Microscale Modeling of Ablative Thermal Protection System Materials

Eric Stern, Graham Candler, Tom Schwartzentruber, Ioannis Nompelis, Michael Barnhardt
• Engineering material response codes in use today take a macroscopic view of the TPS.
• Typically involve heavy empiricism, and many assumptions
The goal of this work is to better model processes at the micro-scale to inform macro-scale models.

- Volume averaging.
- Model reduction!

This will attempt to build and expand on previous efforts in micro-scale modeling by enabling more physics
TPS Modeling

The goal of this work is to better model processes at the micro-scale to inform macro-scale models.

...as well as build a framework where higher fidelity models can be incorporated from the nanoscale.


Lachaud, et al., JSR, 2010
Outline

• Methodology
  – DSMC
  – Surface Generation and Movement
  – Coupled Ablation

• Preliminary Validation and Applications
  – Simplified Darcy Flow
  – Flow-tube Permeability Experiments

• Future Work
Why DSMC?

• First: what is DSMC?
• Knudsen numbers in the porous medium range from high-slip to rarefied regimes.
• DSMC can (in principle) simulate all of the relevant physics.
  – Convection
  – Multicomponent Diffusion
  – Gas-phase Kinetics
  – Sophisticated GSI Models
  – Non-equilibrium handled inherently
• DSMC can simulate arbitrarily complex geometries

Lachaud, et al., JSR, 2010
• Parallel implementation of the DSMC method developed at the University of Minnesota.
  – 3-Level Cartesian Mesh
  – Automated Mesh Refinement
  – Models for dissociation, vibrational/rotational relaxation.

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  – Initialization of simulation to CFD (using US3D).
  – Subsonic Boundary Conditions
  – Simple gas-surface interaction model
  – Ablation modules
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MGDS2

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• Future Work
The objective is to develop a tool that is able to generate triangulated surface meshes of random arrays of “fibers” to use in microscale simulations.

We have developed FiberGen with the following features:

- It can generate 2D and 3D, random and non-random arrays of cylindrical fibers.
- The user specifies a box size to fill with fibers, and a target porosity.
- The user can prescribe properties such as nominal fiber diameter, fiber length, angular biases (i.e. orthotropy), as well as variance and distribution in each.
- Triangulated surface is output in STL format.
- It also includes a post-processor for analyzing the geometry.
FiberGen

• Additionally, the code creates data structures for the mesh which are used for evolving the surface.

• Fiber data structures are written to HDF5 format for efficient I/O in massively parallel applications.

Example geometry having porosity of 0.85, and nominal fiber radius of 6 micron. The figure on the right is of the same geometry after having undergone a prescribed “ablation.”
Surface Data Structure

- The surface is composed of many fibers.
- Each fiber is composed of discrete elements along the axis.
- Each element contains many triangles on their surface.
Now we would like to leverage this framework do develop an efficient method for evolving the surface under the influence of surface reactions (ablation).

We begin by computing and storing the volume of each element for each fiber.

\[
\begin{array}{ccccc}
V1 & V2 & V3 & V4 & V5 \\
\end{array}
\]
Surface Movement

- We then update the *element* volumes as the simulation progresses, and reactions on the *triangles* remove material from the fibers.

- An effective radius that yields a straight cylinder of the same volume is computed for each *element*. 
Surface Movement

- The radius on each side of each element is then defined as the average between it and its neighbor.

- The surface is then reconstructed from conical frustum segments.
Surface Movement

– The surface is then reconstructed from conical frustum segments.

– Note: there is error in the volume of the reconstruction, however we always track and operate on the *actual* volume, so mass is conserved.
Surface Movement

This treatment is able to replicate some of the dominant morphologies we observe at the micro-scale.
- non-uniform thinning
- “needling”
Surface Movement

• This reconstruction method could be thought of as a Axisymmetric Volume of Fluid (VoF) approach.

• Benefits:
  – Relatively easy to implement
  – Error in volume is small and bounded for our work (<1%)
  – Extending code to modeling fiber material response would be (fairly) straightforward (i.e. solving the heat conduction equation is quasi-1D).
  – Surface reconstruction is very fast

• Limitations:
  – Limited to axisymmetric shapes
  – Not easily extensible to tomography-generated surfaces
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• Conclusions
Gas-Surface Interaction Modeling

- In DSMC, the gas surface interaction is modeled by determining the probability that a gas particle will react if it strikes a surface.
- For our current analysis, we use a temperature dependent probability for carbon oxidation given by Park.
- Devising more sophisticated treatments for the GSI is an active area of research.

\[ C(s) + O_2(a) \rightarrow CO(a) + O(a). \]

\[ \alpha = \frac{1.43 \times 10^{-3} + 0.01 \exp(-1450/T)}{1 + 2 \times 10^{-4} \exp(13,000/T)}. \]

*Park, Nonequilibrium Hypersonic Aerothermodynamics, 1991*
• We have found (so far) that the surface update is generally very fast, therefore we update fairly frequently since there is little to no penalty
Ablation of a single fiber

Ablation of a porous geometry
• Methodology
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• Future Work
Simple Darcy Flow

• To begin, we seek to validate the approach for simple Stoke’s flow through idealized porous medium.
  - We compare to both CFD, and models (analytical and empirical) in the literature
  - CFD augmented with Maxwell slip model
Simple Darcy Flow

- Results show good agreement with literature.
- ...as well as intuitive departures due to Knudsen number effects, as well as microstructure changes.

\[ \frac{\partial p}{\partial x} = -\frac{\mu}{K} v'_g \]

Regular Array of Cylinders

Random Array of Cylinders

Lee and Yang, JHMT, 1997
FiberForm Permeability

- Now we want to look at more relevant geometries and conditions.
- Flow-tube experiments performed at NASA Ames.
- Experimental data well-fit by Klinkenberg form of Darcy equation.
- Material permeability tested at various pressures and temperatures
- Significant variation in permeability observed due to rarefied effects.

\[
F = \frac{4 \mu \dot{m} RT L}{\pi D^2 M \Delta P} = K_0 (P_{av} + b)
\]

Marschall and Milos, JTHT, 1998
Preliminary Results

- Simulations were performed near the low end of the pressure range (~1kPa) of the experiments.
- Gas used was N2 at room temperature.
- Size of volume was 200x50x50 microns with a porosity of ~0.85.
- Two nominal fiber radii were used
  - 6 micron (single fiber)
  - 10 micron (fiber bundle)
- Several fiber orientations were simulated.
Fiber orientation is defined as the angle of the fiber with "pressing" plane.

- Error bars are those reported in the paper for all runs.
Permeability Results

• Caveats:
  – Seems to be large scatter in the experimental data

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  – Simulated geometry likely doesn’t constitute a “representative volume element”
  – Experiment gas was air

• Takeaways:
  – Microstructure is important
  – We’re in the ballpark!
**Future Work**

**Gas-Surface Modeling**
- Develop new gas-surface interaction model that takes better advantage of the improved fidelity of DSMC
  - “Active site” based approach
- Incorporate probabilities from Molecular Dynamics simulations

**FiberGen**
- Add analysis toolbox for computing geometric properties and statistics.
- Woven geometries

**Experimental Validation**
- Interested in performing targeted validation experiments in the NASA Flow-tube facility on “simple(r)” microstructure

**Simulate Stuff!...(cool stuff)**


Stern et. al., Gordon Research Conf, 2013
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Questions?