Modeling of the fiber-scale oxidation of highly-porous carbon fiber materials based on synchrotron X-Ray Microtomography

Applied Modeling & Simulation (AMS) Seminar Series

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Thermal Protection Systems

Ceramic Tiles
- Used on the Space Shuttle
- Reusable
- Reentry from LEO

Ablative Heat Shields
- AVCOAT Ablative TPS used on the Apollo capsule
- Single use TPS
- High velocity reentry
Ablative TPS and PICA

- Light weight Carbon / Phenolic Ablator
- Successfully flight tested
- SpaceX development of PICA - X

FiberForm® + Resin = PICA

[Stackpoole et al., AIAA 2008-1202]
PICA Flight Tests

Mars Science Laboratory (Curiosity Rover)  Stardust Capsule  SpaceX Dragon V1, V2
PICA Modeling

- Highly Porous Material
- Ablation can occur at a range of depths
- Models treat PICA as a solid material using a volume-averaged approach
Objectives

- Handle Very Large Data sets of Microtomography
- Framework needed to analyze material properties and run simulations
- Desired Functionality:
  - Material Properties
  - Thermal phenomena
  - Mechanical phenomena
  - Transport phenomena
Synchrotron Microtomography

http://www2.lbl.gov/MicroWorlds/ALSTool/
8.3.2 Beamline

- Hard X-ray microtomography
- 14 KeV X-rays
- Processed through scintillator, magnification lens, and a camera

http://microct.lbl.gov/manual
Projection processing

- Fiji plugin reconstruction algorithm.
- Converts 2048 projections into a 3D image stack.
Grayscale Cutoff

Histogram of grayscale frequencies
Original Slice
Slice with threshold applied
Porous Media Analysis (PuMA)

Domain Generation
- Tomography Import
- Artificial Generator

Image Processing
- Subdomain Extraction and Filtering
- Histogram & Cutoff
- Marching Cubes

Material Properties
- Porosity
- Surface Area

Simulations
- Oxidation Simulation
- Heat Transfer (Under development)

3D Visualization
Image Import
Artificial Geometry Generator

PuMA

Porous Media Analysis
Histogram and Cutoff

Grayscale Value Frequency

- Percent of pixels
  - 0.012 to 0.018
  - 0.024 to 0.03
  - 0.036

- GrayScale value (0=black 255=white)
  - 0 to 40
  - 40 to 80
  - 80 to 120
  - 120 to 160
  - 160 to 200
  - 200 to 240

- Selected Grayscale Value
  - 90

- Lowest Grayscale
  - 0

- Highest Grayscale
  - 255

- Average Grayscale
  - 22

- Highest Frequency
  - 60 with 0.0378133

PuMA
Porous Media Analysis
Marching Cubes Algorithm

- Represent the surface as a collection of triangles.
- Used in visualization and for calculation of specific surface area
- Used in the oxidation model to track the surface of the material
Marching Cubes Algorithm

- Marching Cubes Steps:
  - Define Space in X, Y, Z into voxels
  - Assign value to each voxel vertex
  - Compare each voxel to edge table to determine which edge case applies
  - Linearly interpolate triangle vertex positions
  - Use cross product to calculate normal vector
PuMA Visualization

- Based upon an OpenGL framework written by Tim Sandstrom
- Uses triangle normals to create an appropriate texture
- Capable of showing tomography images in good detail
- Can generate movies of material as well as movies of simulations progressing over time intervals
Material Properties

- Specific Surface Area
  - Requires Marching Cubes
  - Calculated as a sum of individual triangle areas
- Porosity
  - Function of grayscale threshold
Oxidation

- How the material decomposes at the fiber scale
- Simulate this oxidation based upon the microtomography images.
Oxidation Model

Lachaud et al., CMS, 44 (2009]

Model Aspects:
- Material Storage
- Oxygen Storage
- Walker Movement
- Collision Handling
- Verification
- Application to Fiberform
Material Storage

(a) 232 184 94 78 65
    233 198 98 83 70
    237 215 132 92 85
    247 229 166 98 90
    242 205 147 95 89

(b) 255 184 94 0 0
    255 198 98 83 0
    255 215 132 92 0
    255 255 166 98 0
    255 255 147 95 0
Oxygen Storage

\[ N_{walkers} = \frac{y_{O_2} \rho_g V}{n_w M_{O_2}} \]

\( y_{O_2} \): mass fraction of \( O_2 \)
\( V \): volume of the buffer zone
\( n_w \): user-defined number of moles per walker
\( M_{O_2} \): molar mass of oxygen
\( \rho_g \): density of the gas mixture
Walker Movement

Movement of Walker through voxel containing material

\[ \Delta t = \frac{\Delta r^2}{6D} \]

\[ \Gamma' = a + bx' + cy' + dx'y' \]

\[ a = \Gamma_1, \quad b = \Gamma_2 - \Gamma_1, \quad c = \Gamma_4 - \Gamma_1, \quad d = \Gamma_1 - \Gamma_2 + \Gamma_3 - \Gamma_4. \]

\[ (x, y, z) = (x', y', z') + \frac{\Gamma^* - \Gamma'}{\Gamma'' - \Gamma'} [(x'', y'', z'') - (x', y', z')] \]

\[ \Delta t = \text{time increment} \]
\[ \Delta R = \text{random walk length} \]
\[ D = \text{diffusion coefficient} \]
\[ \Gamma_1 \ldots \Gamma_8 = \text{vertex grayscale values} \]
\[ \Gamma' = \text{grayscale at entrance} \]
\[ \Gamma'' = \text{grayscale at exit} \]
\[ \Gamma^* = \text{grayscale threshold} \]
\[
\tilde{P}_s = \frac{1}{1 + \frac{3\gamma D}{2k\Delta r_w}} \quad \alpha = \frac{M_s n_w}{\rho_s \tilde{V}} 256
\]

\( P_s \) = sticking probability

\( D \) = diffusion coefficient

\( \gamma \) = sticking coefficient

\( \Delta r_w \) = walk length before collision

\( k \) = reactivity of material (fiber or matrix)

\( \alpha \) = grayscale attenuation

\( M_S \) = molar mass of solid

\( \rho_s \) = density of solid

\( \tilde{V} \) = voxel volume

\( n_w \) = mols of oxygen per walker
Verification

Exact solution Developed by Lachaud and Vingoles:

\[ A = \frac{k_m \Omega_m}{k_f \Omega_f} \quad Sh = \frac{k_m R_f}{D} \]

- \( A \) = reactivity contrast
- \( k_m \) = reactivity matrix
- \( k_f \) = reactivity fiber
- \( \Omega_m \) = volume fraction matrix
- \( \Omega_f \) = volume fraction fiber
- \( Sh \) = sherwood number
- \( R_f \) = radius of fiber
Diffusion Limited

A = 50  Sh = 5

A = 10  Sh = 10
Reaction Limited

A = 10  Sh = 0.1

A = 2  Sh = 0.2
Oxidation applied to Fiberform

- Volume Ablation
  - High diffusion vs. reaction
- Surface Ablation
  - High reaction vs. diffusion
- Mixed Regime
Summary and Outlook

- Obtained microtomography images to use for material properties and simulations
- Developed framework to import and process images
- Calculation of basic material properties
- Completion of Oxidation simulation

Next Steps:
- Add artificially generation phenolic matrix for oxidation
- Parallelization of Oxidation Model
- Calculation of more material properties (tortuosity, mean pore diameter, etc)
- Module for thermal conductivity
Contributors

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