Progress & Challenges predicting Filtration and Separation

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Filtration and simulation occur on multiple scales
Virtual design cycle of filter media

1. Choose initial structural parameters

2. Generate / modify structure

3. Solve CFD problem

4. Compute particle transport and deposition

5. Compute filtration efficiency and pressure drop

6. Choose new structural parameters
Our simulations are all based on structures of little cubes

Advantages
- Saves grid generation times
- Compatible with computer tomography
- Straight forward structure generation
- Straight forward solver implementation
- Straight forward parallel computations

Disadvantages
- Resolved features require many grid cells
- Leads to very large scale computations
Description of fluid motion: Stationary Stokes flow w/wo slip

\[-\mu \Delta \vec{u} + \nabla \vec{u} \cdot \vec{u} + \nabla p = 0 \text{ (momentum balance)}\]
\[\nabla \cdot \vec{u} = 0 \text{ (mass conservation)}\]
\[\vec{u} = 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)}\]
\[P_{in} = P_{out} + c \text{ (pressure drop is given)}\]

- $\mu$: fluid viscosity,
- $\vec{u}$: velocity, periodic,
- $p$: pressure, periodic up to pressure drop in flow direction.

\[-\mu \Delta \vec{u} + \nabla p = 0 \text{ (momentum balance)}\]
\[\nabla \cdot \vec{u} = 0 \text{ (mass conservation)}\]
\[\vec{n} \cdot \vec{u} = 0 \text{ on } \Gamma \text{ (no flow into fibers)}\]
\[\vec{t} \cdot \vec{u} = -\lambda \vec{n} \cdot \nabla (\vec{u} \cdot \vec{t}) \text{ on } \Gamma \text{ (slip flow along fibers)}\]
\[P_{in} = P_{out} + c \text{ (pressure drop is given)}\]

- $\vec{n}$: normal direction to the fiber surface,
- $\lambda$: slip length,
- $\vec{t}$: any tangential direction with $\vec{t} \cdot \vec{n} = 0$. 
Flow Field Visualization

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Pressure Drop Visualization

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Pressure and Velocity in Clogging Simulation

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Filtration Effects I

A: direct interception
B: inertial impaction
C: diffusional deposition
E: sieving
F: clogging

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Filtration Effects II and modes of particle motion

D: electrostatic attraction

G: Slide
H: Bounce
When particles are **larger** than the grid cells
When particles are smaller than the grid cells
Description of particle motion

\[ d\vec{x} = \vec{v} \, dt, \quad \text{Friction with fluid} \]

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

\[ C_c = 1 + Kn \left( 1.142 + 0.558e^{-0.999/Kn} \right), \]

\[ \gamma = 6\pi \mu R \frac{1}{C_cm}, \]

\[ \sigma^2 = \frac{2k_B T \gamma}{m}, \]

\[ \left\langle dW_i(t), dW_j(t) \right\rangle = \delta_{ij} dt, \quad t: \text{time} \]

\[ \vec{x}: \text{particle position} \quad \vec{v}: \text{particle velocity} \]

\[ Kn = \frac{\lambda}{R}, \quad \overline{\vec{v}}: \text{particle velocity} \quad \overline{R}: \text{particle radius} \]

\[ \lambda = \frac{k_B T}{\sqrt{32\pi R^2 P}}, \quad m: \text{particle mass} \]

\[ q: \text{particle charge} \quad T': \text{ambient temperature} \quad P: \text{total pressure} \]

\[ d\vec{W}(t): \text{3d probability (Wiener) measure} \]
Deposition effects

\[ \alpha = 0.05, \]
\[ d_F = 14, \]
\[ v = 0.1 \text{m/s} \]
Nano Simulations

1.67 cm/sec  10.0 cm/sec

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Nano Simulations

- Deposition patterns and porosity depend on far field velocity, particle size distribution, etc.

Result:

- Find minimal porosity and permeability of the soot layers, $s_{\text{max}}$ and $\kappa_{\text{min}}$
- Derivation by layers from single fiber highly resolved simulations
Stationary Flow with unresolved particles: Stokes-Brinkmann eqs

\[-\mu \Delta \vec{u} + \nabla \vec{u} \cdot \vec{u} + \nabla p + \kappa^{-1} \vec{u} = \vec{f} \ (\text{momentum balance})\]
\[\nabla \cdot \vec{u} = 0 \ (\text{mass conservation})\]
\[\vec{u} = 0 \text{ on } \Gamma \ (\text{no-slip on fiber surfaces})\]

\[\vec{f} = (0, 0, f) : \text{ force in flow(z)-direction,} \]
\[\kappa = \kappa_{min} \max \{1, s_{max}/s\} : \text{ porous voxel permeability,} \]
\[s : \text{ solid volume fraction in a voxel} \]
\[\vec{u} : \text{ velocity,} \]
\[\mu : \text{ fluid viscosity,} \]
\[p : \text{ pressure and} \]
\[\Gamma : \text{ fiber or deposited particle surfaces.} \]

Solid volume fraction in voxel is increased until \(s_{max}\) is reached. Voxel becomes “collision-solid”. Neighbor voxels svf starts increasing upon particle arrival.
Micro Simulations

Final state at 5.1 g / m^2

Darker gray means denser soot.

Filtration_Animation.mp4

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Horizontal layers

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Cross Flow Filtration
Weave Pleat Options

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Oil flow in pleats with support structure: velocity & pressure

- Velocity: 0.15 m/s
- Oil: density 850 kg/m³, viscosity 0.17 m²/s
- Same pleat count
- Different in- and outflow channel widths
- Grid resolution 40 μm
- 50 x 70 x 380 cells

Narrow Channel
Thick Wire
Thin Wire
Conclusions

Challenges

- Measurements
- deposition location
- electric charges
- Requirements: cost, material, space, energy
- Computing power
- Geometric resolution
- Geometry uncertain
- Analytic expressions to be derived

Progress

- 3d media and element models
- Navier-Stokes-Brinkman for gas and liquid
- Fast & low memory solvers
- Prediction of pressure drop for Re < 100
- Low concentration particle transport
- Prediction of filter efficiency
- Cake and porous media build-up
- Prediction of clogging and life time
- Filtration and separation simulation spread in Academic and Industrial R&D

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Outlook

Current “Hot” Simulation Topics:

• Multipass time step control (see my talk tomorrow)
• Re-entrainment of particles, pulse cleaning
• Coalescence
• Filtration in pleats and DPF honeycomb structures
• Nanofibers
• Electric charges
• Two phase flows in filters, rocks, diapers and fuel cells