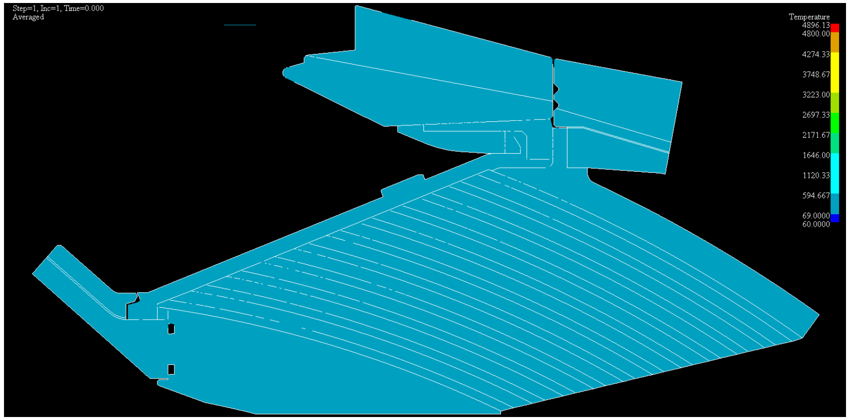
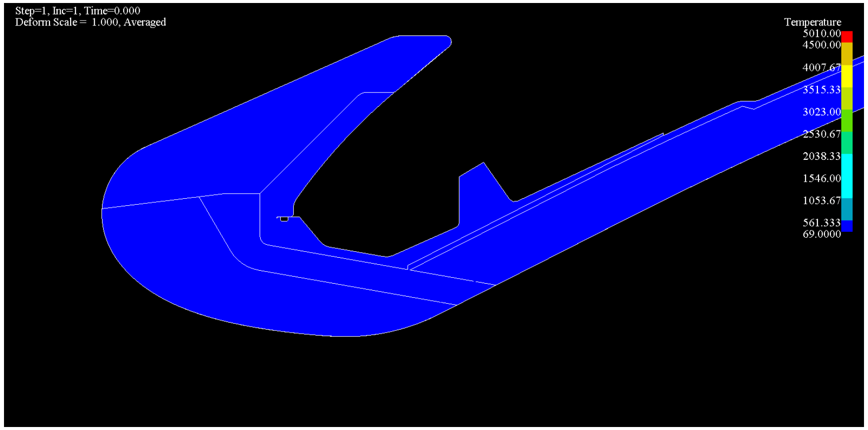
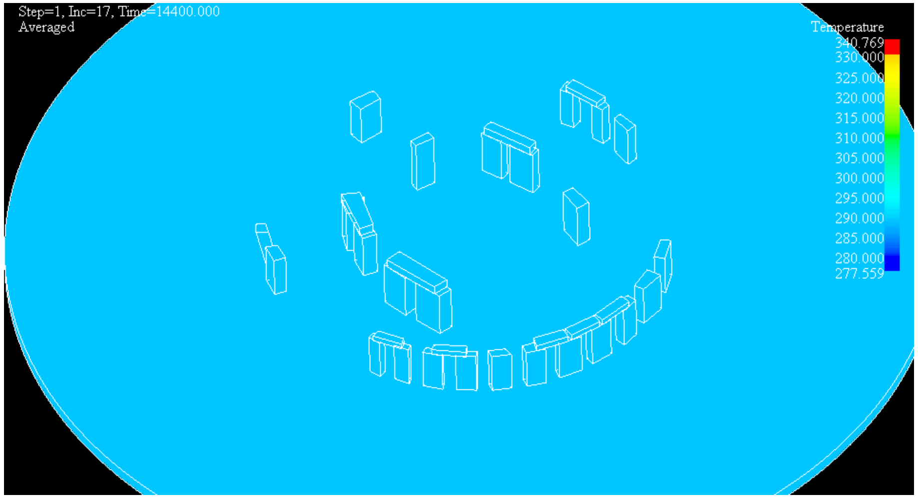


Modeling of Complex Ablation Scenario



Nozzle Thermal Analysis Results



Radiosity with Solar Effects

- **Pyrolysis Properties**

$$\frac{\partial \rho_s}{\partial t} = -(\rho_v - \rho_c)\frac{\partial \alpha}{\partial t}$$

rate of solid density change

$$\alpha = \frac{\sum_i x_i \alpha_i}{\sum_i x_i}$$

overall versus component extent-of-reaction

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overall pyrolysis rate

$$\frac{d\alpha_i}{dt} = A_i e^{\left(-\frac{E_{a,i}}{RT}\right)} (1-\alpha_i)^{m_i}$$

Arrhenius model for component extent-of-reaction

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generation **advection (permeation)** **storage**

  – Neglected storage (quasi-steady)

$$(\rho_v - \rho_c)\frac{\partial \alpha}{\partial t} + \nabla \cdot \left(\frac{\hat{\rho}_g}{\mu_g} \mathbf{\Gamma} \nabla P \right) = 0$$

generation **advection (permeation)**

  – 1-D simplification (with neglected storage)

$$\dot{m}_g''(x_p) = -\frac{1}{A}\int_{x_p}^{x_b} A \frac{\partial \rho_s}{\partial t} dx$$

- **Energy Equation**

$$(Q_s - h_s + h_g)(\rho_v - \rho_c)\frac{\partial \alpha}{\partial t} + \hat{\rho}_g \phi \frac{\partial h_g}{\partial t} + \rho_s \frac{\partial h_s}{\partial t} + \hat{\rho}_g \mathbf{v}_D \cdot \nabla h_g - \nabla \cdot \mathbf{K} \nabla T = 0$$

pyrolysis energy **storage** **advection** **conduction**

Insulator Properties

- Pyrolysis kinetics parameters
  x_i, E_i, A_i, m_i
- Virgin and char densities
  ρ_v, ρ_c
  $\rho_s = \rho_v(1-\alpha) + \rho_c \alpha$
- Virgin and char specific heat
  $c_{p,v}, c_{p,c}$
  $h_v = \int_{T_{ref}}^{T} c_{p,v}\, dt \quad h_c = \int_{T_{ref}}^{T} c_{p,c}\, dt$
  $h_s = h_v(1-\alpha) + h_c \alpha$
- Virgin and char conductivity
  k_v, k_c
  $k_s = k_v(1-\alpha) + k_c \alpha$
- Elemental compositions (v & c)
  $K_{k,v}, K_{k,c} \xrightarrow{\text{equilibrium analysis}} h_g, MW_g$
- Heats of formation
  $h_{f,v}^o, h_{f,c}^o \rightarrow Q_s$

Input for Surface Modeling

$$q''_{cond} = \rho_e u_e C_H \left[(H_r - h_w)_{f.e.g.} + \frac{C_M}{C_H} \sum_i (K_{i,e} - K_{i,w}) h_i^{T_w} + B'_g h_g + B'_c h_c - B' h_w \right] + \alpha q''_{rad,inc} - \varepsilon \sigma T_w^4$$

Boundary Conditions

- Transport coefficient
- Enthalpy (recovery and frozen)
- Incident radiation heat flux

Propellant Properties

- Stanton number ratio
- Elemental composition

Surface Product Properties

- Elemental composition
- Enthalpy of products

Insulator Properties

- Char enthalpy (specific heat) and pyrolysis gas enthalpy
- Radiation properties (emissivity and absorptivity)

Property Summary

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Pyrolysis kinetic parameters

Density

- Virgin and char

Specific heat

- Virgin and char
- Versus temperature

Thermal conductivity

- Virgin and char
- Versus temperature

Elemental compositions

- Virgin and char
- Pyrolysis gas calculated

Heats-of-formation

- Virgin and char
- Pyrolysis gas value calculated
- Used to calculate heat-of-pyrolysis
- Used in surface thermochemistry

Radiation properties

- Emissivity and absorptivity

For pore pressure

- Porosity
- Permeability
- Pyrolysis gas molecular weight
- Pyrolysis gas viscosity

Structural Modeling

Structural modeling is often required for accurate assessment of structural integrity (including phenomena such as pocketing, ply-lifting, wedge-outs, and delamination)

- Phenomena can have significant impact on thermal protection
- Integrally tied to thermal responses
- Accurate modeling of heat transfer, material pyrolysis, pore pressure, thermochemical ablation, etc. is critical

Structural – High Temperature Issues

Pocketing involves the expulsion of carbon-cloth phenolic (CCP) material due to a combination of stresses from thermal expansion and pore pressure driven stresses

- Can significantly affect thermal protection

Structural – High Temperature Issues

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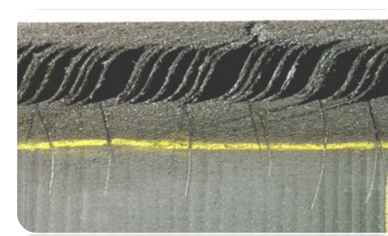
Ply lifting involves the lifting of a char cap of CCP material. Initial failure is caused by thermal expansion/contraction, lifting is caused by pore pressures



Structural – High Temperature Issues

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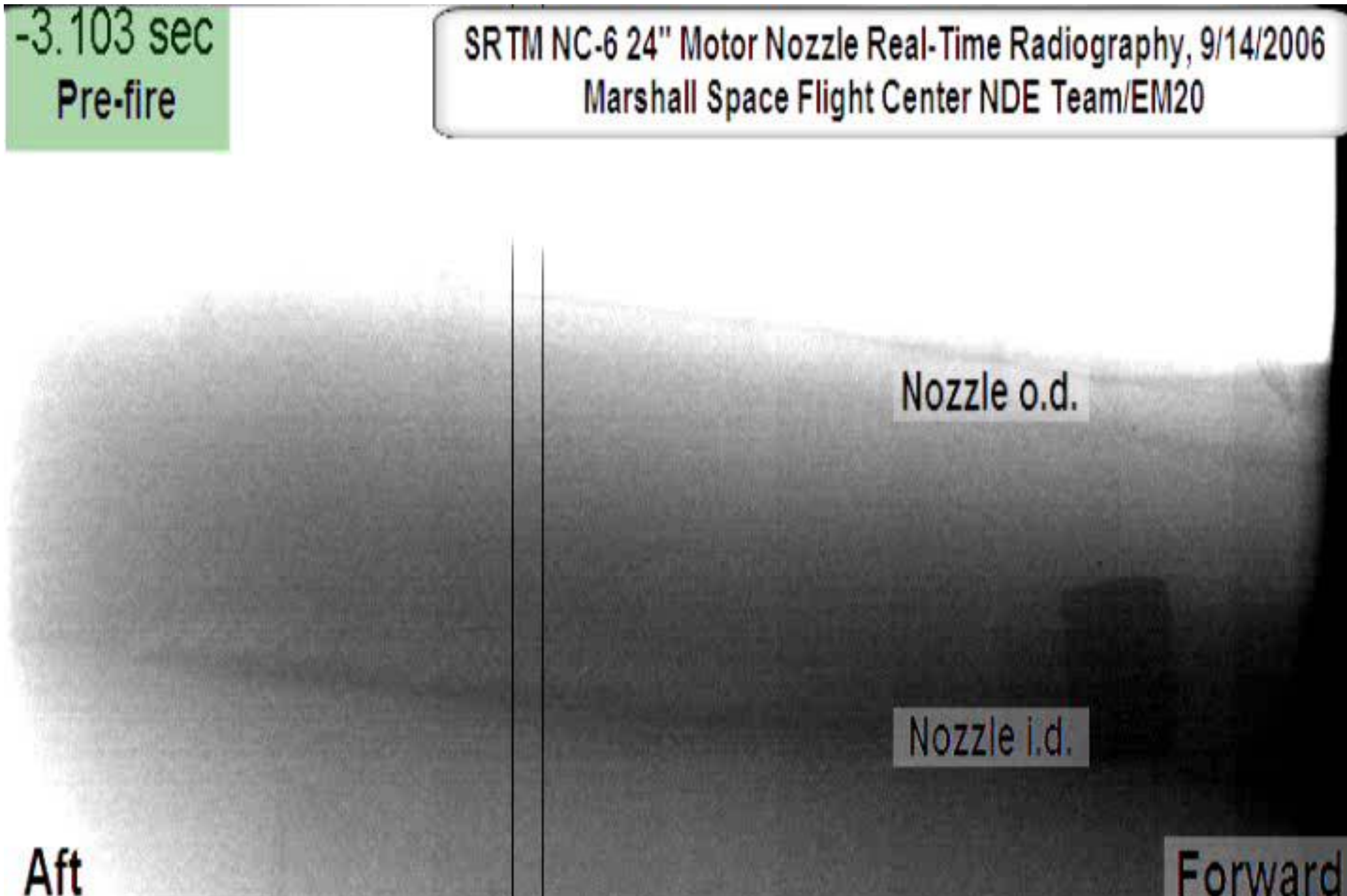
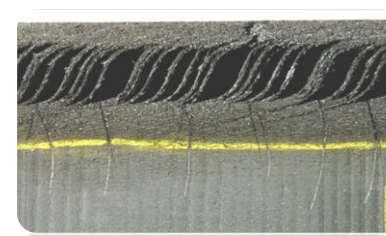
Ply lifting char caps can slough, causing loss of thermal protection

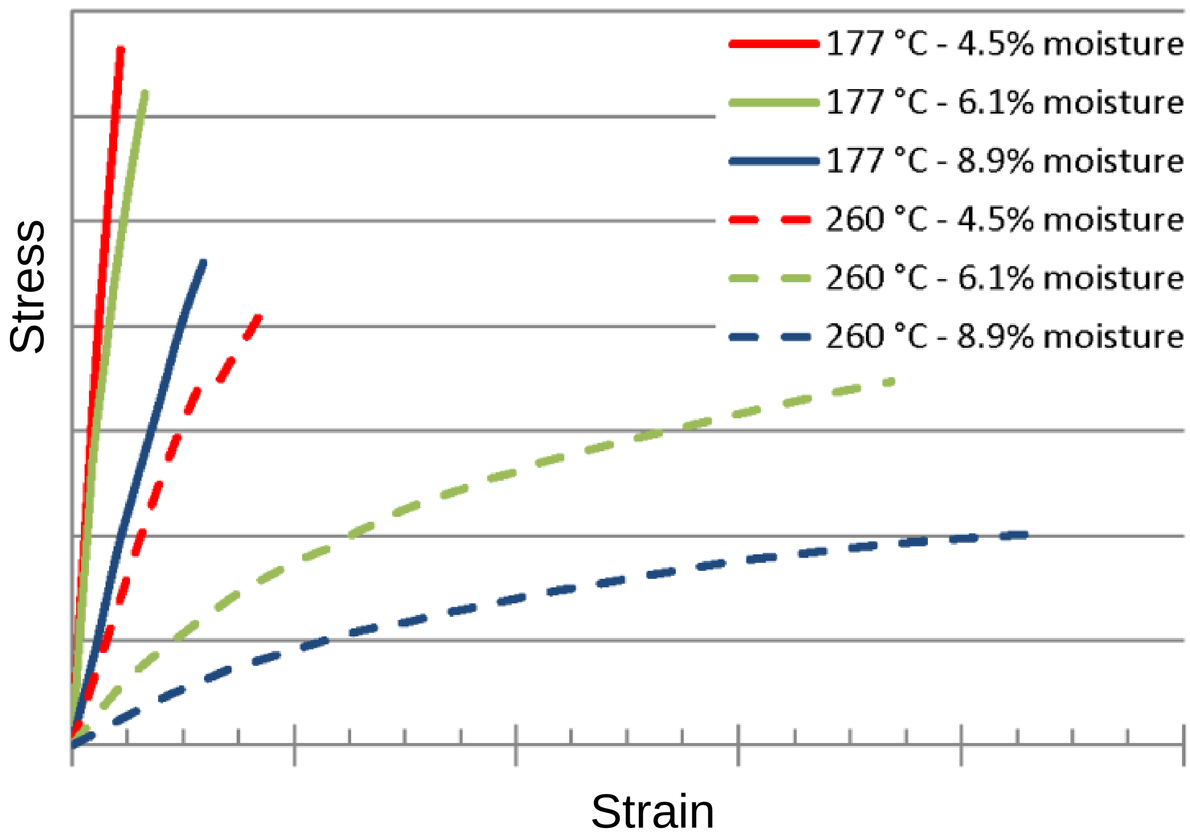




Structural Dependent on Thermal

Structural modeling is dependent on thermal modeling, for example:

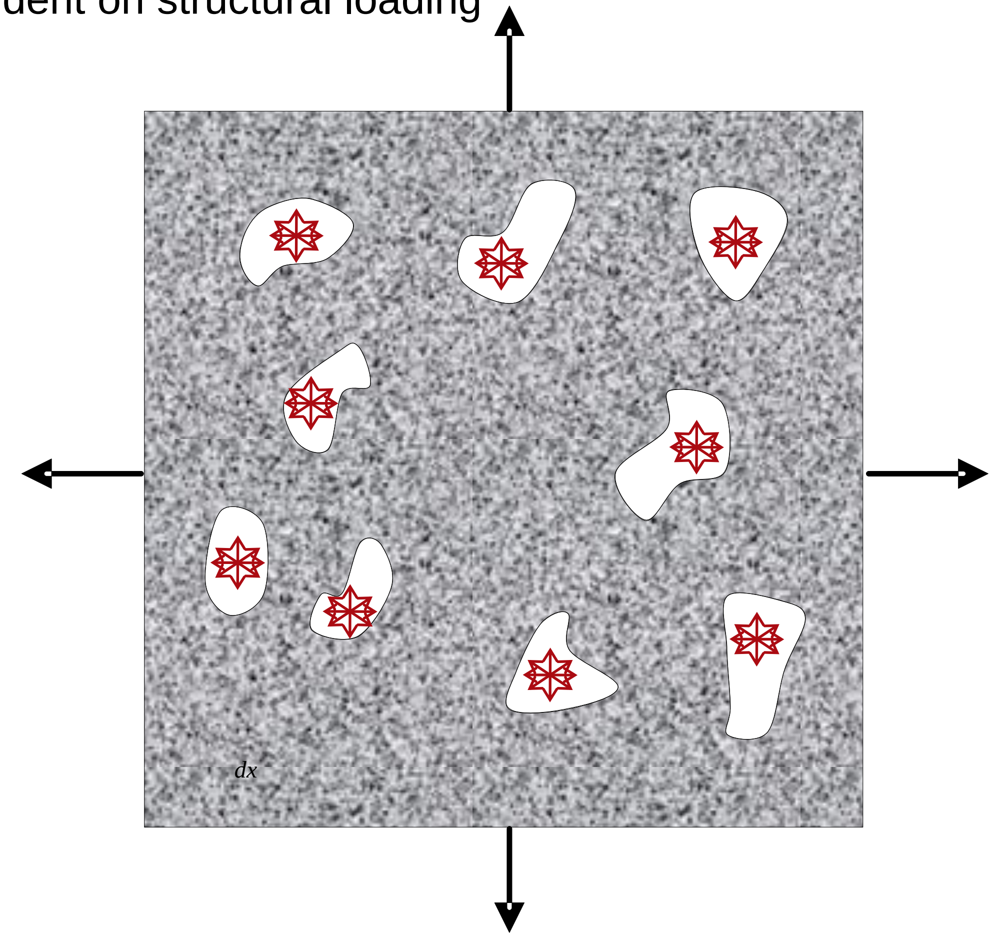
- Stiffness can be dependent on degree-of-char and presence of moisture
  - Charring causes material changes that affect the magnitude of the modulus
  - Moisture causes a plasticization of the matrix material



Structural Dependent on Thermal

Structural modeling is dependent on thermal modeling, for example:

- Structural behavior is also influenced by pressures
- Pressure magnitudes are highly dependent on structural loading
  - Permeability is affected by load
  - Pressure is affected by permeability



Property Summary

The following is a simple first principles equation that may be used for the structural model (complexity is usually added to address nonlinearities)

$$\underbrace{\varepsilon_{ij} = S_{ijkl}\sigma_{kl}^{m}}_{\text{stress loading}} + \underbrace{\eta_{ij}\Delta P}_{\text{pore pressures}} + \underbrace{\alpha_{ij}\Delta T}_{\text{thermal expansion}} + \underbrace{\beta_{ij}\Delta M}_{\text{moisture swelling}} + \underbrace{\chi_{ij}\Delta v_c}_{\text{decomposition}}$$

Material properties summary (dependent on thermal state)

- Stiffness matrix (includes moduli and Poisson's ratios) S_{ijkl}
- Pressure stress coupling, η_{ij}
- Coefficient of thermal expansion, α_{ij}
- Moisture expansion coefficient, β_{ij}
- Decomposition coefficient, χ_{ij}
- Failure criteria

Conjugate models are required for accurate simulation of thermal and structural behavior

On-going Work

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Thermal

- 3-D surface ablation in Hero
- General thermal contact in Hero
- Advanced surface thermochemistry code (ACE replacement)
  - Alumina impingement
  - Chemical kinetics
- Material properties
- Comprehensive validations against historical nozzle data

Flow modeling

Advanced carbon-cloth phenolic CCP modeling

- Moisture
- Structural coupling

Related References

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