Nano Filtration Media – Challenges of Modeling and Computer Simulation

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GeoDict

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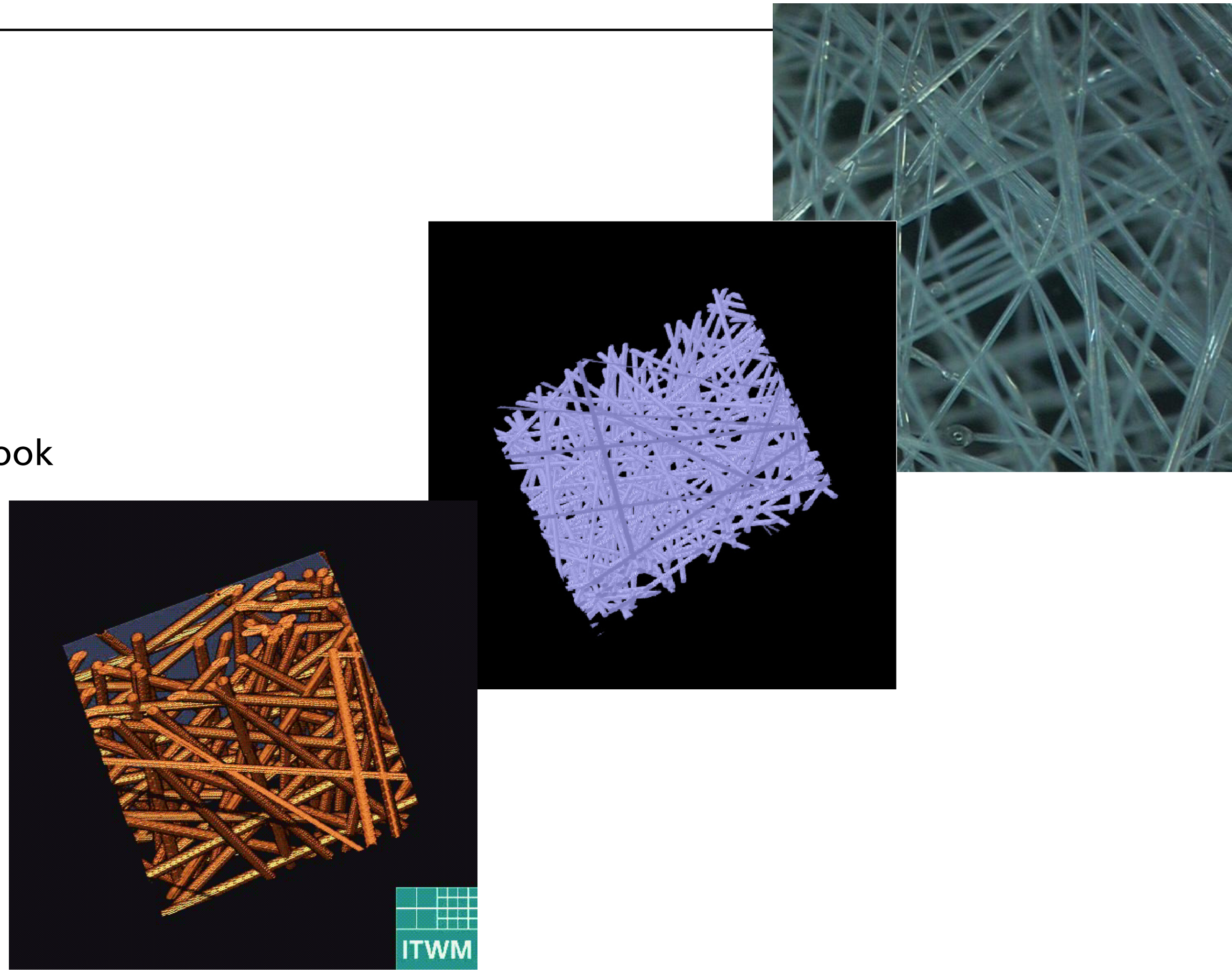
Outline

- Introduction
- Method
- Simulation results
- Conclusion and outlook



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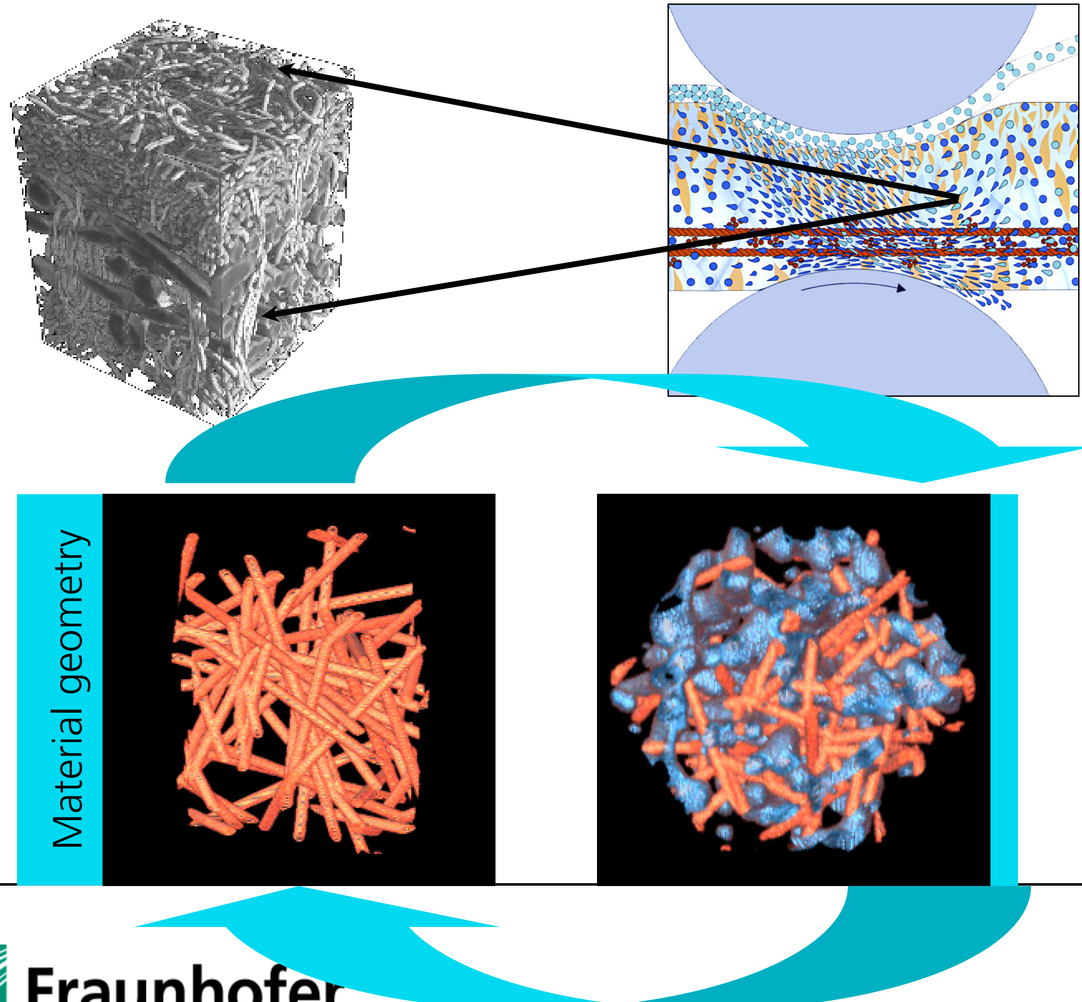
Introduction

- Filtration media: porous microstructures, or even nanostructrues
- Physical phenomena:
  - Fluid flow
  - Particle adhesion effects
  - Deposition
  - …
- Nano fiber filtration process
  - Benefits: improvements of filter efficiency and low increase of pressure drop
  - Simulation challenges: the structures become huge; new physical effects such as nano slip have to be considered.

Method

➢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.



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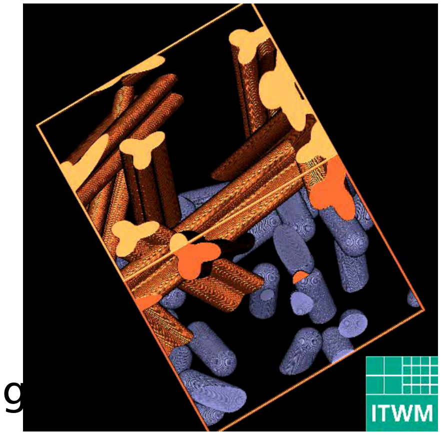
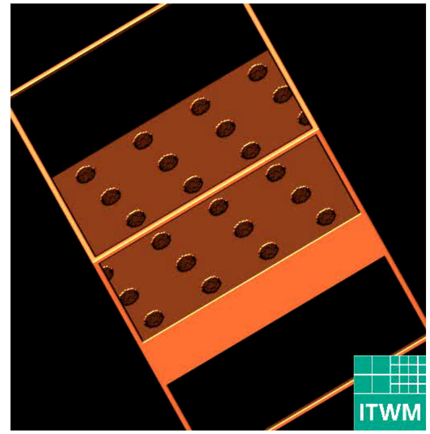
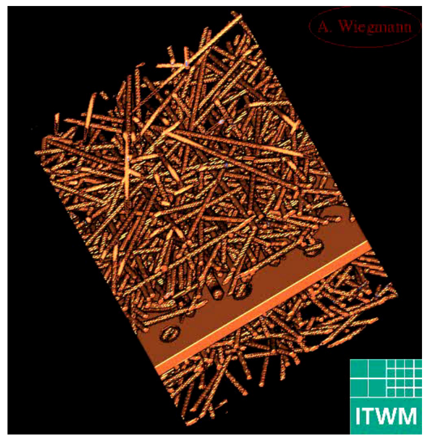
Method

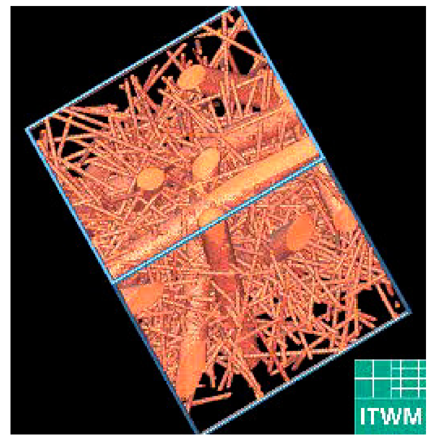
➢Design Parameters for Nonwoven Filter Media

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









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Method

➢Transverse Isotrope Fiber Orientation Probability and Nonwoven Material Density

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

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

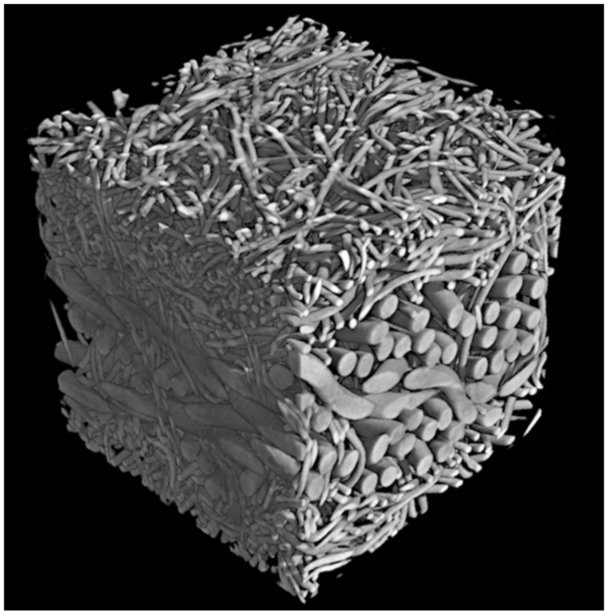
- For two fiber types with probability $0 \leq p \leq 1$ and $1-p$, generate random number n between 0 and 1 and select first type if $n \leq p$ and second type if $n>p$.

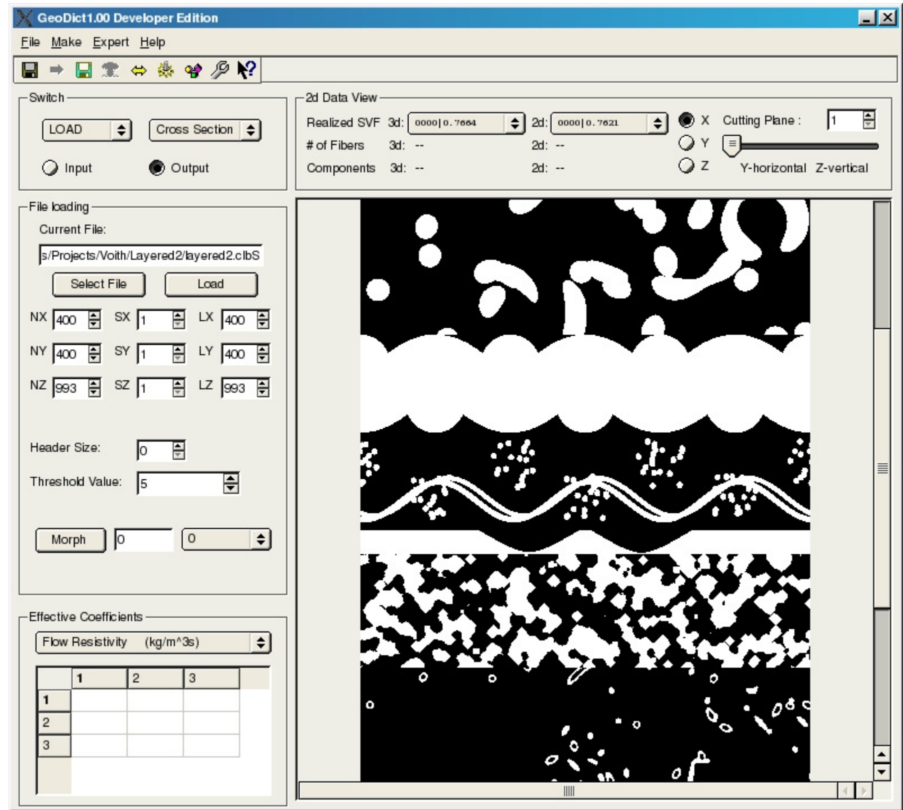
- Generate fibers until the desired solid volume fraction f_V is reached based on comparing the voxels occupied by the generated fibers with the total amount of voxels in the volume.

- Can select overlapping and nonoverlapping fibers, the latter with limits on the desired solid volume fraction.

Method

➢Real and Generated Three Dimensional Images





Synchrotron image vs.
generated structure
(paper dewatering felt)

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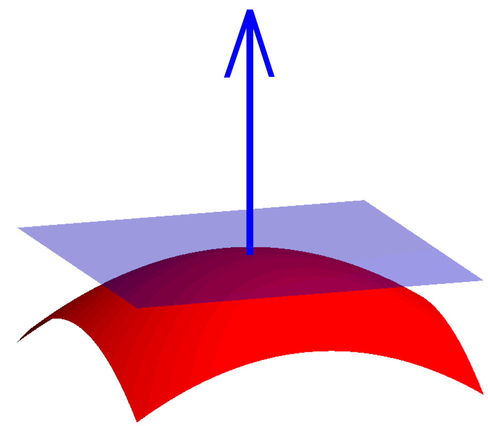
Method

- **Eulerian Description of Stationary Stokes Flow**
  No slip vs fractional slip



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

μ : fluid viscosity,

$\vec{u}$: velocity, periodic,

p : pressure, periodic up to pressure drop in flow direction.

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

$\vec{n}$: normal direction to the fiber surface,

λ : slip length,

$\vec{t}$: any tangential direction with $\vec{t}\cdot\vec{n}=0$.

Method

➢Particle Motion

$$d\vec{v} = -\gamma \times \left(\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t)) \right) dt + \sigma \times d\vec{W}(t),$$

$$d\vec{x} = \vec{v}(\vec{x}(t))dt,$$

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

$$\gamma = 6\pi\rho\mu \frac{R}{m},$$

$$\langle dW_i(t), dW_j(t) \rangle = \delta_{ij} dt.$$

[Latz & Wiegmann, Filtech 2003]

$\vec{u}$: fluid velocity

$\vec{v}$: particle velocity

t : time

T : temperature

γ : friction coefficient

R : particle radius

ρ : fluid density

μ : fluid viscosity

$\vec{W}$: Wiener Measure (3d)

k_b : Boltzmann constant

m : particle mass

Kn : Knudsen number

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Method

➢ Mechanisms of Filtration

A: direct interception

B: inertial impaction

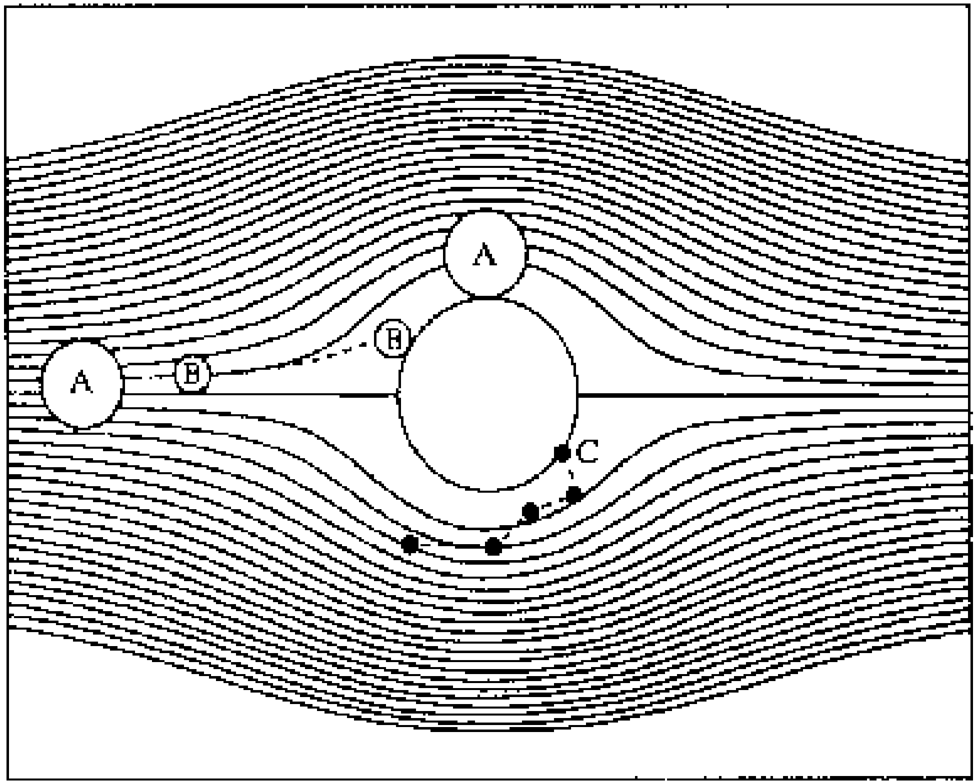
C: diffusional deposition

D: electrostatic attraction/repulsion

E: sieving

F: clogging

G: other effects (gravity,...)



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Method

➢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 & C
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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Method

➢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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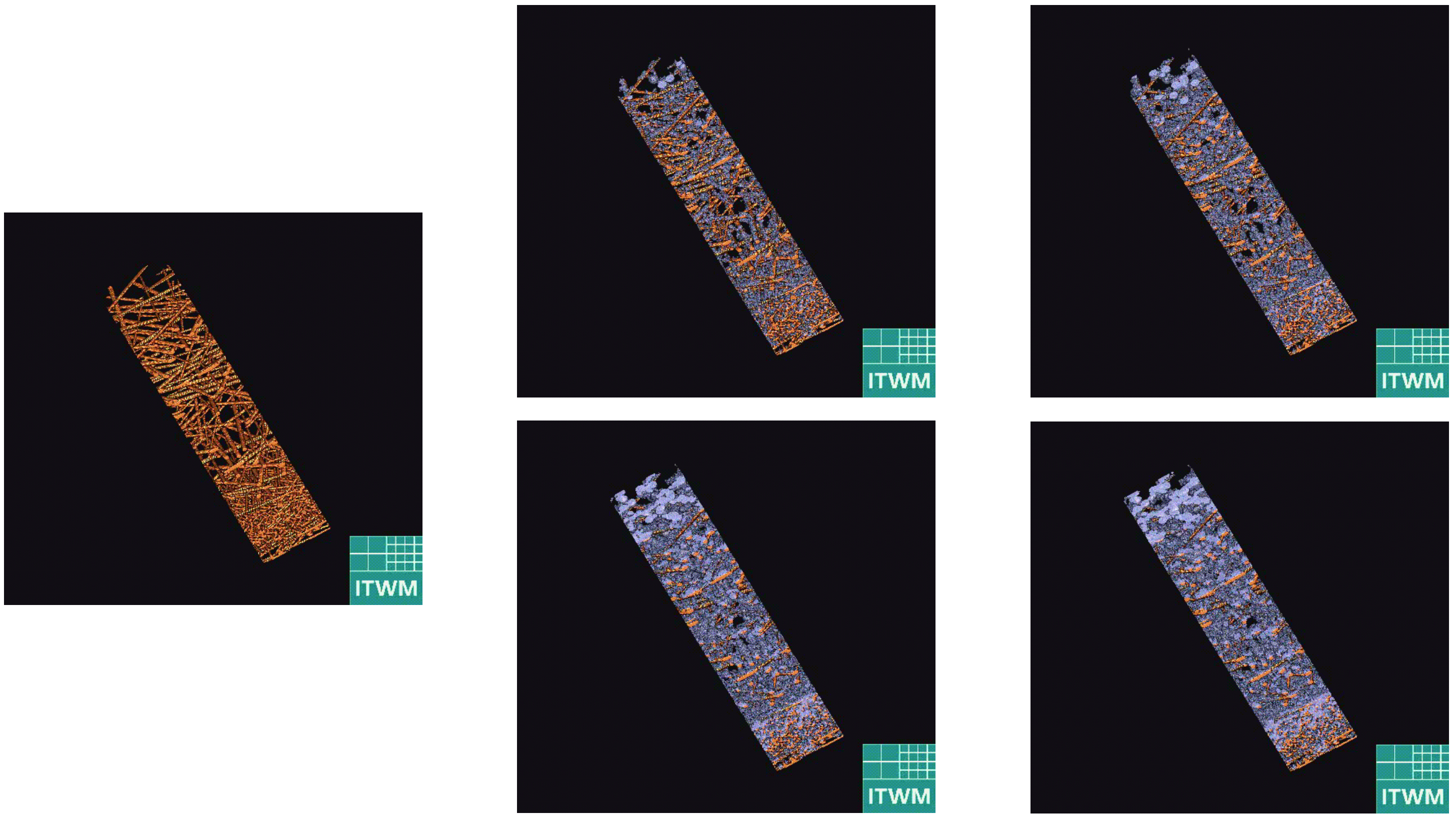
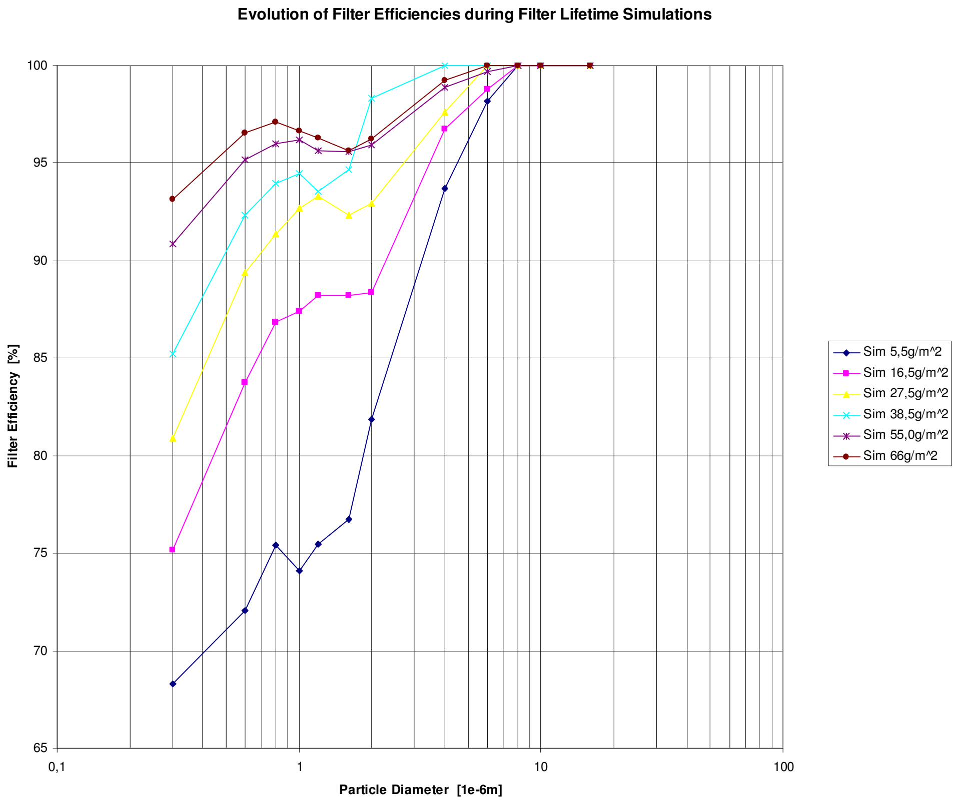
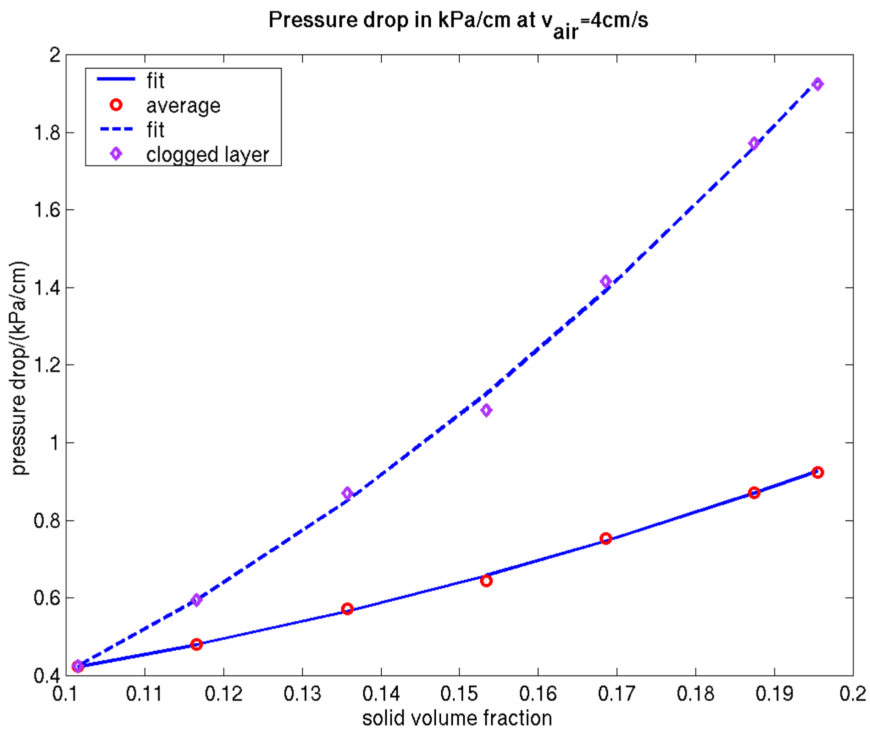
Method

➢Filter Lifetime Simulation: from Clean to End-of-Life



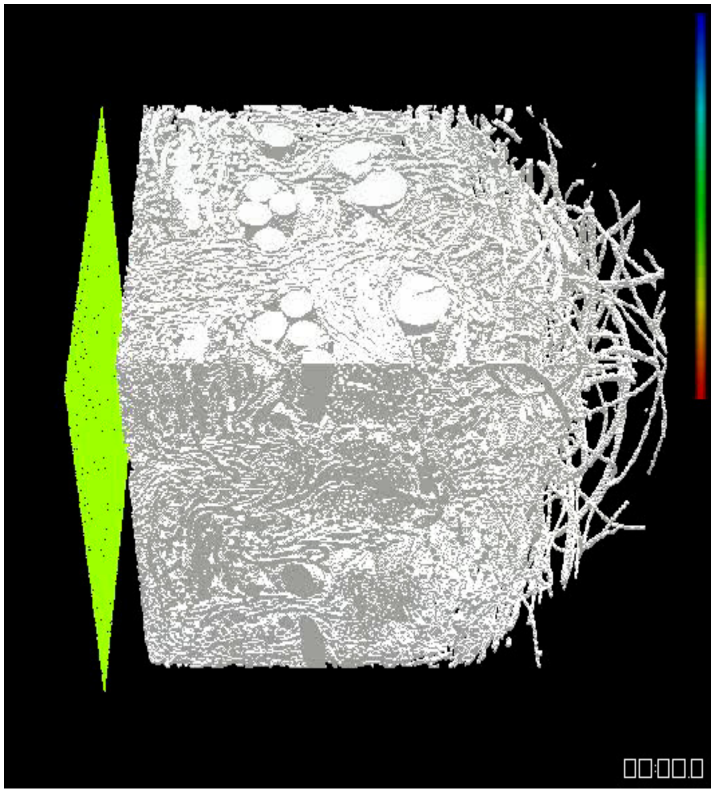
Method

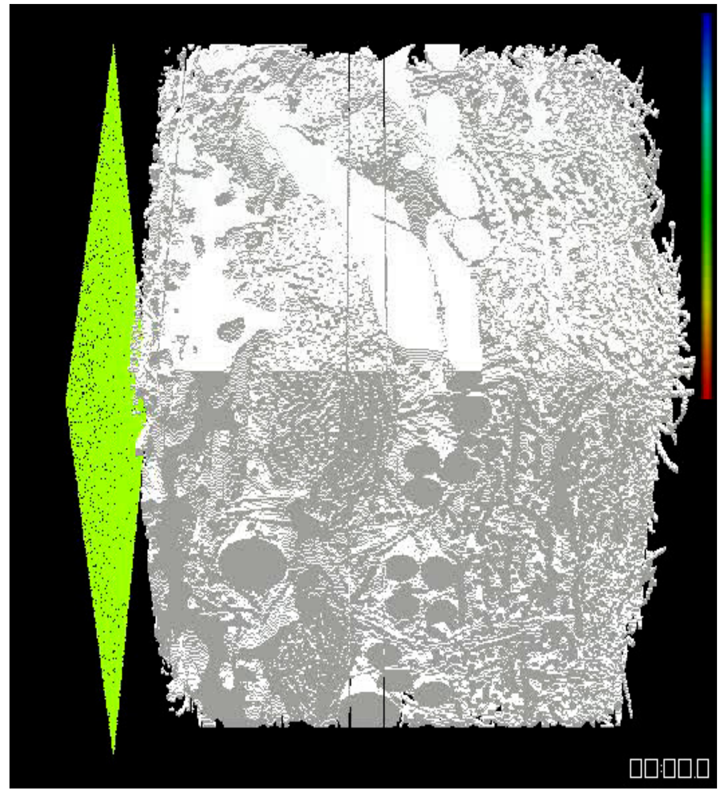

Evolution of Filter Efficiencies during Filter Lifetime Simulations
Filter Efficiency [%]
Particle Diameter [1e-6m]
Sim 5,5g/m^2
Sim 16,5g/m^2
Sim 27,5g/m^2
Sim 38,5g/m^2
Sim 55,0g/m^2
Sim 66g/m^2


Pressure drop in kPa/cm at v_air=4cm/s
pressure drop/(kPa/cm)
solid volume fraction
fit
average
fit
clogged layer

Method

➢Visualization





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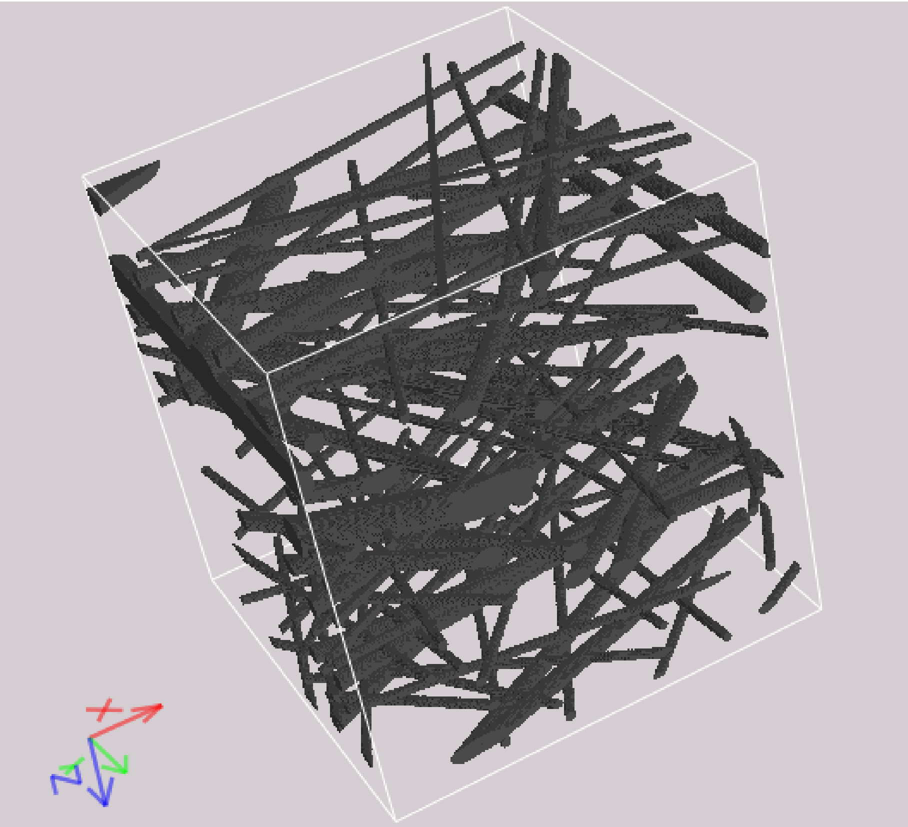
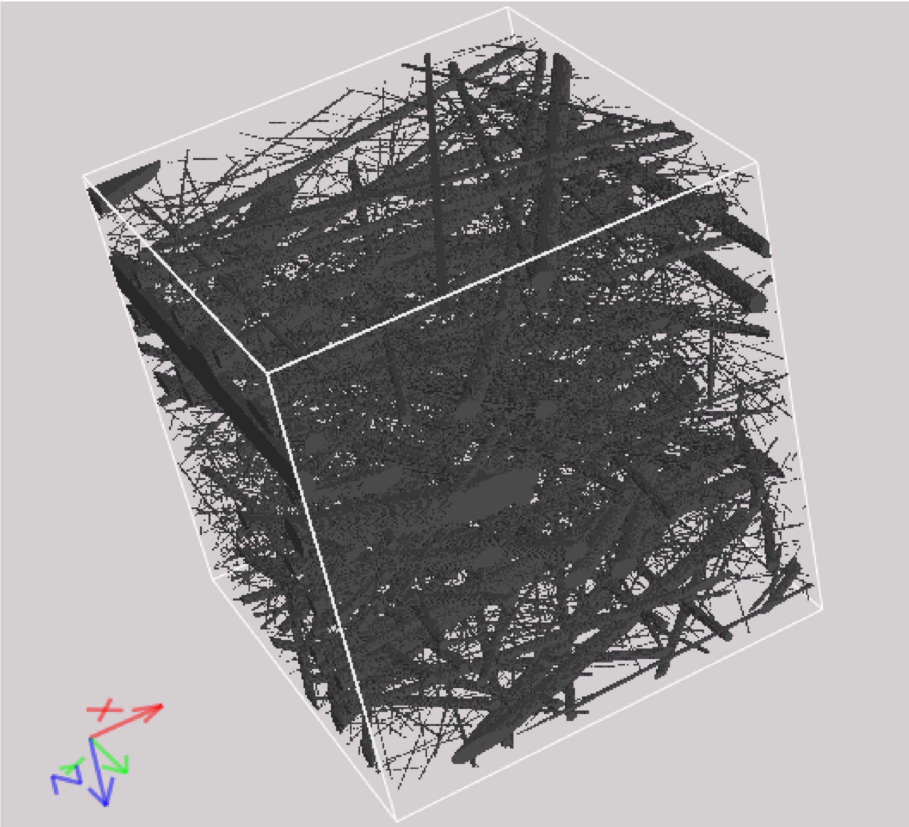
Results

Medium 1: volumetrically equally distributed with 1, 2, and 4 μm; fiber content 5%
Medium 2: Medium 1 + nanofibers with 100, 200, 400 nm (fiber content 0.5%)



Medium 1



Medium 2

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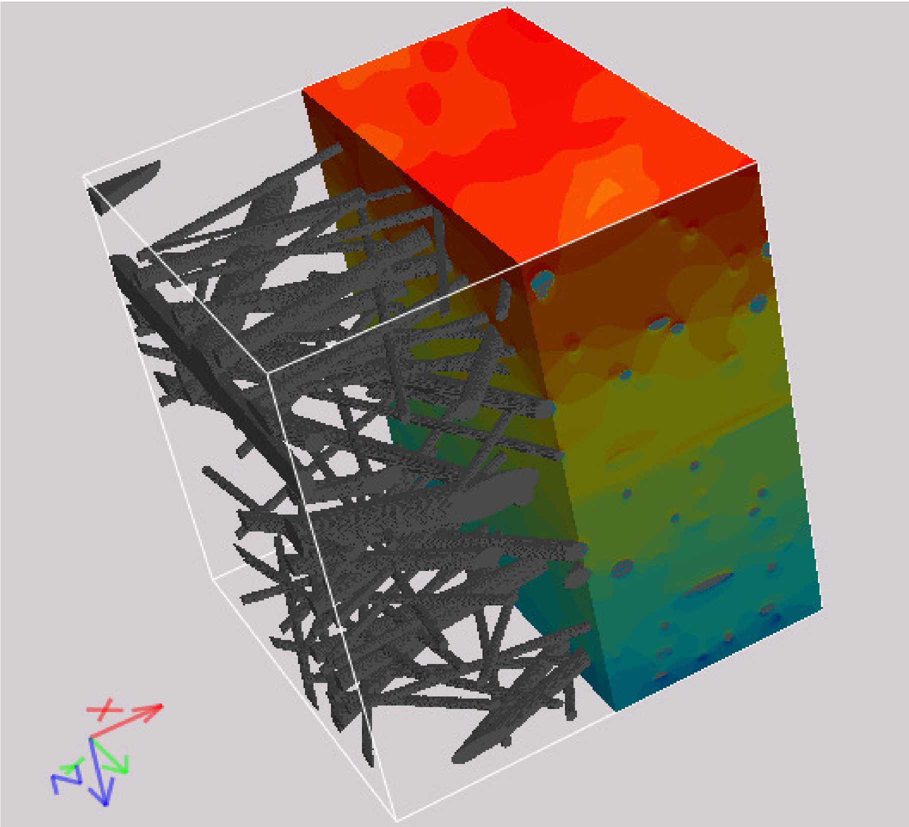
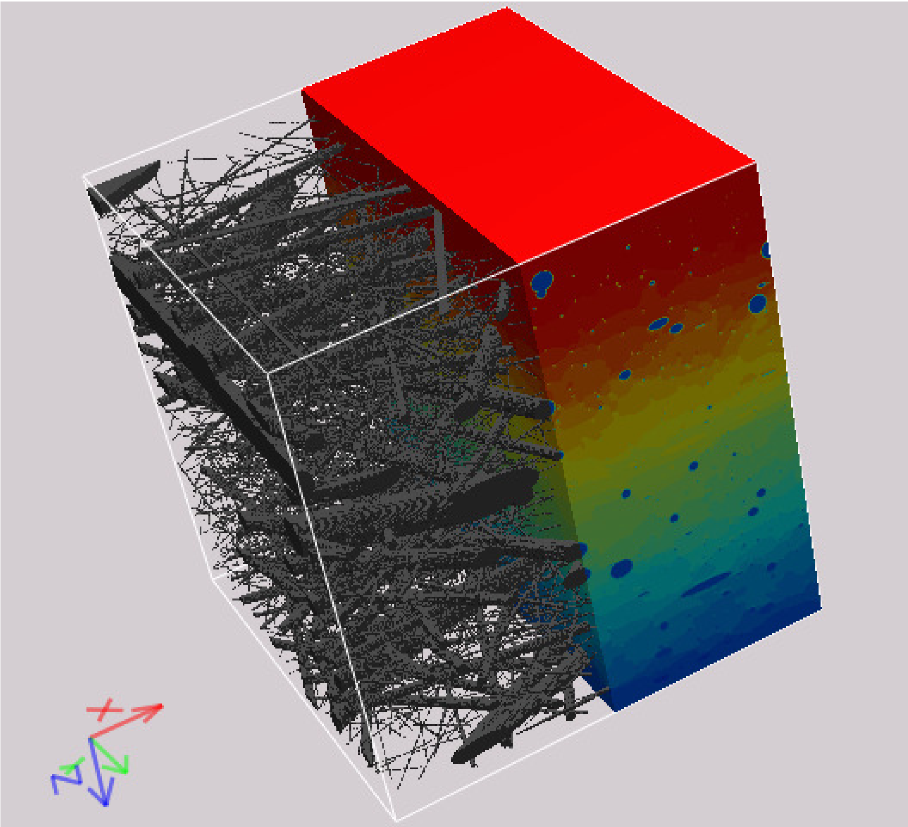
Voxel length: 100nm
Size: 512 x 512 x 512

Results

Pressure distributions



Medium 1



Medium 2

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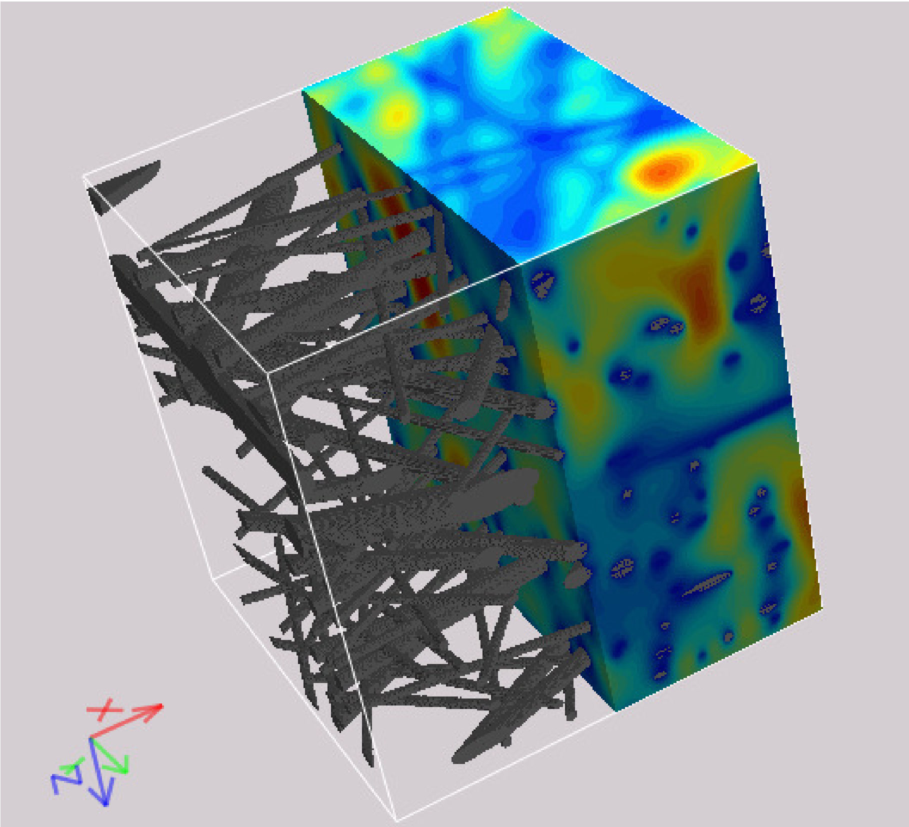
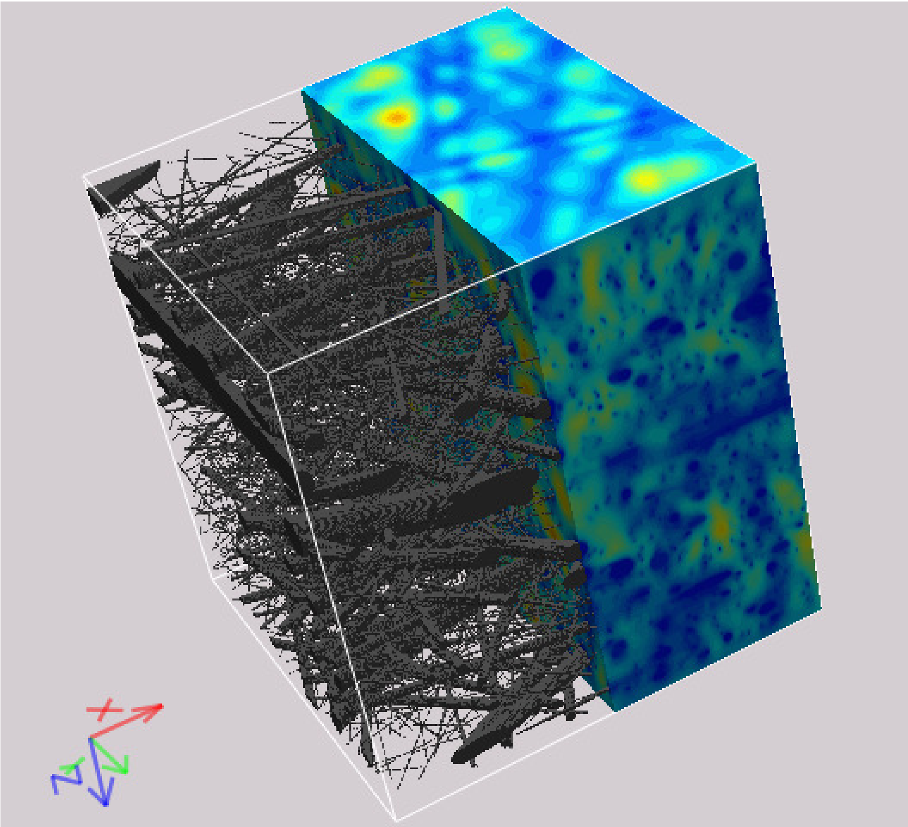
Results

Velocity distributions



Medium 1



Medium 2

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Results

- Permeabilities at 20℃, slip length of 118nm[1]

Media	1	2
Permeability	3.89e-12	6.44e-13

- Filter efficiency

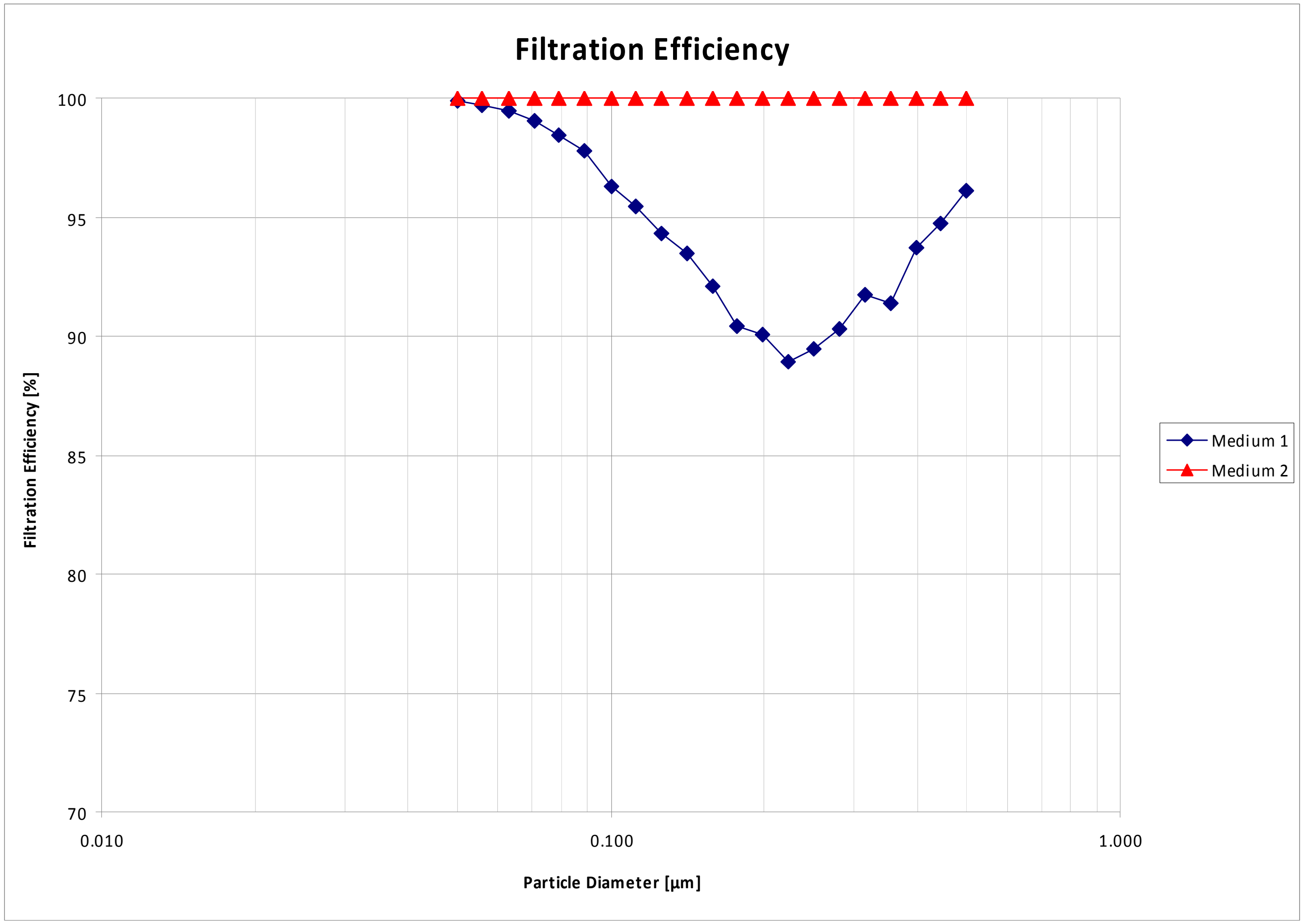
NaCl particles in the range of 50 to 500 nm

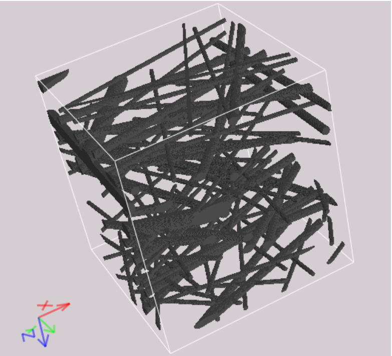
fluid: air at 20°C

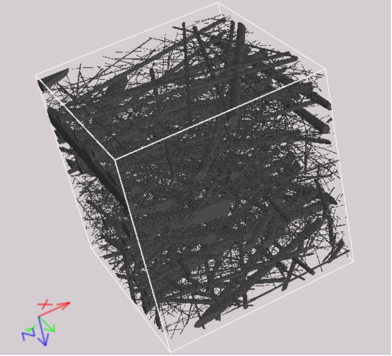
mean flow velocity: 5 cm/s

[1] M.D. Allen, and O.G. Raabe, *Slip correction measurements of spherical solid aerosol-particles in an improved Milikan apparatus,* Aerosol Sci. Technol. 4(3):269-286, 1985.

Results







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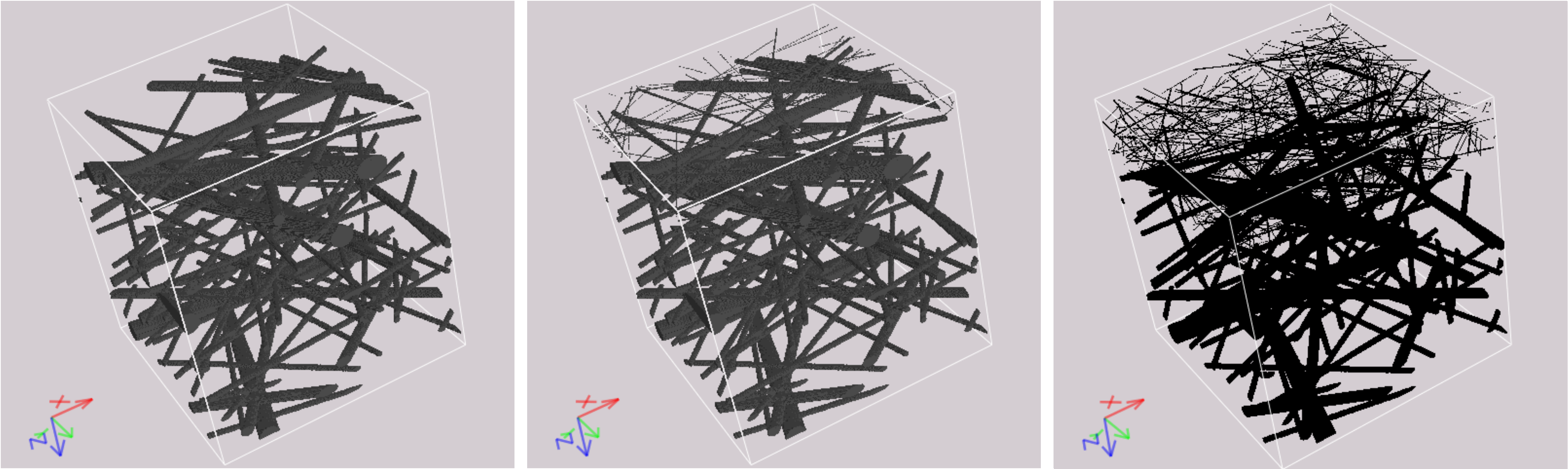
Results

Medium 3: similar to Medium1, but with different random structure generator

Medium 4: Medium 3, top replaced with a nanofiber layer with 2.5μm thickness

Medium 5: Medium 3, top replaced with a nanofiber layer with 10μm thickness



Medium 3 | Medium 4 | Medium 5

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Voxel length: 100nm

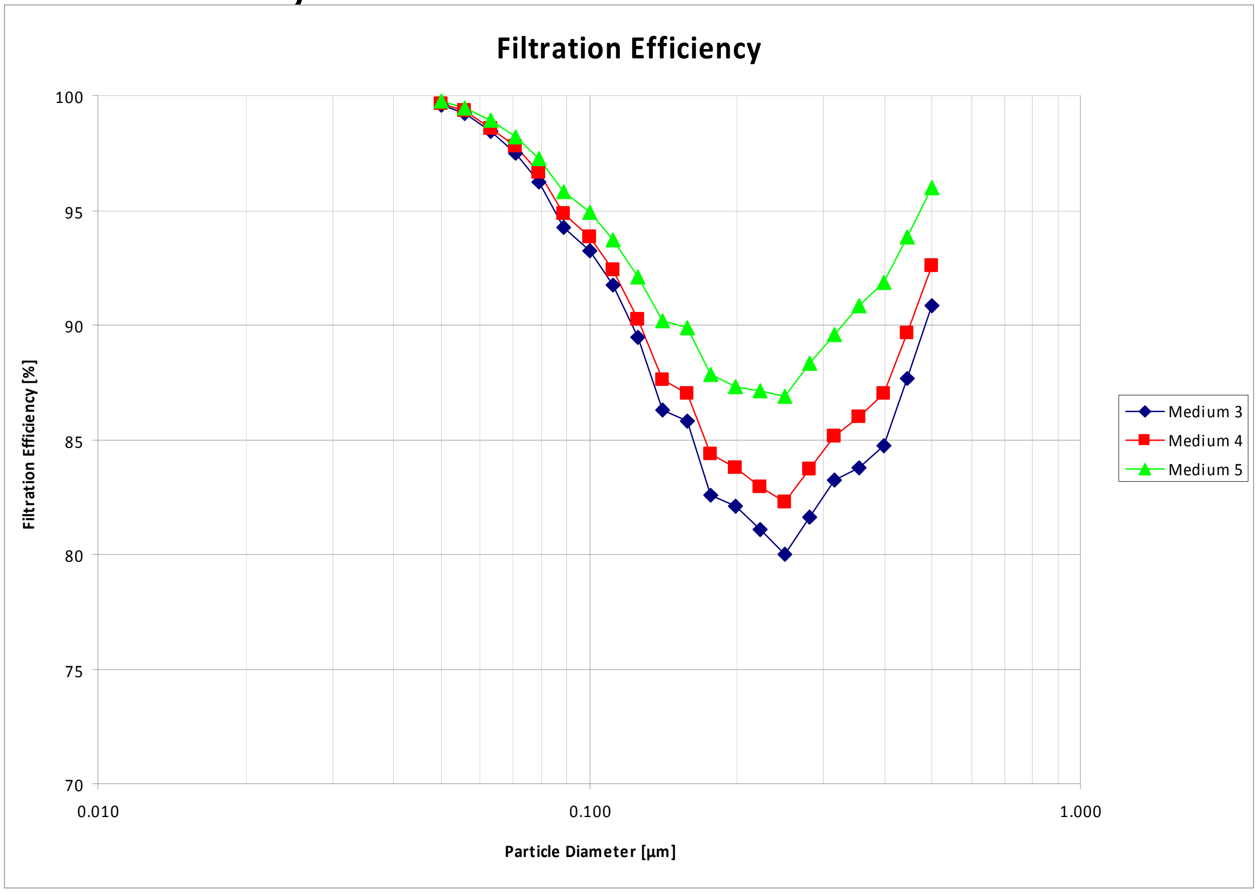
Size: 512 x 512 x 512

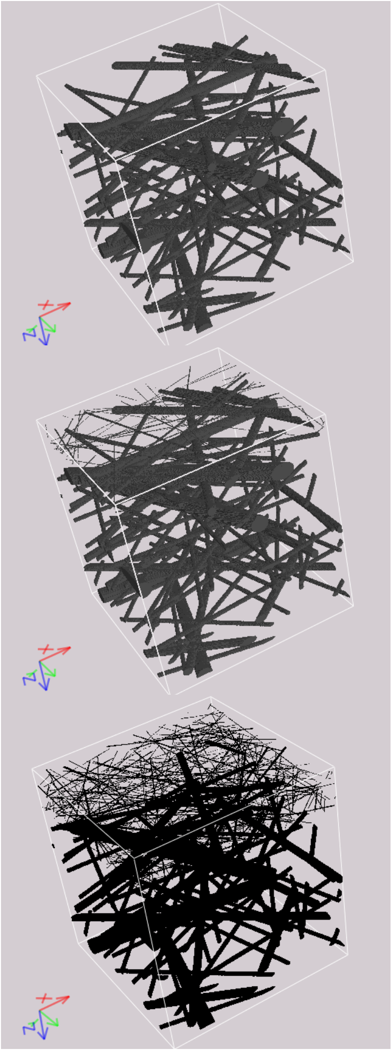
Results

➢ Permeabilities

Media	3	4	5
Permeability	4,35e-12	3,71e-12	2.48e-12

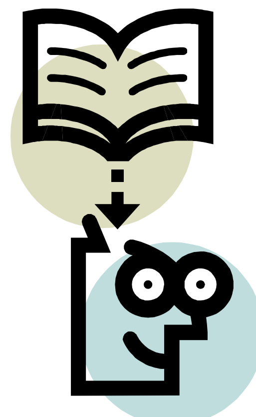
➢ Filter efficiency





Conclusion and outlook

- Numerical simulation of filter media properties
- Comparison between microfiber media and media with additional nanofibers
- Additional nanofibers lead to a big improvement of the filter efficiency
- To simulate the filter lifetime the whole thickness of the media has to be resolved, which leads to much larger geometries.
- Adaptive grid solver under development for GeoDict FilterDict software suite.



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Find out more:

www.geodict.com

Thank you for you attention!

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