Computer Models of Nonwoven Geometry and Filtration Simulation

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Part I: 3d Nonwoven Model

- Fiber diameter, length
- Fiber shapes
- Fiber directions
- Fiber crimp, overlap
- Porosity
- # of Layers, thicknesses

[Images of 3D nonwoven model components: Shape, Layers, Directions, Diameters]
Model parameters and realization

“Manufacturable” parameters:

- Porosity
- Fiber diameter & length (distributions)
- Fiber orientation distribution

Generator:

- Choice of uniform Cartesian REV
- Random center point location
- Random fiber orientation
- Discretization via distance from axis
- Until desired porosity is reached

Extra effects:

- Partly exterior fibers
- Overlapping fibers
Geometric meaning of anisotropy

- Planar isotropy
- Parallel
- 2-fold anisotropy
Real and generated nonwoven

Microscopy (real)

ZY-cross section

XY-cross section

3D view
Nonwoven with binder; under compression

XY-cross section

ZY-cross section

XY-cross section, with binder

ZY-cross section, compressed
Compression for oil filtration

- Currently purely geometric
- Must still be connected to the oil pressure
Model validation

- Simulated and real nonwoven
- Simulated and real mercury intrusion (porosimetry)
Part II: Flow through Nonwoven

\[-\mu \Delta \bar{u} + \nabla \bar{u} \cdot \bar{u} + \kappa^{-1} \bar{u} + \nabla p = \vec{f} \text{ (momentum balance)}\]

We do NOT use Fluent, but

- A proprietary Lattice Boltzmann code Parpac
- A proprietary Finite Volume code EJ-Stokes
Pressure and velocity

Pressure (p)

Velocity (u)
Permeability from Stokes equations

Mean velocity from nano simulation: $\bar{u}_i$ is mean value of solution of a periodic Stokes problem

$$\nabla \cdot u_i = 0 \text{ (mass conservation)},$$
$$u_i = 0 \text{ on } \Gamma \text{ (no-slip on solid surfaces)},$$
$$-\mu \Delta u_i + \nabla p = \begin{pmatrix} \delta_{i1} \\ \delta_{i2} \\ \delta_{i3} \end{pmatrix}.$$ 

Then make Darcy-Ansatz $\bar{u}_i = -\frac{\kappa}{\mu} \begin{pmatrix} -\delta_{i1} \\ -\delta_{i2} \\ -\delta_{i3} \end{pmatrix}$ and get

$$\kappa_{*1} = \mu \bar{u}_1,$$
$$\kappa_{*2} = \mu \bar{u}_2,$$
$$\kappa_{*3} = \mu \bar{u}_3.$$
Permeability (in $10^{-11}m^2$)

- Computations require ca. 17 iterations or 5 minutes per column (45 minutes for all 3 tables) for 2 digits on $160^3$ data sets on my 512 MB laptop
- Geometric anisotropy in Cartesian directions results in almost diagonal & symmetric (up to precision) tensor
Permeability (in $1e-011m^2$)

\[
\begin{align*}
\kappa_{11} &= 93 \quad \beta_1 = 10 \\
\kappa_{22} &= 120 \quad \beta_2 = 3 \\
\kappa_{33} &= 80 \quad \rho = 5\% \\
\end{align*}
\]
\[
\begin{align*}
d &= 8\mu m
\end{align*}
\]

\[
\begin{align*}
\kappa_{11} &= 82 \quad \beta_1 = 0.1 \\
\kappa_{22} &= 79 \quad \beta_2 = 1 \\
\kappa_{33} &= 124 \quad \rho = 5\% \\
\end{align*}
\]
\[
\begin{align*}
d &= 8\mu m
\end{align*}
\]

\[
\begin{align*}
\kappa_{11} &= 103 \quad \beta_1 = 10 \\
\kappa_{22} &= 108 \quad \beta_2 = 1 \\
\kappa_{33} &= 80 \quad \rho = 5\% \\
\end{align*}
\]
\[
\begin{align*}
d &= 8\mu m
\end{align*}
\]

\[
\begin{align*}
\kappa_{11} &= 104 \quad \beta_1 = 10 \\
\kappa_{22} &= 121 \quad \beta_2 = 1 \\
\kappa_{33} &= 195 \quad \rho = 5\% \\
\end{align*}
\]
\[
\begin{align*}
d &= 10\mu m
\end{align*}
\]

\[
\begin{align*}
\kappa_{11} &= 40 \quad \beta_1 = 10 \\
\kappa_{22} &= 40 \quad \beta_2 = 1 \\
\kappa_{33} &= 67 \quad \rho = 7\% \\
\end{align*}
\]
\[
\begin{align*}
d &= 8\mu m
\end{align*}
\]

\[
\begin{align*}
\kappa_{11} &= 28 \quad \beta_1 = 10 \\
\kappa_{22} &= 29 \quad \beta_2 = 1 \\
\kappa_{33} &= 48 \quad \rho = 9\% \\
\end{align*}
\]
\[
\begin{align*}
d &= 8\mu m
\end{align*}
\]

Expect now at most 10% deviation of mean values compared with measurements for nonwoven
Part III: Particle Motion & Filtration

\[ d\vec{\dot{v}} = -\gamma \times (\vec{v}(\vec{x}) - \vec{v}_0(\vec{x})) \, dt + \frac{Q \vec{E}_o(\vec{x})}{m} \, dt + \sigma \times d\vec{W}(t) \]

\[ \frac{d\vec{x}}{dt} = \vec{v} \]

\[ \gamma = 6\pi \rho \mu \frac{R}{m} \quad t: \text{ time} \]

\[ \sigma^2 = \frac{2k_B T \gamma}{m} \quad \vec{x}: \text{ particle position} \]

\[ \vec{v}: \text{ particle velocity} \]

\[ \langle dW_i(t), dW_j(t) \rangle = \delta_{ij} dt \quad R: \text{ particle radius} \]

\[ m: \text{ particle mass} \]

\[ Q: \text{ particle charge} \]

\[ T: \text{ ambient temperature} \]

\[ k_B: \text{ Boltzmann constant} \]

Description applies to:

- Oil filtration
- Air filtration
- [Aerosol filtration]

\): 3d probability (Wiener) measure
electric field
fluid velocity
fluid density
fluid viscosity
Influence of electric charge (air filtration)

No charges

Low charges

High charges
Snapshot of small & large particles

- Particles at fixed travel time, do not interact
- Blue: largest
- Green
- Yellow
- Red: smallest
Filter efficiency, measured & simulated
Deposition Diagram

- Deposition locations are 20 64µm layers.
- Orange: particle numbers
- Lines: mean value and standard deviation of number of collisions
- Example: Layer 15 contains 7% of the filtered particles. Those had on average 13.15 collisions with standard deviation 1.9
- 4 layers of gradient material indicated by thick black lines:
Evolution of pressure drop

- Pressure drop over time or amount
Particle filtration: soot, oil, blood, air, ...

Optimization of
• Filter efficiency of filter media
• Pressure drop
• Life time
• Manufacturing cost

Solve ca. $500^3$ Stokes flow problems in hours. Unfortunately, in filtration applications must iterate this over many geometries.

Treatment of
• „intelligence“
• deformation
of white blood cells

• Soot deposition on single fiber, resolved
• Computation of soot cake on fiber, derive permeability of cake
• Computation of time-dependent clogging of filter media.

Deposition in filter media, with porous voxels, 2d and 3d
The Virtual Filter Material Design Cycle

1. Identify parameters for real, existing material
2. Generate volume image for parameters
3. [Solve electric potential]
4. Solve Stokes(-Brinkmann) equations
5. Solve particle motion & deposition
6. Compute filter efficiency, pressure drop/ filter life time
7. Modify material parameters
Summary

• I: Nonwoven model
  • Porosity, Fiber direction, Fiber shape
  • Random, voxelized
• II: Flow through Nonwoven
  • Stokes equations, Permeability (= flow resistivity, = flow rate)
• III: Filtration
  • Brownian motion, friction w. fluid
  • Particle size distribution
  • Particle deposition, clogging
  • Pressure drop, efficiency, life time
Find out more:

GEO DICT

www.geodict.com

FILTER DICT

Thank you for attending this presentation.