Virtual Material Design and Air Filtration Simulation Techniques inside GeoDict and FilterDict

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Micro Structure Simulation and Virtual Material Design

- Structure generator + property simulator GeoDict / FilterDict
- Virtual three dimensional nonwoven models
- Computation of material properties
  - flow resistivity
  - permeability, capillary pressure
  - particle filtration, filter efficiency
  - filter lifetime
  - acoustic absorption
  - effective elasticity properties
- Sequences of simulations to optimize material geometry
The Virtual Material Design Cycle

1. Identify parameters for real, existing material
2. Generate 3d geometry for parameters
3. Solve Stokes equations in 3d geometry
4. Compute filter efficiency in 3d geometry
5. Modify material parameters
6. Go back to 2.
The Geometric Nonwoven Model

Possible variations: for example
• Cross sections
• Layers
• Anisotropy
Design Parameters for Nonwoven Filter Media

1. Layer thicknesses
2. Porosity of each layer (via voxel count)
3. Fiber diameters in each layer
4. Fiber anisotropy in each layer
5. Fiber shapes in each layer
6. Combination with other types of layers, e.g. porous membranes
7. Fibers may or may not overlap
8. Fiber crimp can be modeled
9. Fibers are “infinitely long”
10. Enough voxels in all directions to have representative elementary volume
11. Resolution critical for fibers surface roughness, particle sizes and flow
Transverse Isotrope Fiber Orientation Probability and Nonwoven Material Density

- Transverse isotrope fiber orientation probability: compression in theta-direction, isotrope for $\beta=1$, compressed for $\beta>1$.

$$p(\vartheta, \varphi) = \frac{1}{4\pi} \frac{\beta \sin \vartheta}{(1 + (\beta^2 - 1) \cos^2 \vartheta)^{3/2}} , \quad \vartheta \in [0, \pi), \, \varphi \in [0, 2\pi)$$

- For two fiber types with probability $0 \leq p \leq 1$ and $1-p$, generate random number $n$ between 0 and 1 and select first type if $n \leq p$ and second type if $n > p$.

- Generate fibers until the desired solid volume fraction $f_V$ is reached based on comparing the voxels occupied by the generated fibers with the total amount of voxels in the volume.

- Can select overlapping and nonoverlapping fibers, the latter with limits on the desired solid volume fraction.
Real and Generated Three Dimensional Images

Synchrotron image vs. generated structure (paper dewatering felt)
Eulerian Description of Stationary Stokes Flow

\[ \mu \Delta \vec{u} + \vec{f} = \nabla p \]  \hspace{1cm} \text{: momentum balance}

\[ \text{div} \, \vec{u} = 0 \]  \hspace{1cm} \text{: incompressible conservation of mass}

\[ \vec{u} = 0 \text{ on } \Gamma \]  \hspace{1cm} \text{: no-slip on fiber surfaces}

- \( \vec{f} \): force in direction of the flow,
- \( \vec{u} \): velocity,
- \( \mu \): fluid viscosity,
- \( p \): pressure and
- \( \Gamma \): fiber or deposited particle surfaces.

The flow can be solved with periodic boundary conditions if the cutout is large enough and empty space is added in front.
Filter Efficiency Model

A) Testdust:
- Sphere radii
- Specific weight
- Electrostatic charges

B) Fluid:
- Viscosity
- Density
- Temperature
- Mean flow velocity

C) Nonwoven geometry:
- Electrostatic charges
- No-slip boundary conditions

D) Interaction:
- Flow & pressure drop: B & C
- Electrostatic field: C
- Friction: A & B
- Diffusion: A & B
- Collision: A & B
- Adhesion: A & C
- Electrostatic attraction: A & C
- Particle Paths: A, B & C

E) Deposition due to:
- Inertial impact + adhesion
- Diffusion + adhesion
- Electrostatic attraction + adhesion
- Sieving

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Filter Efficiency

- Measurement
- Simulation M1
- Simulation M4
- Simulation M5

Filter Efficiency [%] vs Particle Diameter [1e-6m]
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:
Particle Diameter = 0.3 µm

Layer of Deposition
Deposition of Different Sized Particles in the Different Layers

![Graph showing deposition efficiency across different particle diameters and layers.]

- **Layer 1**
- **Layer 2**
- **Layer 3**
- **Layer 4**

**Particle Diameter [µm]**
- 0.255
- 1.077
- 16.591

**Filter Efficiency [%]**
- 0
- 10
- 20
- 30
- 40
- 50
- 60
- 70
- 80
- 90
- 100

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Influence of Electrostatic Surface Charges

Deposition of uniform sized particles on a single fiber in the absence and in the presence of an electric field:

- deposition rate doubles,
- particles also stick to the “back” of the fiber.
Filter Life Time Model

A) Testdust:
- Sphere radii
- Specific weight
- Electrostatic charges

B) Fluid:
- Viscosity
- Density
- Temperature
- Mean flow velocity

C) Nonwoven geometry:
- Electrostatic charges
- No-slip boundary conditions

D) Efficiency:
- Flow & pressure drop: B & C
- Electrostatic field: C
- Friction: A & B
- Diffusion: A & B
- Collision: A & C
- Adhesion: A & C
- Electrostatic attraction: A & C
- Particle Paths: A, B & C

E) Deposition due to:
- Inertial impact + adhesion
- Diffusion + adhesion
- E-static attraction +adhesion
- Sieving

F) Clogging:
- Deposited particles determine new geometry model, including permeable voxels

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Filter Lifetime Simulation: from Clean to End-of-Life
Evolution of Filter Efficiencies during Filter Lifetime Simulations

Filter Efficiency [%]

Particle Diameter [1e-6m]

- Sim 5.5g/m²
- Sim 16.5g/m²
- Sim 27.5g/m²
- Sim 38.5g/m²
- Sim 55.0g/m²
- Sim 66g/m²
Time Dependent Pressure Drop

Pressure drop in kPa/cm at \( v_{\text{air}} = 4 \text{cm/s} \)

- Graph showing pressure drop in kPa/cm versus solid volume fraction.
- The graph shows the pressure drop in the loaded portion of the media (closed diamonds) and on average over the whole media (open circles).

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Summary

Filtration properties of filter media can be computed and optimized

1. 3d geometry from tomography or mathematical model
2. Model media, fluid flow and the dirt as well as their interactions
3. MPPS: small particles filtered by diffusion, large ones by sieving
4. Layered materials give more uniform clogging, can have multiple properties
5. Study of electrostatic effects on filtration is on its way
6. Study of subvoxel effects is on its way
7. Virtual filter material design is possible!
GeoDict and FilterDict: Contributors from ITWM

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