GeoDict and FilterDict: Software for the Virtual Material Design of new Filter Media

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New Developments in Filtration Technology

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ITWM

Fraunhofer Institut Techno- und Wirtschaftsmathematik

Overview

I. Virtual Material Design Cycle

II. Filter Media

III. Fluid & Electric Field

IV. Dirt model & dirt motion

V. Deposition

VI. Life time

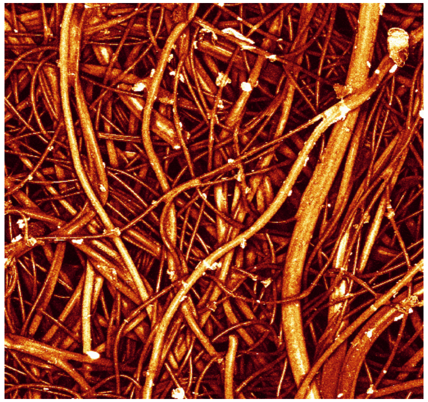
VII. Nano model

VIII. Summary

I. The Virtual Filter Material Design Cycle

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

REM



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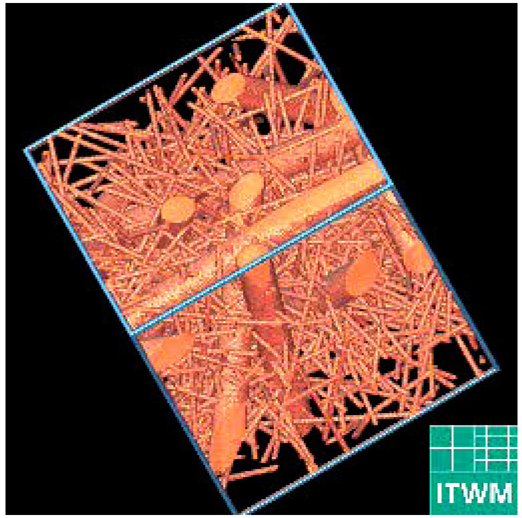
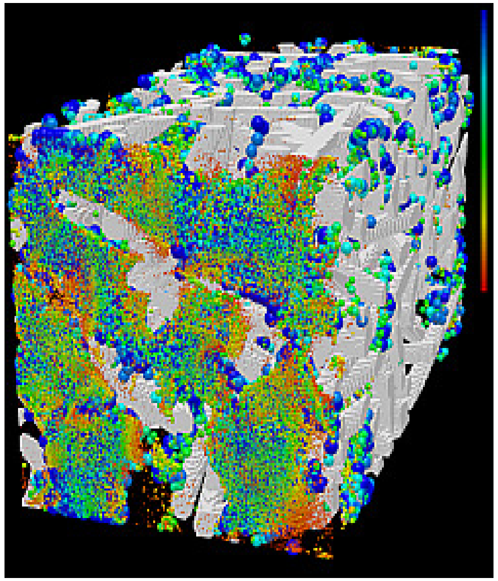




Clogged nonwoven

Overview

II. What constitutes ITWMs designable Virtual Materials?

The **real media**, porous or composite [e.g. nonwoven vs. carbon fiber-enforcement]

The mathematical **model** with (few) parameters [e.g. fiber diameter, etc.]

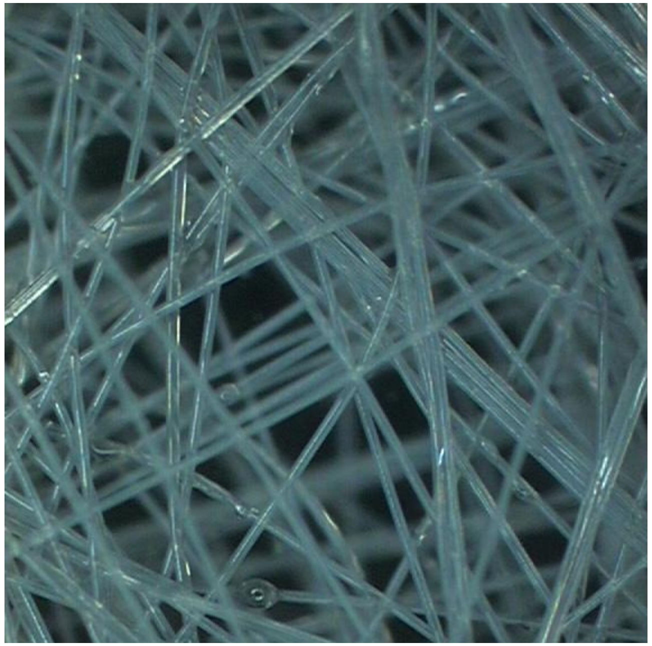
The **Realizations** in volume images, **independent of the model**

The **Validation**

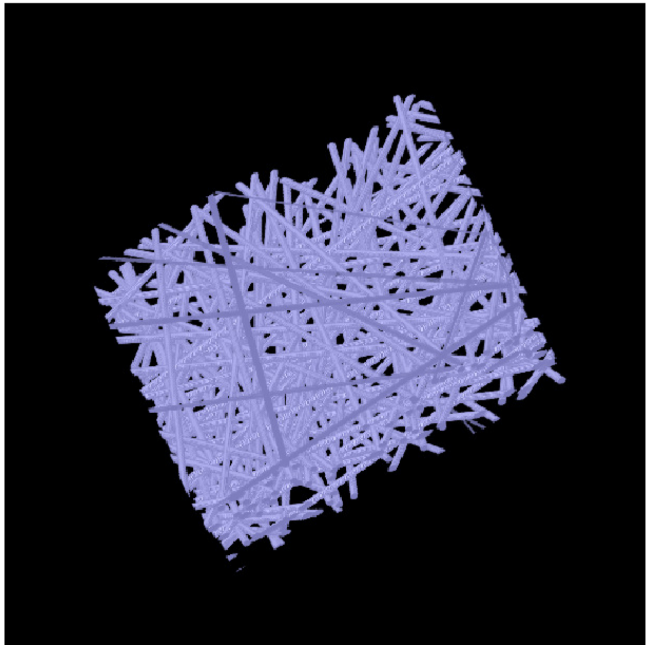
- inspection [2d & 3d visualization, comparison with microscopy & tomography]
- geometric analysis [e.g. porosity, pore size distribution, etc.]
- agreement of computed properties for existing media

The **Design;** based on model parameters, not the volume images

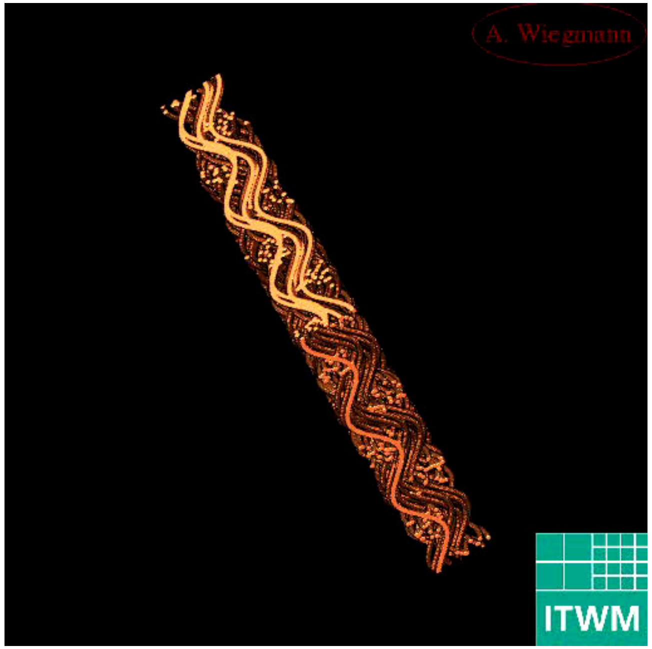
II. Material Models for Nonwoven, Woven & Layers



Microscopy



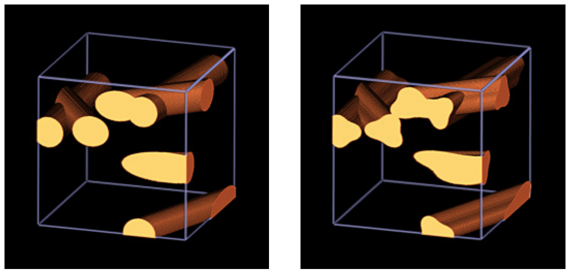
Nonwoven model



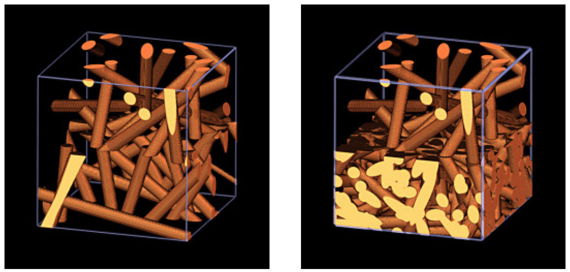
Multifilament woven model

Possible variations: for example

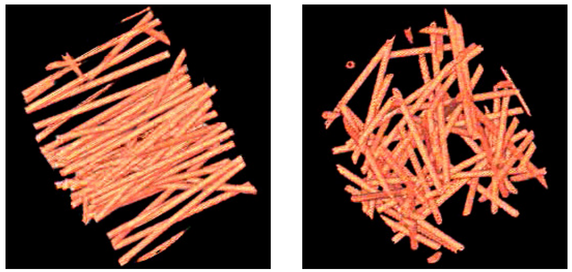
- Cross sections



- Layers

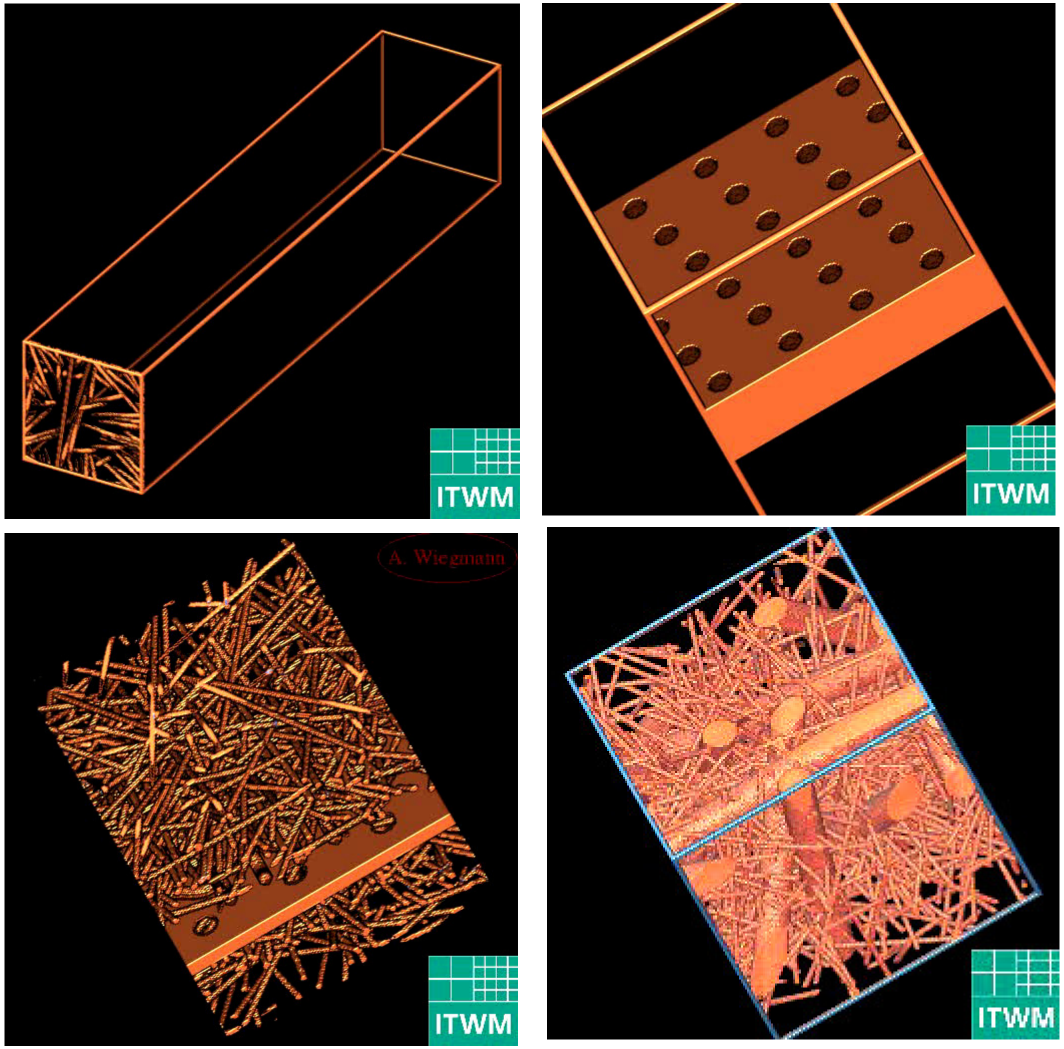


- Anisotropy



II. Simulation and Design Parameters for Filter Media

1. Nonwoven model
2. Sinter model
3. Layers
4. Layer thicknesses
5. Porosity
6. Fiber diameters
7. Fiber anisotropy
8. Fiber shapes
9. Fiber overlap
10. Fiber crimp
11. Fiber length
12. …



Overview

III. Fluid & Electric Field:

For very sparse particles, the influence of the particles on the flow field and on the electrical field can be neglected.

The fluid enters the model through its viscosity μ. For example,

Oil at -25°C : μ = 1.50e+0 kg/(m s)

Blood at 22°C : μ = 2.00e-2 kg/(m s)

Air at 20°C : μ = 1.84e-5 kg/(m s)

Mean flow velocity is an output of the model. It is controlled by the pressure drop, which enters the model as a volume force, e.g. for 200 Pa, sample thickness L:

$$f = \frac{200\,Pa}{L}$$

Electric field enters the model as charges on fiber surfaces

III. Flow: Navier-Stokes-Brinkmann equations

$$
\begin{aligned}
-\mu\Delta\vec{u} + \nabla\vec{u}\cdot\vec{u} + \kappa^{-1}\vec{u} + \nabla p &= \vec{\mathrm{f}} \text{ (momentum balance)} \\
\nabla\cdot\vec{u} &= 0 \text{ (mass conservation)} \\
\vec{u} &= 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)}
\end{aligned}
$$

$\vec{\mathrm{f}} = (0, 0, f)$: force in flow(z)-direction,

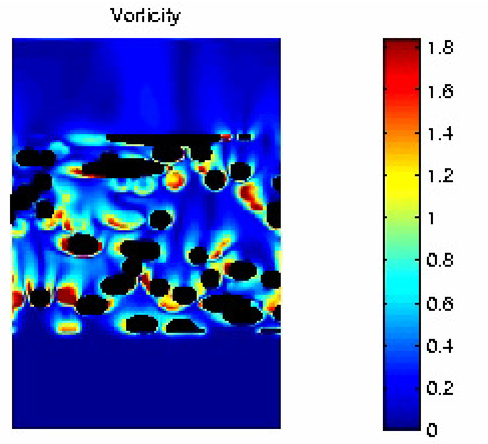
κ : porous voxel permeability,

$\vec{u}$: velocity,

μ : fluid viscosity,

p : pressure and

Γ : surfaces of fibers or deposited particles.



Cross section views of vorticity

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

III. Electric field: Poisson equation for the potential

$$\Delta u = \rho\chi(\delta\Omega): \text{ Poisson equation}$$
$$\vec{\mathbf{E}} = \nabla u : \text{ Field equation}$$

$\delta\Omega$: boundary of domain occupied by fibers (surface),

ρ : source strength,

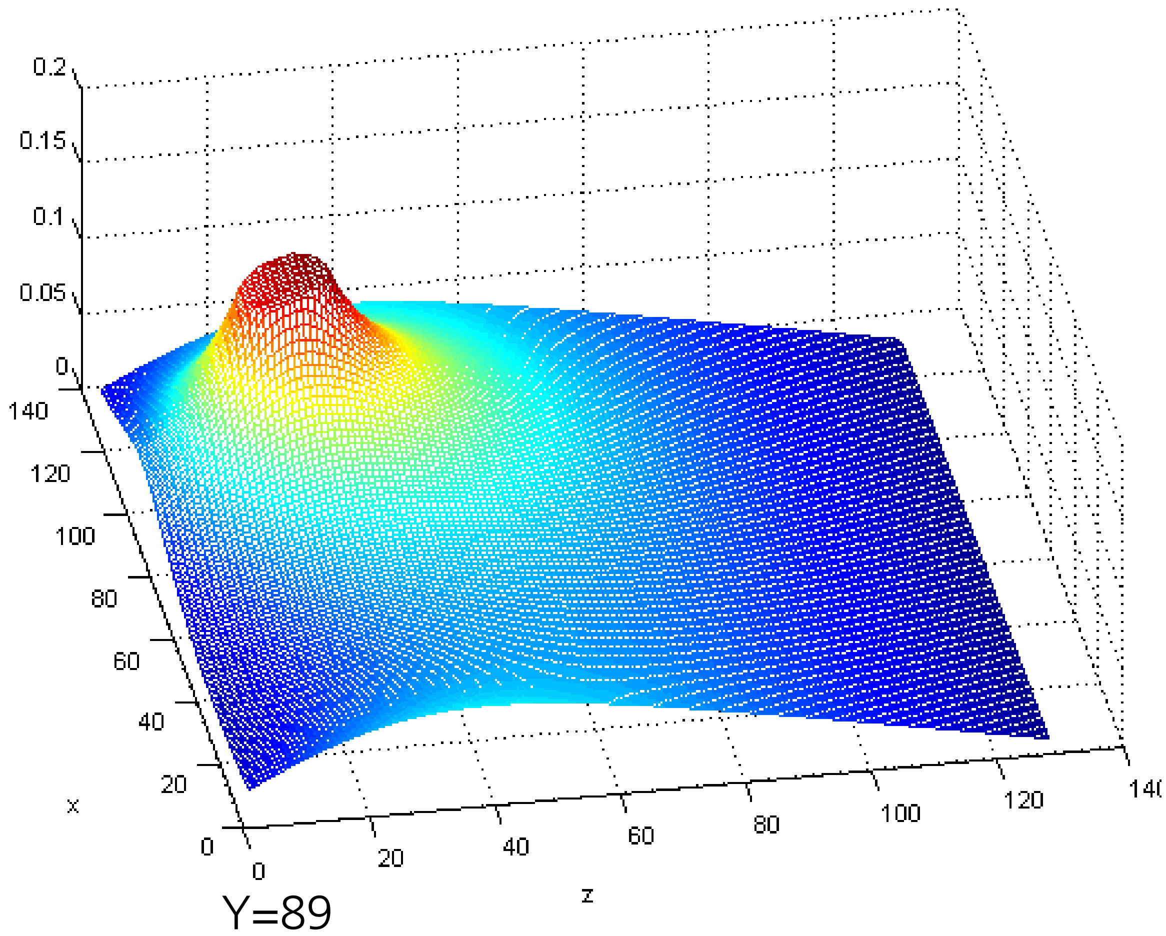
χ : surface Dirac delta function,

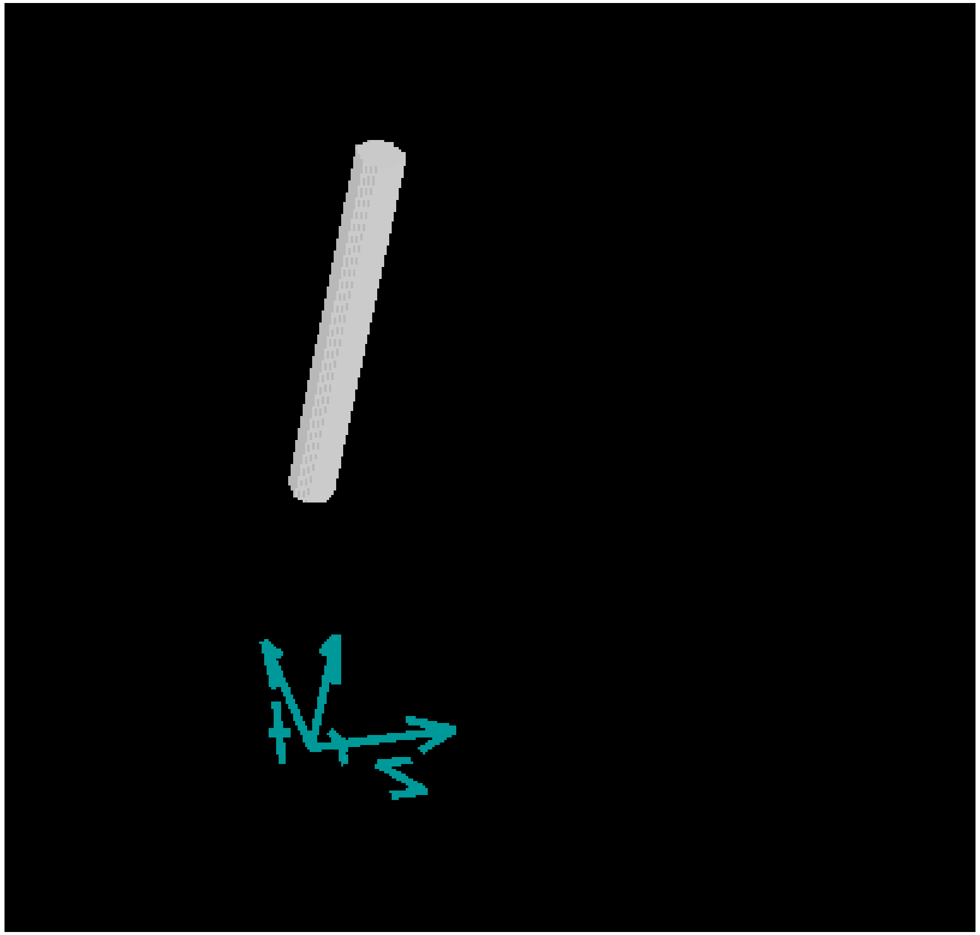
u : the electric potential,

$\vec{\mathbf{E}}$: the electric field (the gradient of the potential).

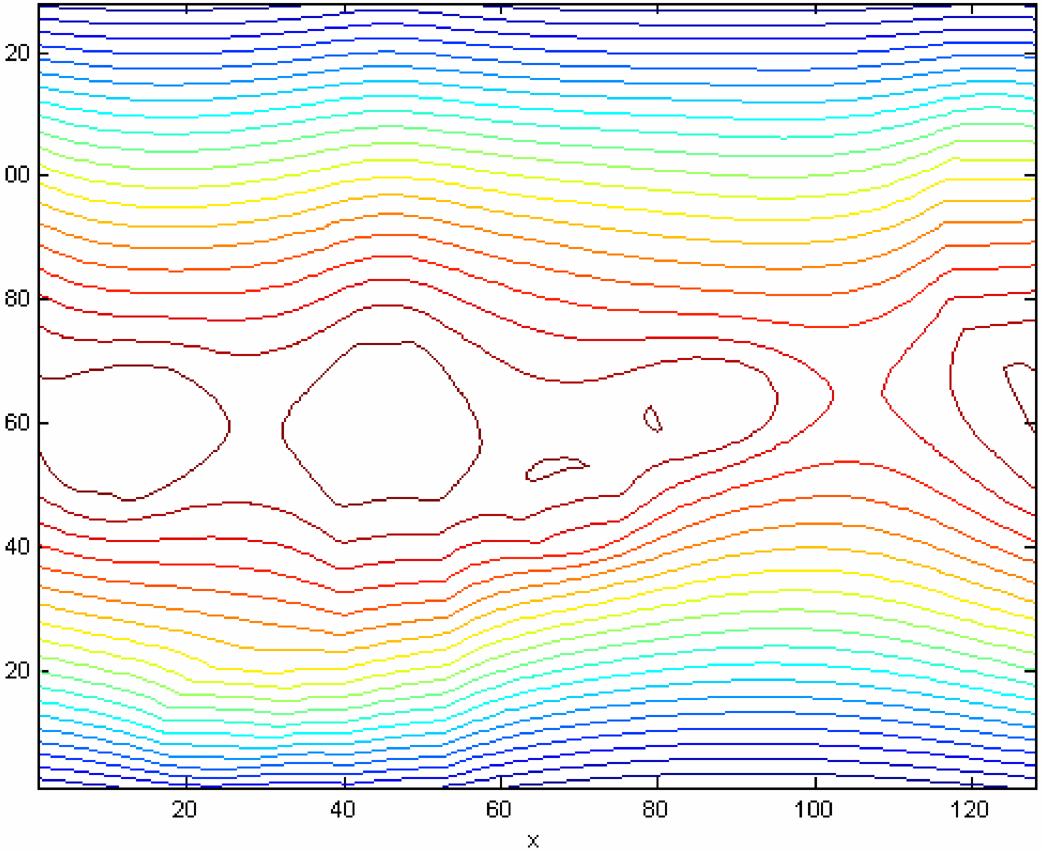
The field can be solved with periodic boundary conditions in the lateral direction and zero potential at appropriately chosen distances outside the media.

III. Electric potential (cross section Y=89) for a single fiber

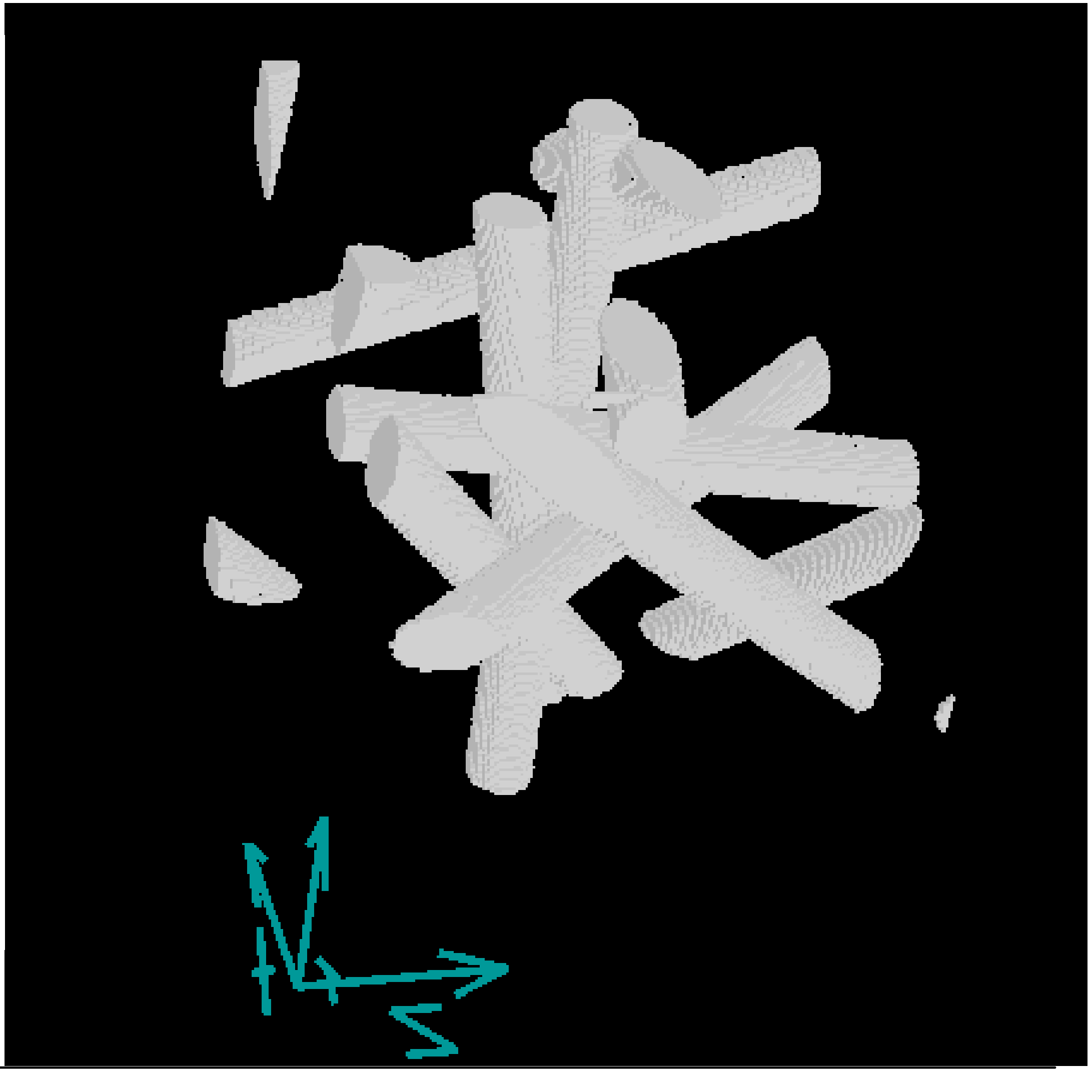




III. Electric potential (contour Y=89) for random fibers



Y=89



Overview

IV. Dirt Model

- probability distribution of diameters of spherical particles of given material
- Size and material determine the particle mass
- Particles move with fluid via friction
- Particles move diffusively in fluid dependent on size and temperature
- Particles move based on their own charge and the electric field

IV. Lagrangian description of particle motion

$$\frac{d\vec{v}}{dt} = -\gamma \times (\vec{v}(\vec{x}) - \vec{v}_\circ(\vec{x})) + \frac{Q\vec{E}_\circ(\vec{x})}{m} + \sigma \times \frac{d\vec{W}(t)}{dt}$$

Friction with fluid — Electric attraction — Diffusive motion

$$\frac{d\vec{x}}{dt} = \vec{v}$$

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

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

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

t:	time
$\vec{x}$:	particle position
$\vec{v}$:	particle velocity
R:	particle radius
m:	particle mass
Q:	particle charge
T:	ambient temperature
k_B:	Boltzmann constant
$d\vec{W}(t)$:	3d probability (Wiener) measure
$\vec{E}_\circ$:	electric field
$\vec{v}_\circ$:	fluid velocity
ρ:	fluid density
μ:	fluid viscosity

Overview

V. Mechanisms of filtration

Particle impact by:

A: direct interception

B: inertial impaction

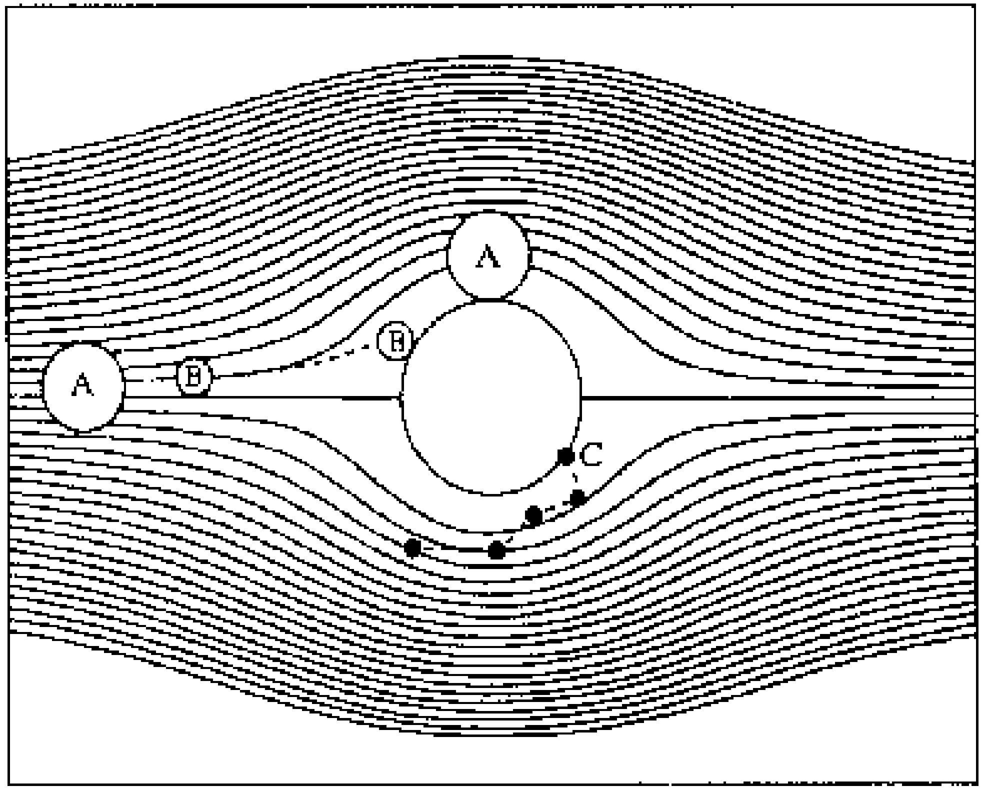
C: diffusional deposition

D: electrostatic attraction

E: sieving

F: clogging

G: other effects (gravity,...)



Detect collisions of particles with fibers and previously deposited particles!

V. 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

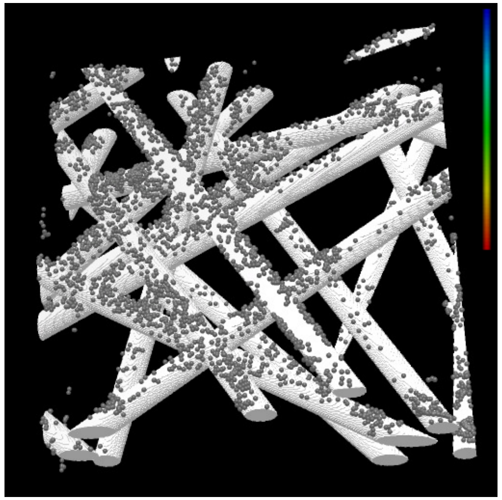
D) Efficiency:

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:
Adhesion
- Inertial impact
- Diffusion
- **Electrostatic attraction**

Sieving

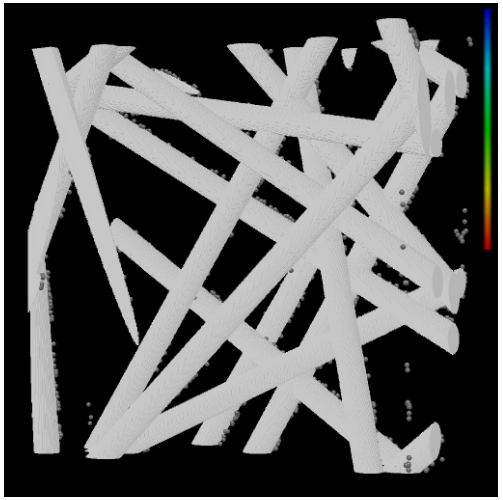
V. Simulation results with(out) electric surface charge

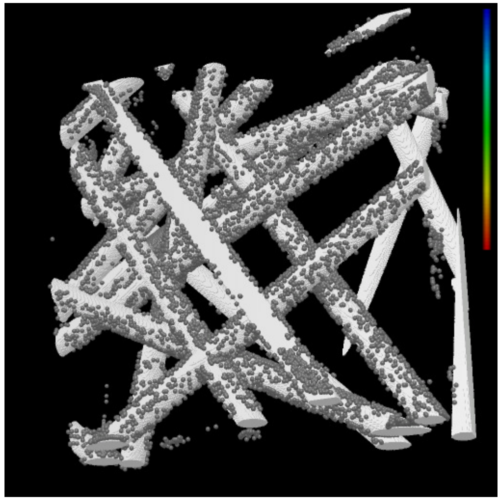


Simulation result without the influence of electric surface charges on the fibers.

Front view

back view



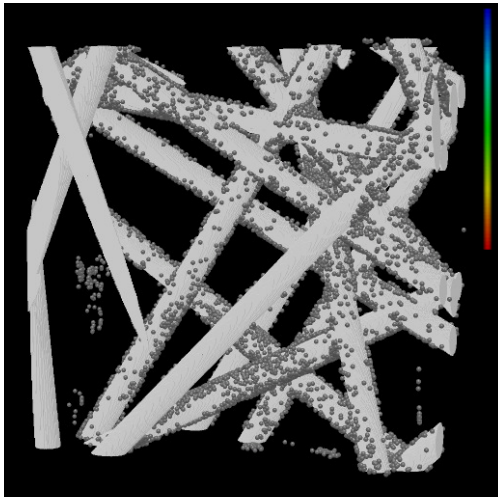


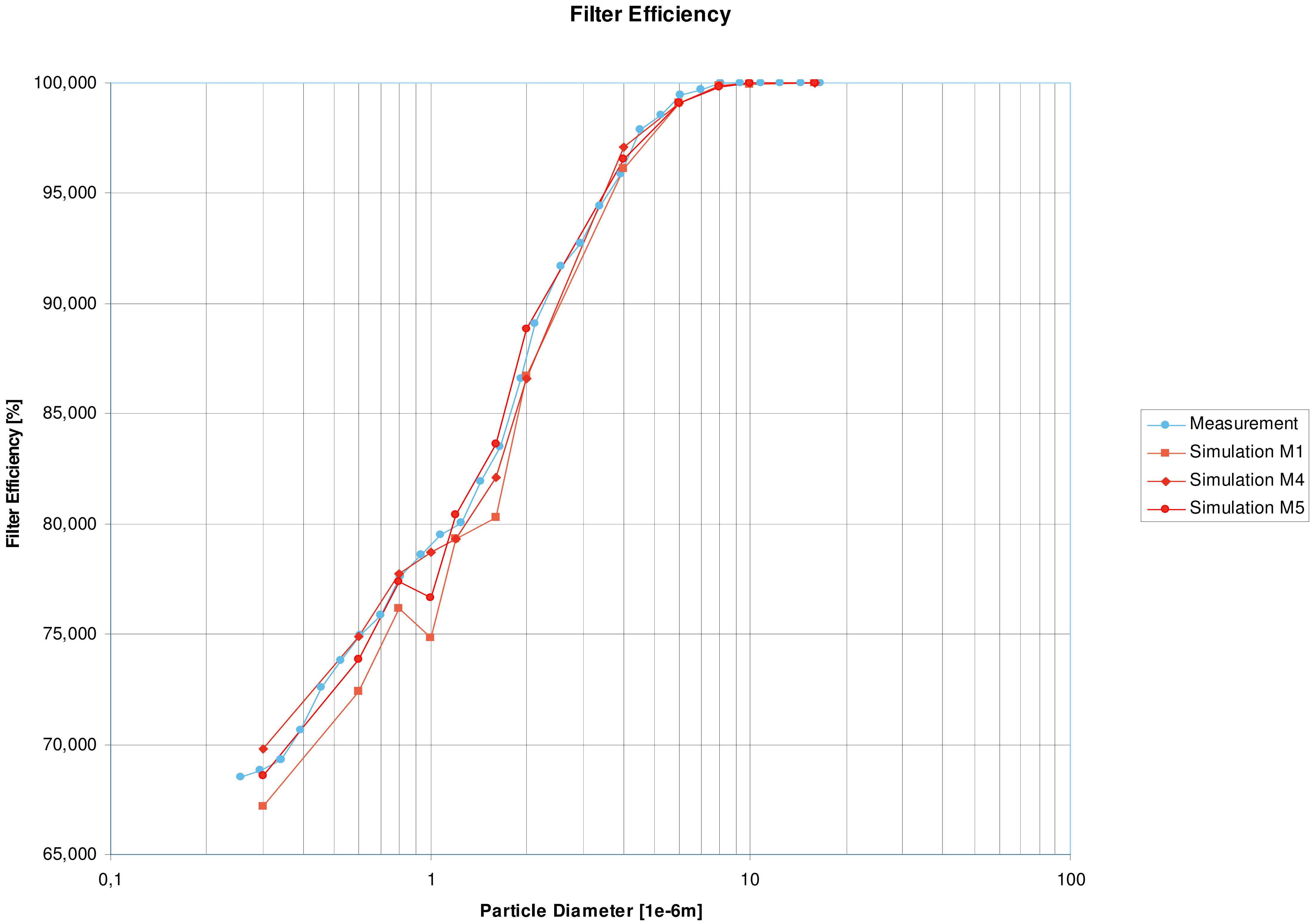
Simulation result under the influence of electric surface charges on the fibers.

Retention rate increased by about 50%!

Front view

back view

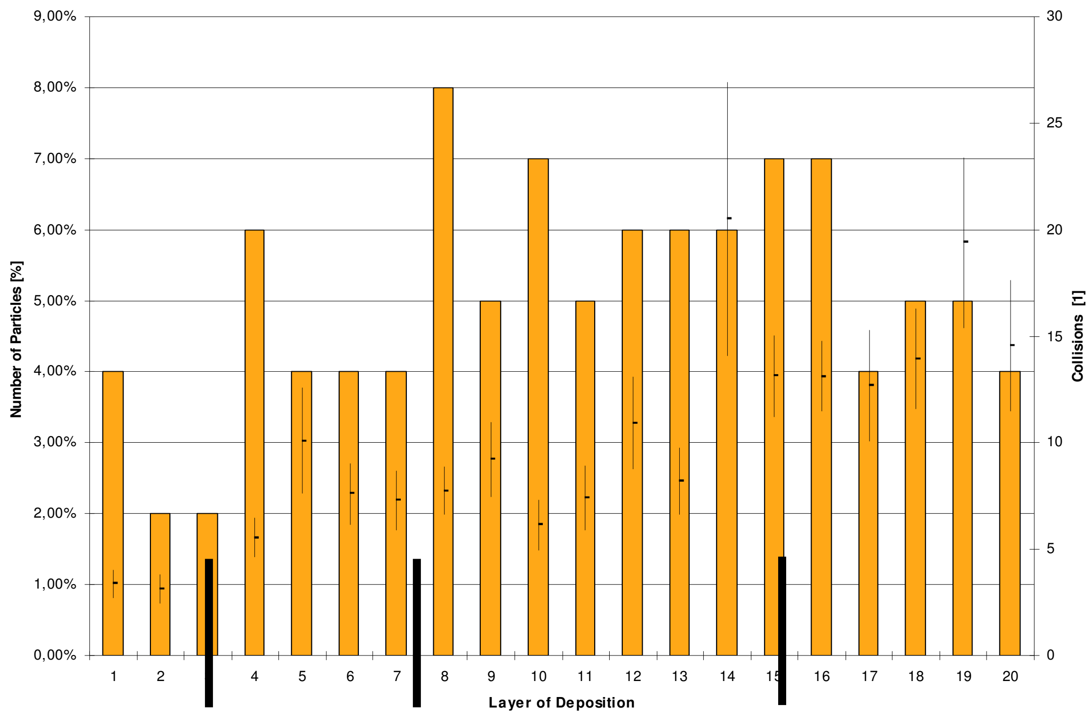


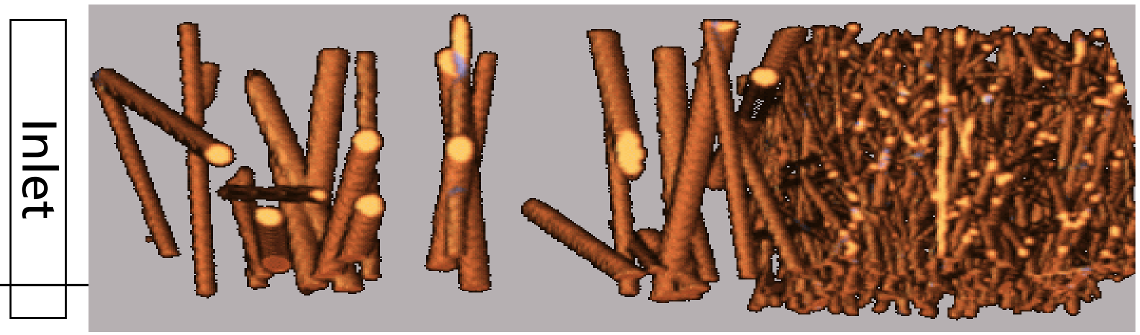


Filter Efficiency
100,000
95,000
90,000
85,000
80,000
75,000
70,000
65,000
Filter Efficiency [%]
0,1
1
10
100
Particle Diameter [1e-6m]
Measurement
Simulation M1
Simulation M4
Simulation M5

V. 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:





Overview

VI. Decoupling of fluid flow and particle motion simulations

Assume particle density is very low, then:

- Particles move and deposit independently, they do not collide in the air.
- When many particles have deposited, the fluid flow is significantly altered.
- So, for clogging, the volume image is periodically updated by deposited particles and the flow field in this volume image is recomputed.
- Subsequent particle motion is computed based on the updated flow field, particle deposition is based on the updated volume image.

VI. Filter Life Time Model

G) Multipass:
Unfiltered particles change particle size distribution

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:

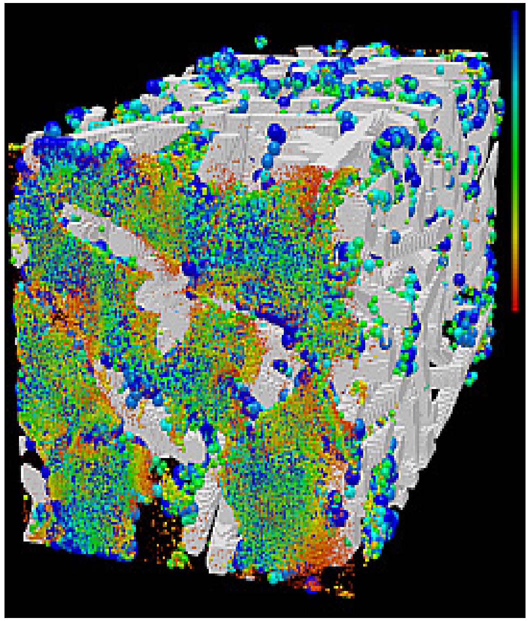
Flow & pressure drop:	B & C
Electrostatic field:	C
Friction:	A & B
Diffusion:	A & B
Collision:	A & C
Adhesion:	A & C
Electrostatic attraction:	A & C
Particle Paths:	A, B & C

E) Deposition due to:
Adhesion
- Inertial impact
- Diffusion
- Electrostatic attraction

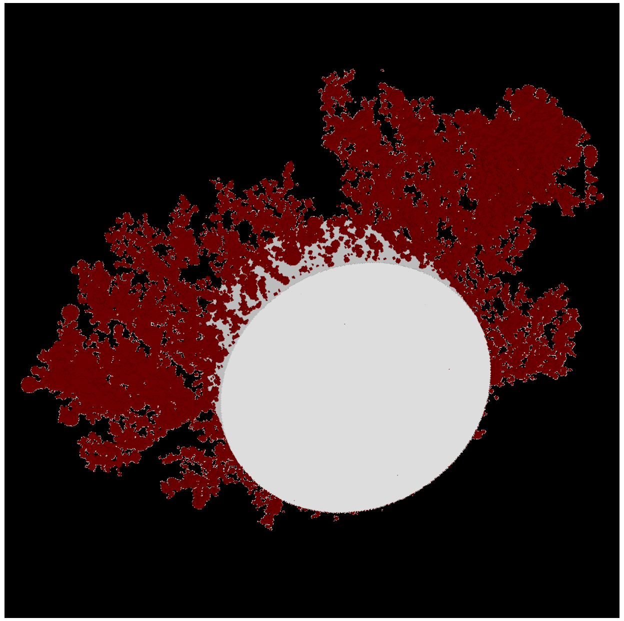
Sieving

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

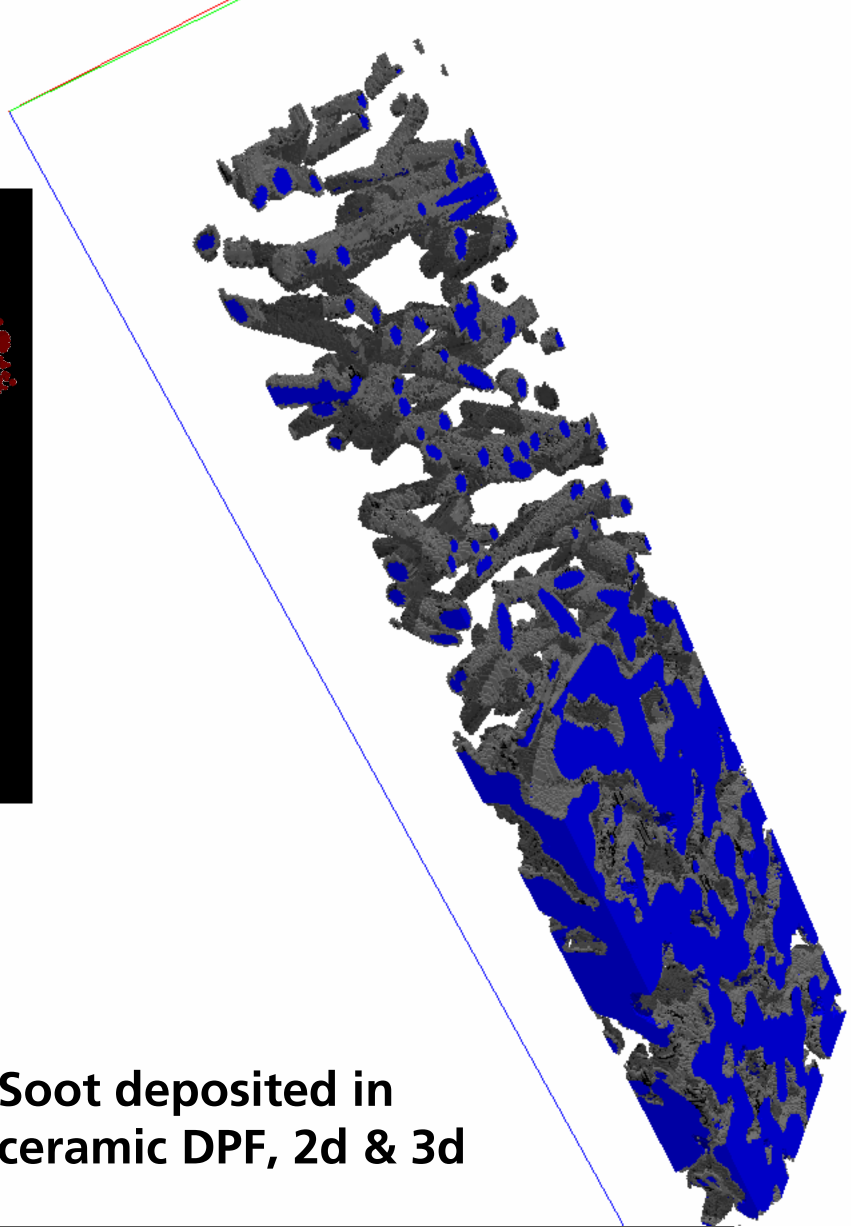
VI. Clogging of nonwoven & ceramic; dendrites on single fiber



Clogged nonwoven



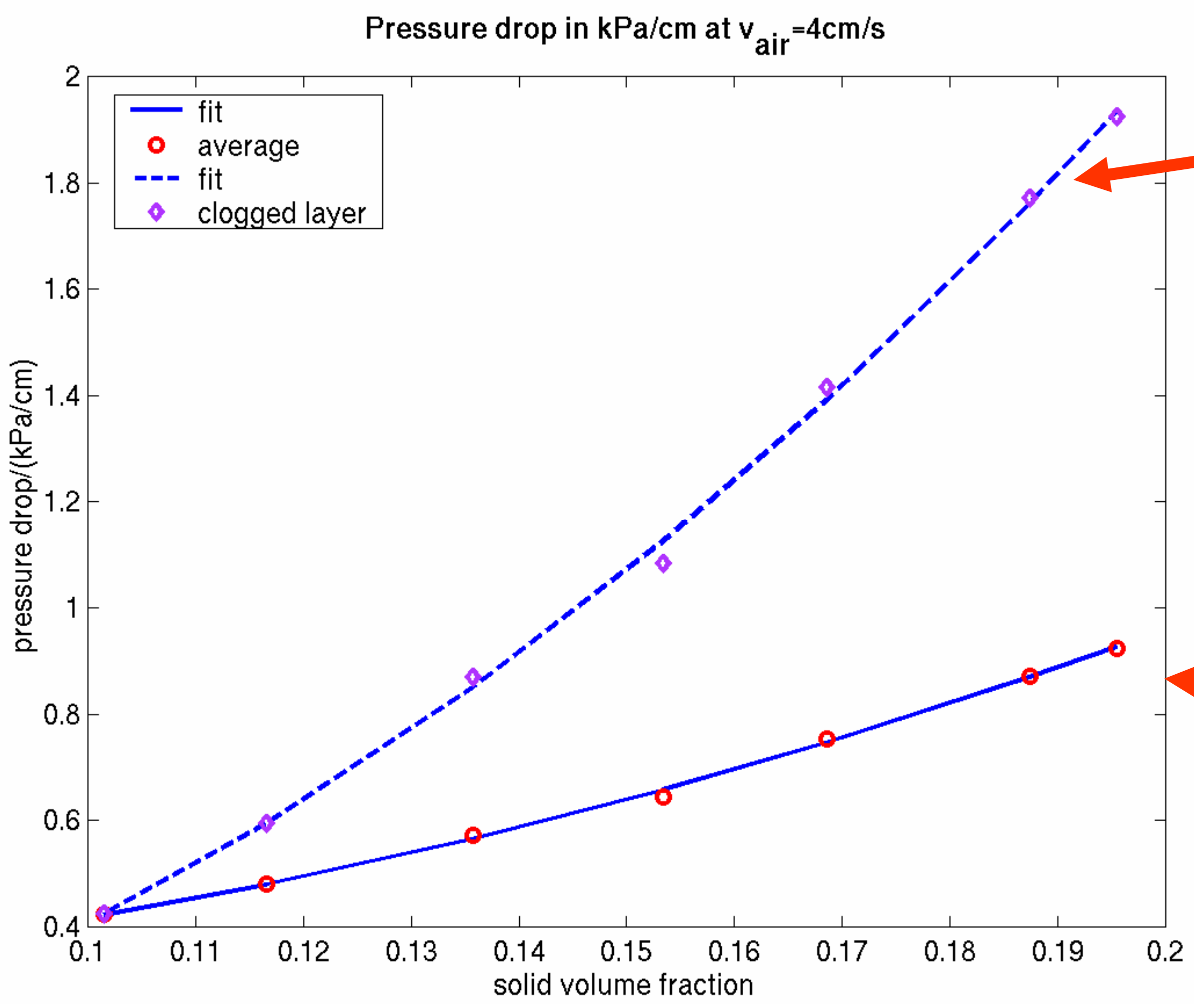
Soot deposition on a single fiber



Soot deposited in ceramic DPF, 2d & 3d

Deposition occurs on fibers and on previously deposited particles

VI. Time Dependent Pressure Drop



in the loaded portion of the sample

on average over the whole sample

VIII. Summary

Complex geometry of real textiles ⇨ high resolution volume image

"Slow" flow ⇨ Stokes equations

Highly diluted ⇨ Particles do not modify fields

Material & Dirt models

Fluid & electric models

Deposition & Clogging models

Output are models, predicted filter properties, and optimized material geometries

Models & equations are fairly standard. Completeness of approach is new.

Difficulties: knowledge of parameter settings, high resolution for large cutouts.

Goals: "generic agreement with reality", little need for recalibration for new application areas. Material must be manufactured; predictions must be verified.

Development of the Software

- GeoDict virtual material generator:
- http://www.geodict.com
- geodict@itwm.fraunhofer.de
- **FilterDict filtration simulation (GeoDict module):**
- **http://www.geodict.com/filterdict**
- **filterdict@itwm.fhg.de**

GeoDict2006 – development teams

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