Particle methods for tortuosity factors in porous media

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Ablation WS, 2017
Bozeman, MT
Ablative Thermal Protection Systems

FiberForm® + Resin

PICA

Artist rendering of MSL entry

http://mars.nasa.gov/mer/gallery/artwork/entry_br.html
Material Design and Modeling
X-ray micro-tomography

• Advanced Light Source (ALS) at the Lawrence Berkeley Natl. Laboratory
• Synchrotron electron accelerator used to produce 14KeV X-rays
• Used for many research areas, including optics, chemical reaction dynamics, biological imaging, and X-ray micro-tomography.

http://www2.lbl.gov/MicroWorlds/ALSTool
X-ray micro-tomography

Collect X-ray images of the sample as you rotate it through 180°

Use this series of images to “reconstruct” the 3D object

Penetrating power  Multiple angles

X-ray Camera View

Courtesy of D. Parkinson (ALS)
X-ray micro-tomography

Visualization of FiberForm in PuMA at multiple scales
Porous Materials Analysis (PuMA)

Technical Specifications

- Written in C++
- GUI built on QT
- Visualization module based on OpenGL
- Parallelized using OpenMP for shared memory systems

Domain Generation

- Artificial Material Generator
- Micro-tomography Import, Processing, and Thresholding

Visualization

- Marching Cubes
- OpenGL Surface Rendering

Material Properties

- Porosity
- Specific Surface Area
- Effective Thermal Conductivity
- Effective Electrical Conductivity
- Diffusivity / Tortuosity (Bulk and Knudsen)
- Representative Elementary Volume

Material Response

- Oxidation Simulations
- Transient Heat Transfer *

*Under Development
Tortuosity Factors

- Quantifies a material's resistance to a diffusive flux.
- Important in modeling diffusion/reaction systems – such as ablative TPS response.

\[ \eta = \varepsilon \frac{D_{\text{ref}}}{D_{\text{eff}}} \]

- \( \eta \): tortuosity factors
- \( \varepsilon \): porosity
- \( D_{\text{ref}} \): reference diffusion coefficient
- \( D_{\text{eff}} \): effective diffusion coefficient

Surface rendering of FiberForm tomography in PuMA V2.1. Visualization contains \( \approx \) 500 million triangles.
Knudsen Number

- Non-dimensional number which defines the diffusion regime

\[ \text{Kn} = \frac{\bar{\lambda}}{l_D} = \frac{\text{Mean Free Path}}{\text{Characteristic Length}} \]

- Continuum: \( \text{Kn} \ll 1 \)
- Transitional: \( \text{Kn} \approx 1 \)
- Rarified: \( \text{Kn} \gg 1 \)

2D diffusivity simulations using a random walk method in PuMA. Particle paths are visualized in red.
Tortuosity Factors

- Quantifies a materials resistance to a diffusive flux
- Important in modeling diffusion/reaction systems – such as ablative TPS response

\[ \eta = \varepsilon \frac{D_{\text{ref}}}{D_{\text{eff}}} \]

- \( \eta \) = tortuosity factors
- \( \varepsilon \) = porosity
- \( D_{\text{ref}} \) = reference diffusion coefficient
- \( D_{\text{eff}} \) = effective diffusion coefficient

Surface rendering of FiberForm tomography in PuMA V2.1. Visualization contains \( \approx \) 500 million triangles.
Reference Diffusion Coefficient

- $D_{ref} = \text{reference diffusion coefficient}$

<table>
<thead>
<tr>
<th><strong>Continuum</strong></th>
<th><strong>Free Molecular</strong></th>
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<tbody>
<tr>
<td>$D_{ref} = D_{bulk}$</td>
<td>$D_{bulk}$ does not exist</td>
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- $D_{bulk} = \frac{1}{3} \bar{v} \bar{\lambda}$, which is undefined as the mean free path approaches infinity
- $D_{ref}$ therefore must be based on a length scale. In this case, the Diffusion coefficient through a capillary of diameter $l_D$

$\bar{v} = \text{mean thermal velocity}$

$\bar{\lambda} = \text{mean free path}$
Bosanquet Approximation

• Used to approximate $D_{ref}$ based on known values for $D_b$ and $D_k$. [1]

$$\frac{1}{D_{ref}} = \frac{1}{D_b} + \frac{1}{D_k}$$

• Rewritten for single species diffusion in a capillary, $D_{ref}$ becomes [2]

$$D_{ref} = \frac{1}{3} \bar{v} \left( \frac{\bar{\lambda} l_D}{\bar{\lambda} + l_D} \right)$$

1. Define $l_D$ based on an approximate geometric length scale for the material. Typically $\frac{4\varepsilon}{S}$ or mean intercept length. (Tomadakis, Lachaud, Geodict)

2. Define $l_D$ after the simulations are complete as the value which makes the tortuosity factor vs. Knudsen number plot converge to a single value. (Zalc)
Define $l_D$ based on an approximate geometric length scale for the material. Typically $\frac{4\varepsilon}{S}$ or mean intercept length. (Tomadakis, Lachaud, Geodict, PuMA)

- Most often used in the literature and software
- Requires values of $\eta_b$, $\eta_k$ and $l_D$ in order to apply the Bosanquet approximation
- $\eta$ is no longer a purely geometrical property, as it is now a function of the Knudsen number
- Since $\eta_b$ had no physical meaning without $l_D$, this can produce confusing results of $\eta_k < 1$

Figure from Tomadakis, 1993
Define $l_D$ after the simulations are complete as the value which makes the tortuosity vs. Knudsen number plot converge to a single value. (Zalc, PuMA)

- Requires only one value of $\eta$ and a computed length scale, $l_D$, in order to apply the Bosanquet approximation
- $\eta$ is now longer a purely geometrical property, no longer a function of Kn
- Easier to understand and implement

Tortuosity factor vs Knudsen Number for 1D fibers, computed in PuMA, showing the parallel and perpendicular tortuosity factors for Option #1 and Option #2
1. Define $l_D$ based on an approximate geometric length scale for the material. Typically $\frac{4\varepsilon}{S}$ or mean intercept length. (Tomadakis, Lachaud, Geodict)

2. Define $l_D$ after the simulations are complete as the value which makes the tortuosity factor vs. Knudsen number plot converge to a single value. (Zalc)
Applying Tortuosity Factors

• Used to compute $D_{eff}$ within a porous media, with known tortuosity factor, $\eta$, known length scale, $l_D$, and known gas properties.

\[ D_{eff} = \varepsilon \frac{D_{ref}}{\eta} \]

• Using Bosanquet approximation to approximate $D_{ref}$, the equation becomes

\[ D_{eff} = \frac{\varepsilon}{3\eta} \tilde{v} \left( \frac{\tilde{\lambda}l_D}{\tilde{\lambda} + l_D} \right) \]
Numerical Methods

Continuum

• Can be solved using typical numerical methods such as finite volume and finite difference

1. Geodict - Explicit Jump Solver
2. PuMA – Explicit Jump Solver
3. TauFactor – Finite Volume solver

Rarified

• Must be solved using particle methods to account for Knudsen effects

1. PuMA – Random walk solver
2. Geodict – Random walk solver (Knudsen regime)
3. SPARTA – Direct Simulation Monte Carlo
Random Walk Solver

- Particle method for solving diffusion
- Velocity and mean path for each particle based on exponential distribution
- Diffuse reflections are used for surface collisions
- Symmetric boundary conditions

\[ D_{eff_i} = \frac{\langle \xi^2 \rangle}{2t} \]

- \( \langle \xi^2 \rangle \) is the mean square displacement of the particles
- Mean thermal velocity, \( \bar{v} \), and mean free path, \( \bar{\lambda} \), are imposed to simulate the desired gas species and conditions.
Wall Collisions

- Diffuse reflections used for surface collisions
- Collision detection can be based on isosurface or cuberille grid

Isosurface (a) and cuberille (b) approximations of a cylinder with radius 3 voxels.
Wall Collisions

- Diffuse reflections used for surface collisions
- Collision detection can be based on isosurface or cuberille grid

Percent difference (isosurface vs cuberille) vs Knudsen number for three different ideal geometries
Comparison to Literature

Test Case #1

- 3D Fibers, $512^3$
- Intersecting, isotropic
- 0.6 porosity

The 5% error is likely due to the limitations of computing in 1993. Simulations by Tomadakis were using only 200 particles and likely on a small dataset. The PuMA simulations were run on 200,000 particles for a total walk length of 10,000 times the domain length.
Comparison to Literature

Test Case #2

- 1D Fibers, 512 x 512 x 256
- Non intersecting
- 0.7 porosity

The 5% error is likely due to the limitations of computing in 1993. Simulations by Tomadakis were using only 200 particles and likely on a small dataset. The PuMA simulations were run on 200,000 particles for a total walk length of 10,000 times the domain length.
Test Case #1

- 3D Fibers, $512^3$
- Intersecting, isotropic
- 0.6 porosity
Bosanquet Analysis

Test Case #2

- FiberForm, 0.8 mm³
- Transverse isotropic
- 0.89 porosity
Direct Simulation Monte Carlo

- DSMC is a particle method to simulate transitional and rarified flows with high fidelity
- Very computationally expensive, preventing large or frequent simulations
- DSMC diffusion simulations conducted in SPARTA, developed at Sandia National Labs.
- Pressure varied to change the mean free path, and therefore the Knudsen number
- **Used as a verification case for the random walk method**

DSMC simulation of transitional flow over the Space Shuttle. Sparta.sandia.gov
Direct Simulation Monte Carlo

Test Case #1

- 3D Fibers, $512^3$
- Intersecting, isotropic
- 0.6 porosity
Conclusion and Outlook

- Implemented finite difference and random walk tortuosity factor solvers into PuMA V2.1
- Demonstrated the necessity of using an isosurface collision detection for complex 3D media, a capability which currently only exists in PuMA
- Verified random walk model for tortuosity factors against Direct Simulation Monte Carlo (DSMC) simulations.
- Recommend changing current definitions of tortuosity factor to restore the value as a purely geometrical property.
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Questions?

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