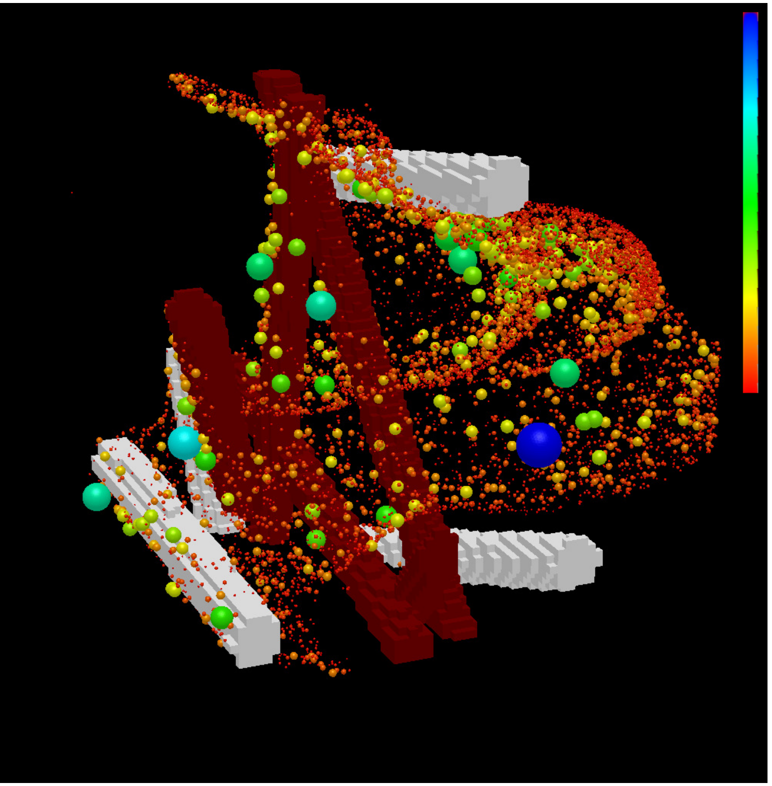
Computer simulation of air filtration including electric surface charges in three-dimensional fibrous microstructures



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Filtech Europa 2005

Wiesbaden, October 13th, 2005.

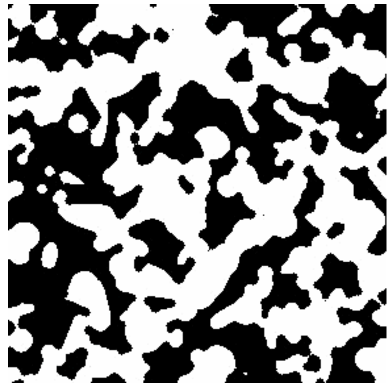
Fraunhofer Institut Techno- und Wirtschaftsmathematik

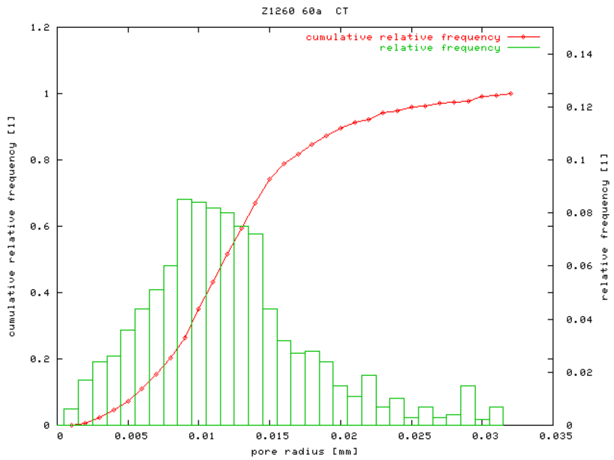
The virtual filter media design cycle

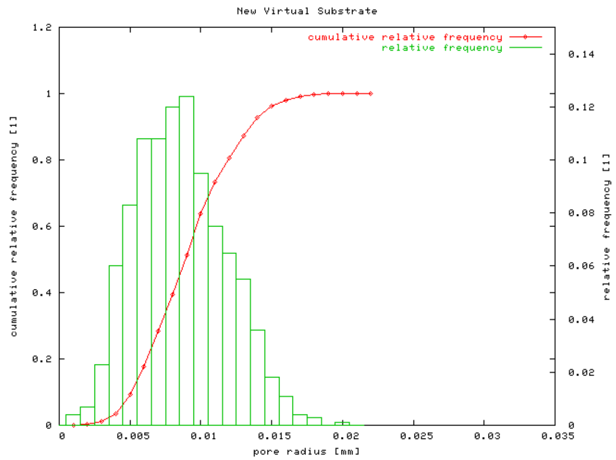
1. Identify parameters for real, existing material
2. Generate 3d geometry for parameters
3. Solve Stokes-Brinkmann equations
4. Solve electric potential
5. Solve particle motion & deposition
6. Compute filter efficiency or filter life time
7. Modify material parameters
8. Go back to 2.

REM

Generated







Pore size distributions

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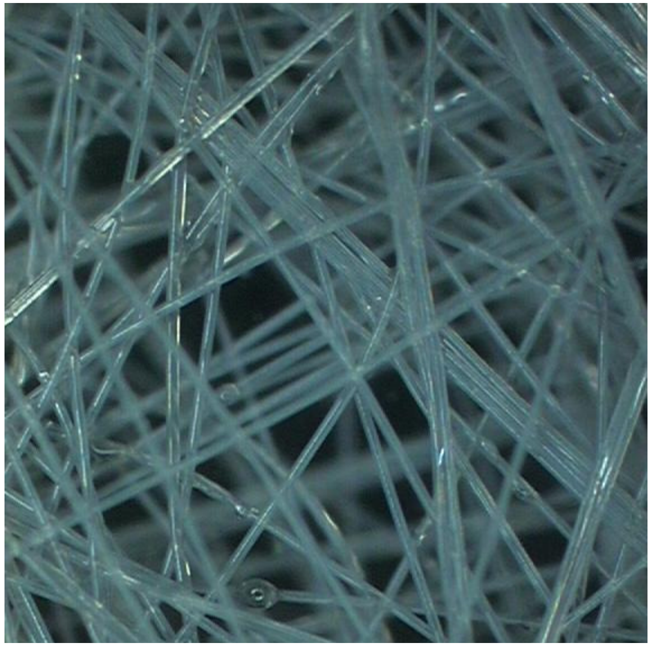
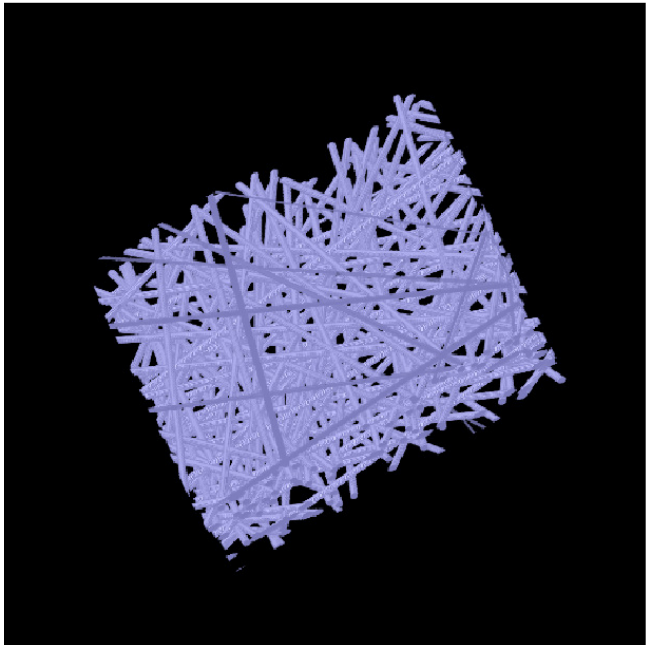
October 13th, 2005

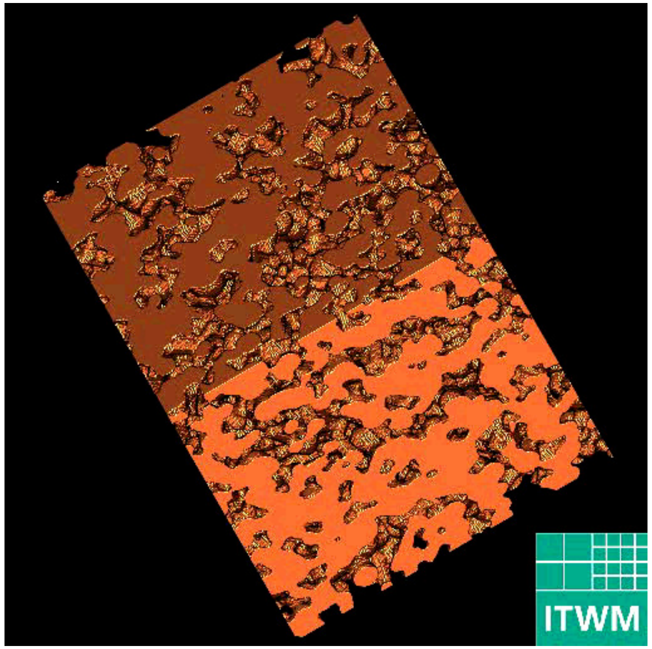
Material Models



Microscopy



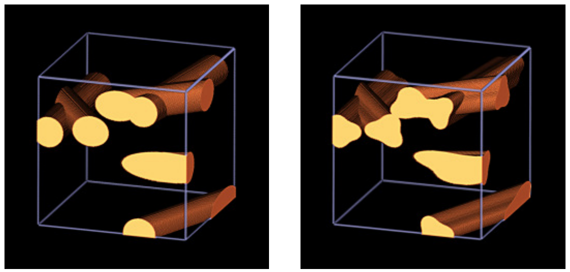
Fiber model



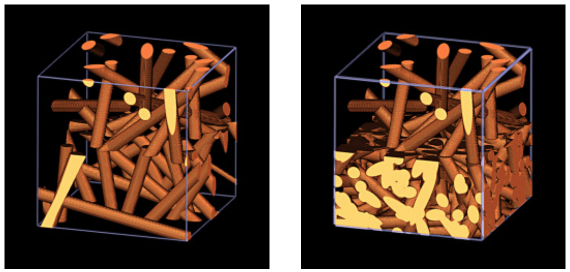
Sinter model

Possible variations: for example

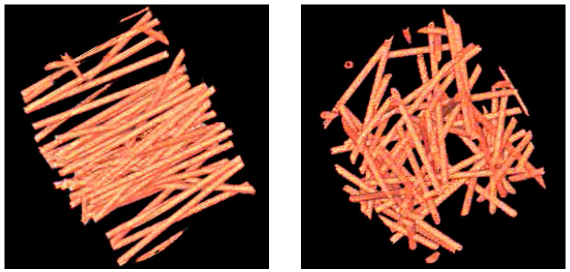
- Cross sections



- Layers

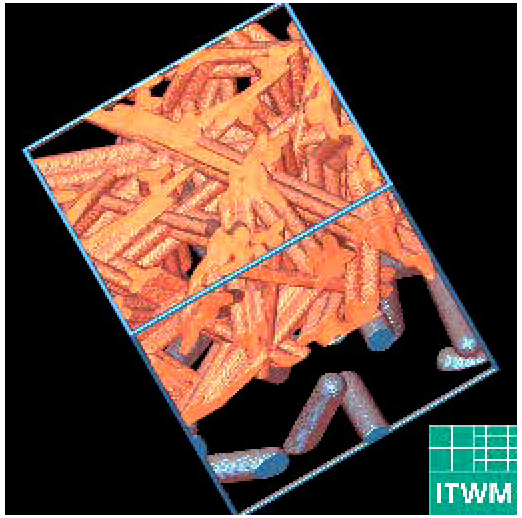


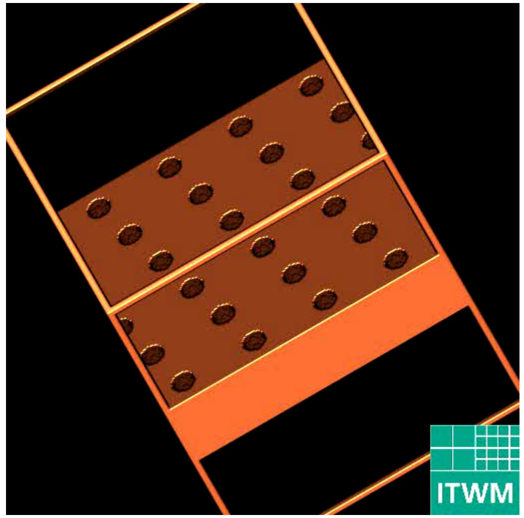
- Anisotropy

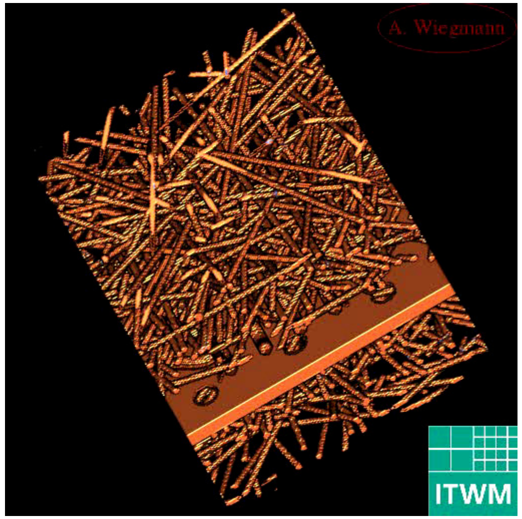


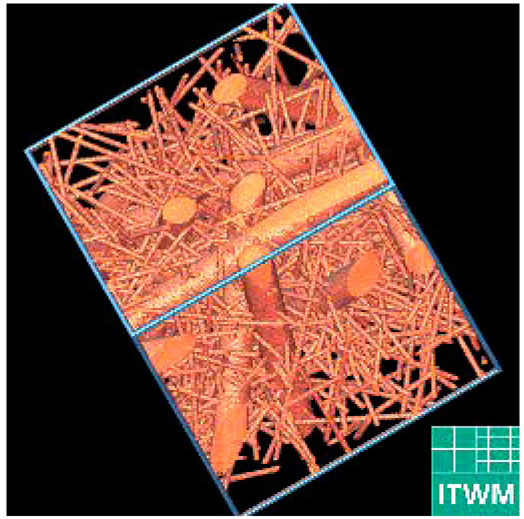
Simulation and Design Parameters for Filter Media

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. …









Flow: Stokes-Brinkmann equations

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

- $\vec{f}$: force in direction of the flow,
- κ : porous voxel permeability,
- $\vec{u}$: velocity,
- μ: fluid viscosity,
- p: pressure and
- Γ: 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.

Electric field: Poisson equation for the potential

$$\Delta u = \rho\chi(\partial\Omega) \quad : \text{ singular force Poisson equation}$$

$$\vec{E} = \nabla u \quad : \text{the electric field}$$

- u : potential
- χ : characteristic function of the fiber boundary

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

Lagrangian description of particle motion

$$
\begin{aligned}
\frac{d\vec{x}}{dt} &= \vec{v} \\
d\vec{v} &= -\gamma \times (\vec{v} - \vec{v}_\circ(\vec{x}(t)))\, dt + \frac{Q\vec{E}}{m} dt + \sigma \times d\vec{W}(t) \\
\gamma &= 6\pi\rho\nu\frac{R}{m} \\
\sigma^2 &= \frac{2\kappa T\gamma}{m} \\
\left\langle dW_i(t), dW_j(t) \right\rangle &= \delta_{ij} dt
\end{aligned}
$$

$\vec{x}$:	particle position
R:	particle radius
m:	particle mass
Q:	particle charge
$\vec{E}$:	electric field
$\vec{v}$:	particle velocity
$\vec{v}_\circ$:	fluid velocity
$d\vec{W}(t)$:	three-dimensional Wiener measure
ρ:	fluid density
ν:	fluid viscosity

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:
Inertial impact + adhesion
Diffusion + adhesion
E-static attraction +adhesion
Sieving

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

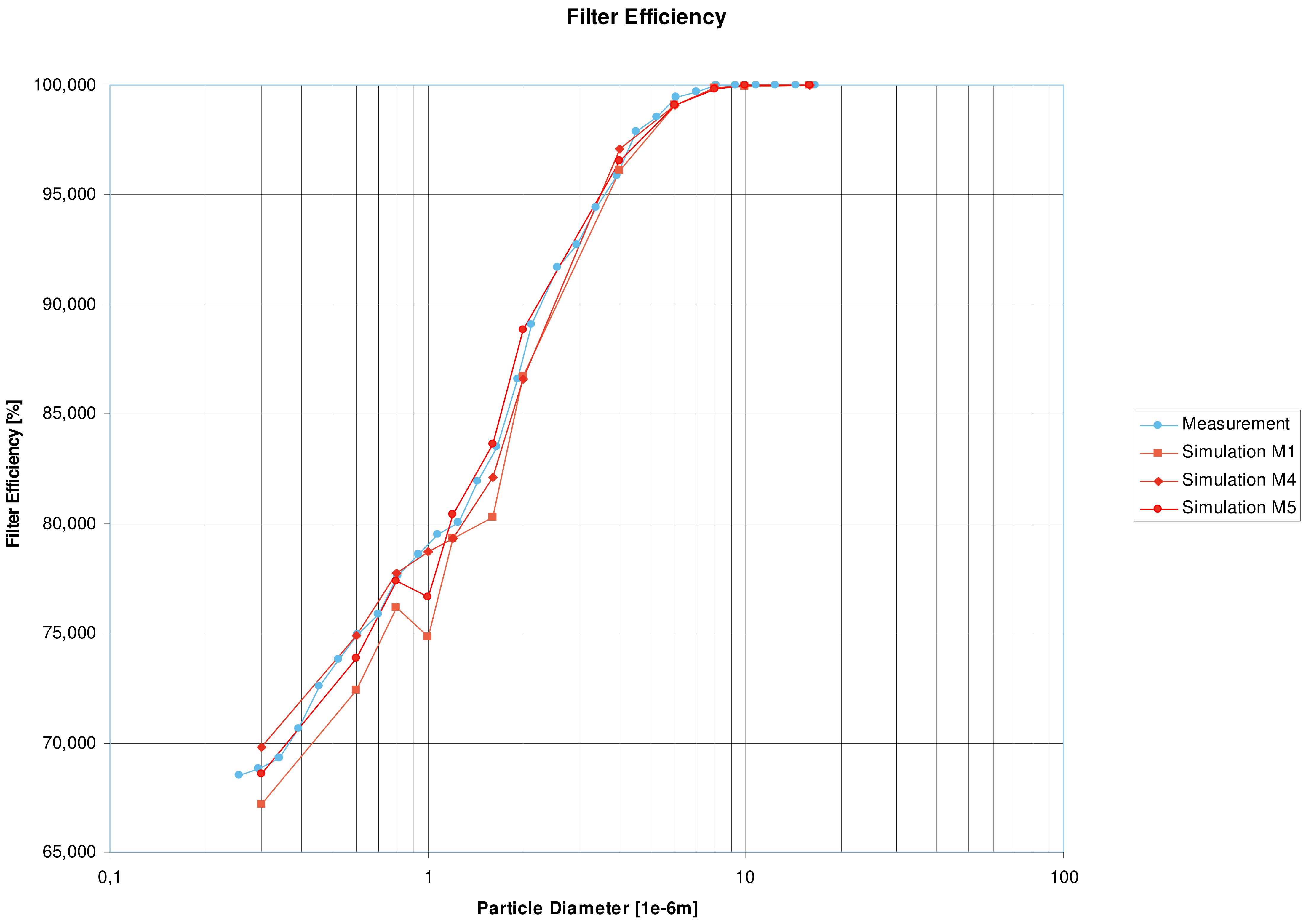
C) Nonwoven geometry:
Electrostatic charges
No-slip boundary conditions

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

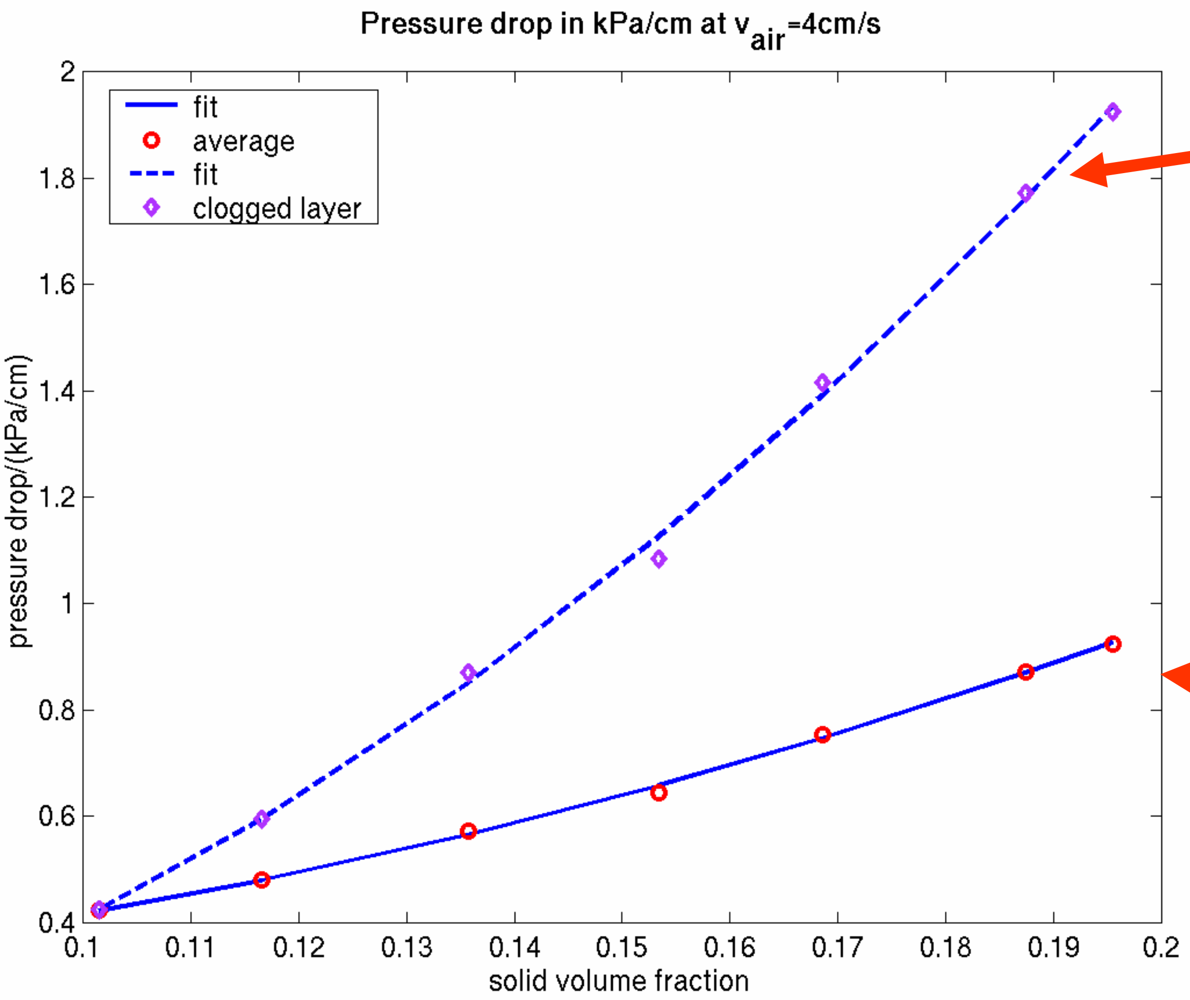
E) Deposition due to:
Inertial impact + adhesion
Diffusion + adhesion
Electrostatic attraction+adhesion
Sieving

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



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

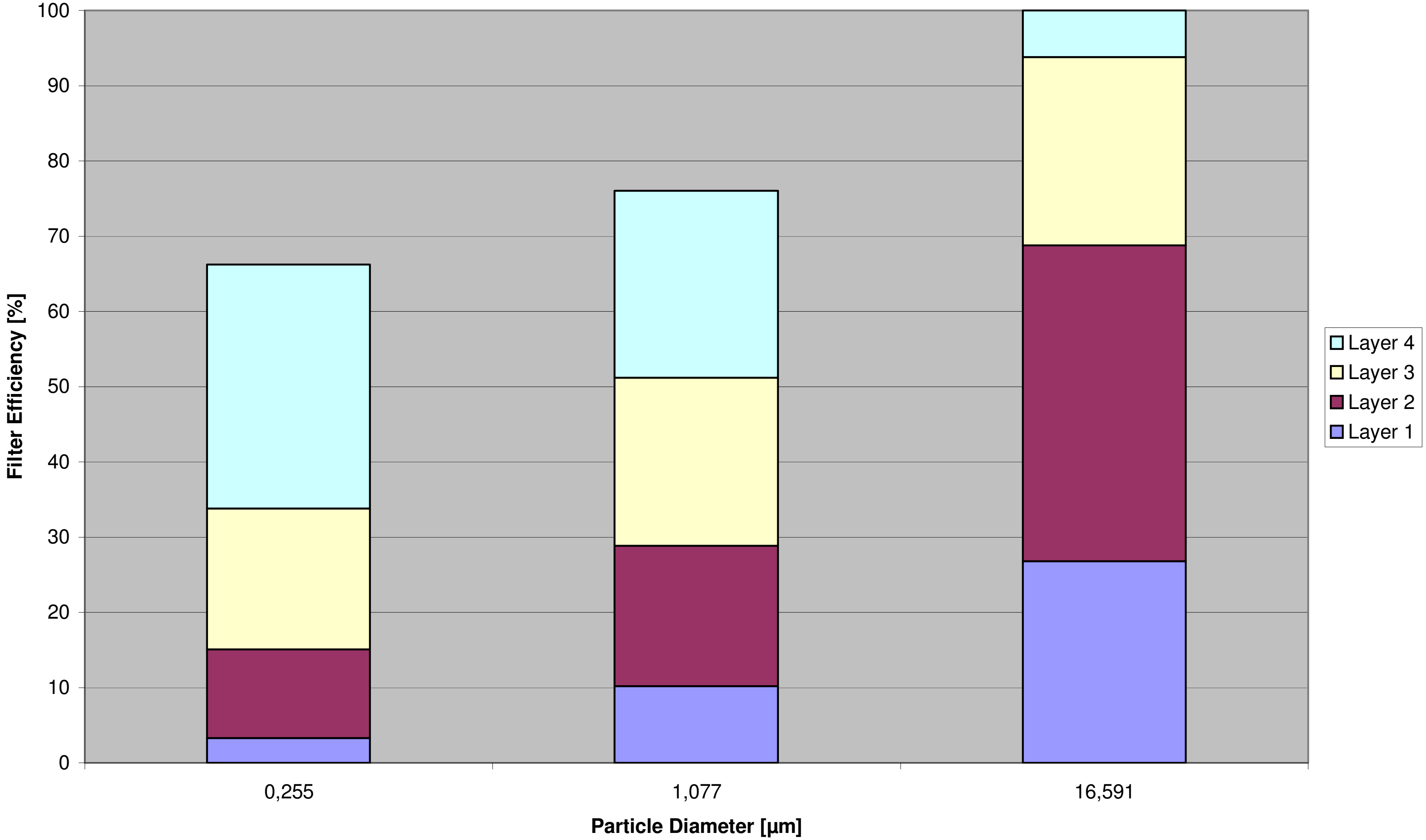
Time Dependent Pressure Drop



in the loaded portion of the media

on average over the whole media

Deposition of Different Sized Particles in the Different Layers



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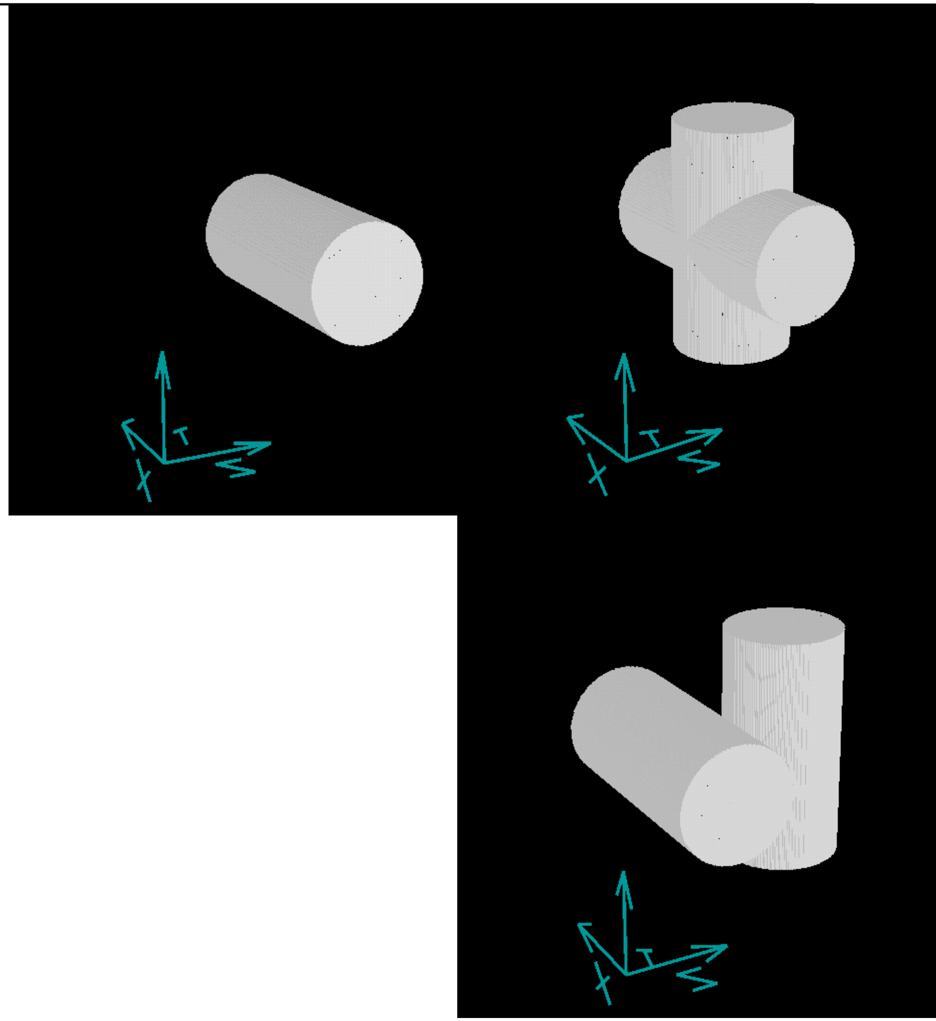
October 13th, 2005

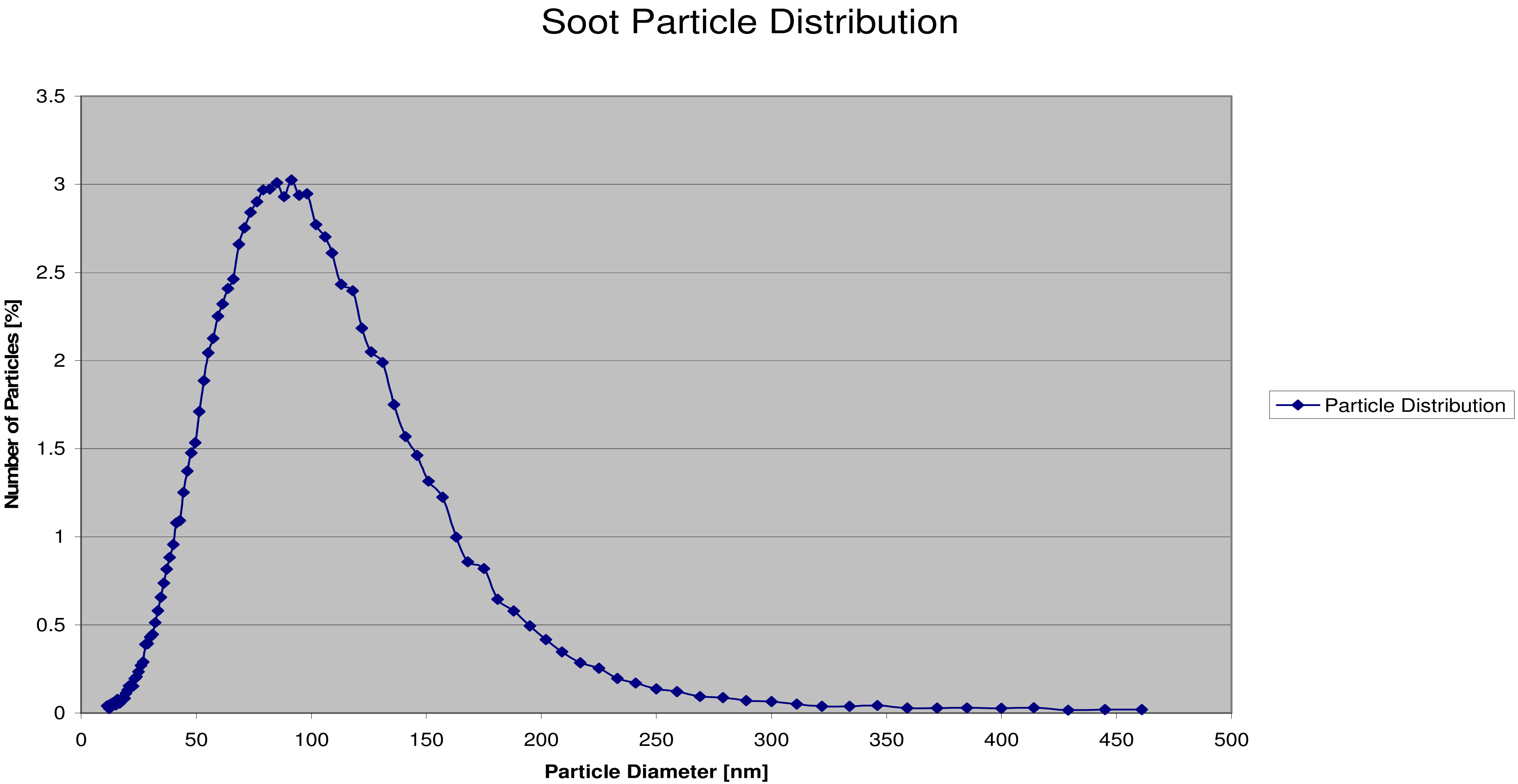
Nano Simulations of Soot Deposition

Setup

- Geometry: 240x240x300voxels
- Resolution: 25nm
- 3 fiber arrangements
- Fiber diameters 3µm = 120voxels
- Far field velocities: 1.67cm/sec, 5cm/sec, 10cm/sec
- Flow direction: z
- 1000 soot particles at each iteration step
- Soot particle density: 35kg/m^3
- Soot particle distribution



Nano Simulations of Soot Deposition



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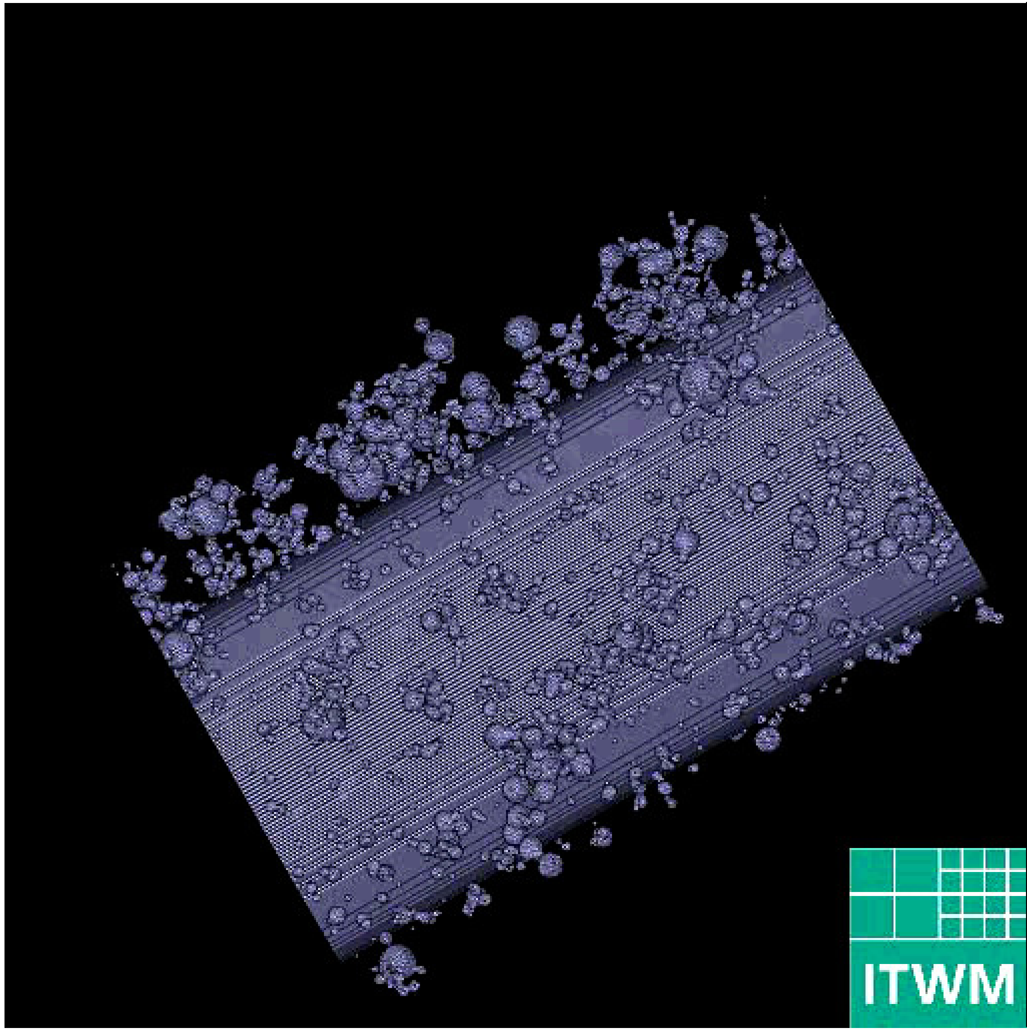
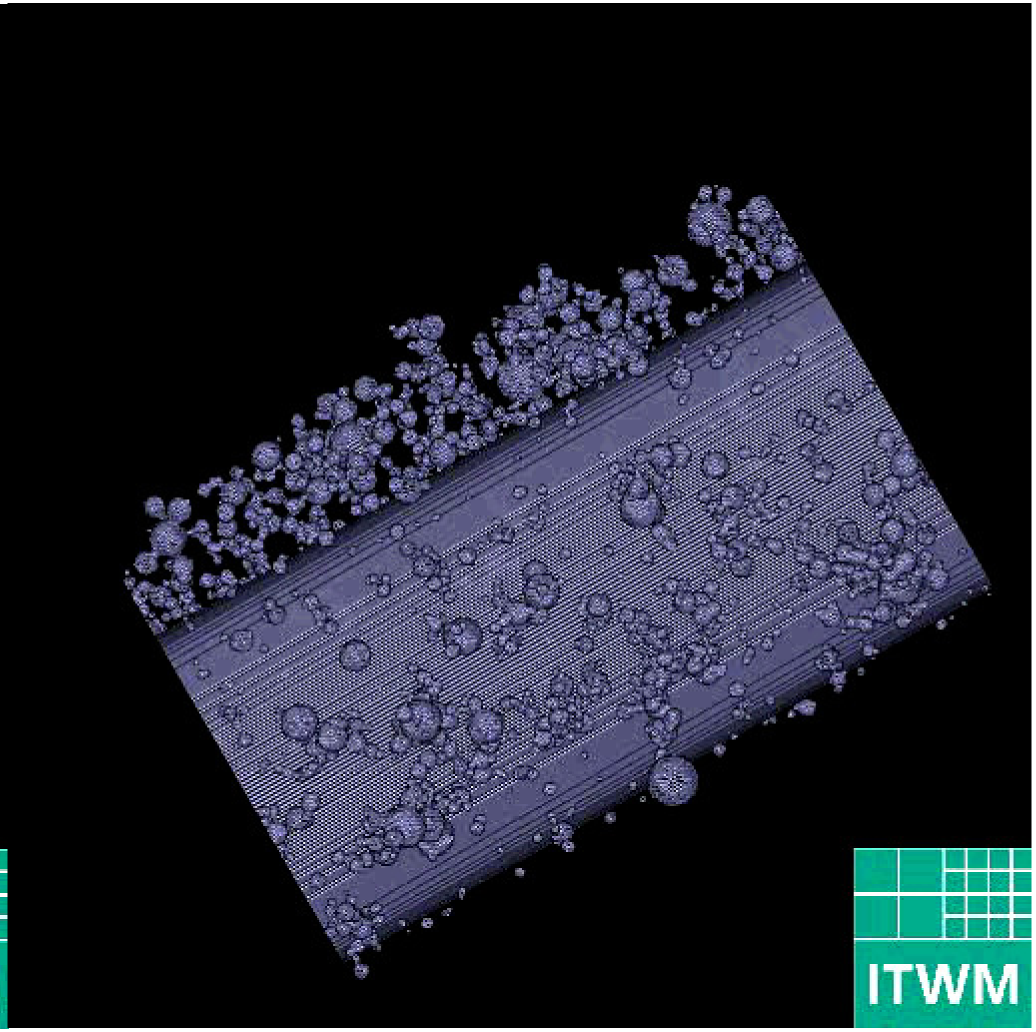
Nano Simulations of Soot Deposition

1.67cm/sec



10.0cm/sec



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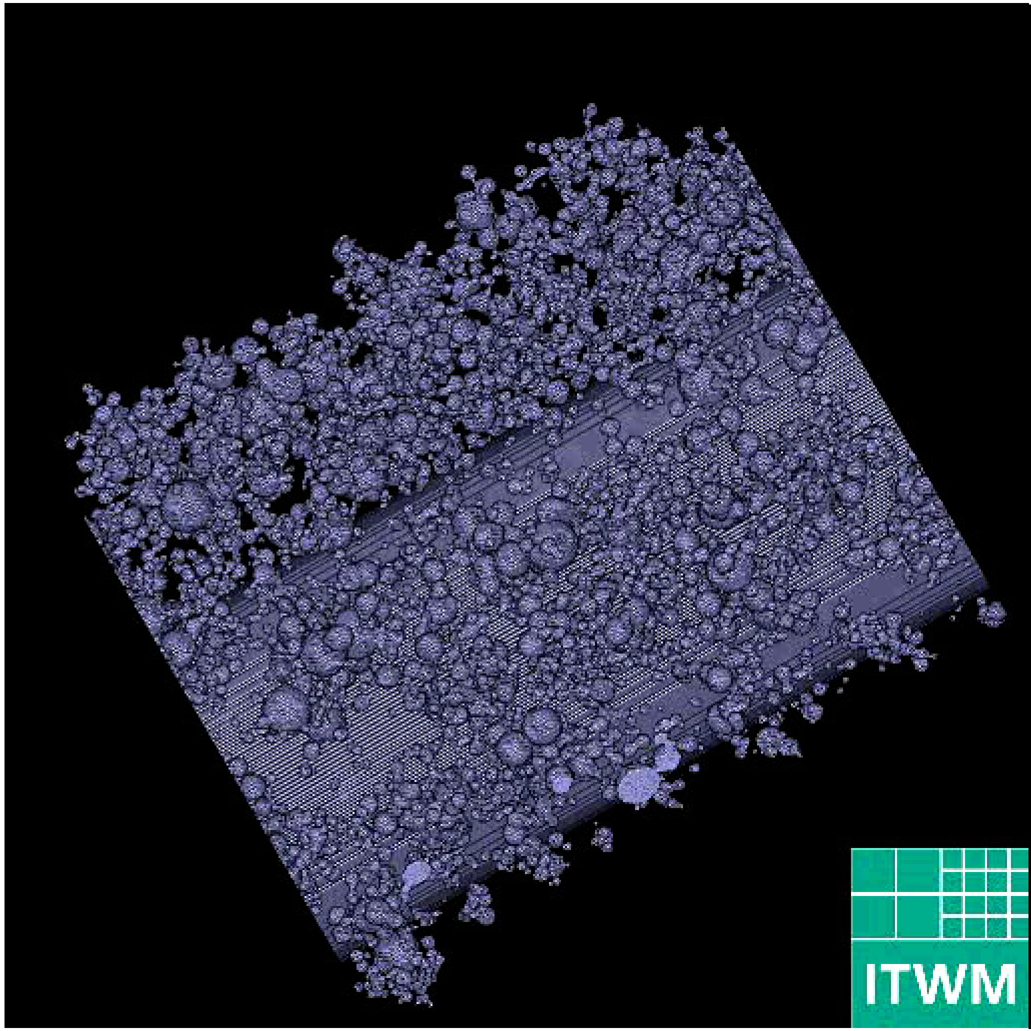
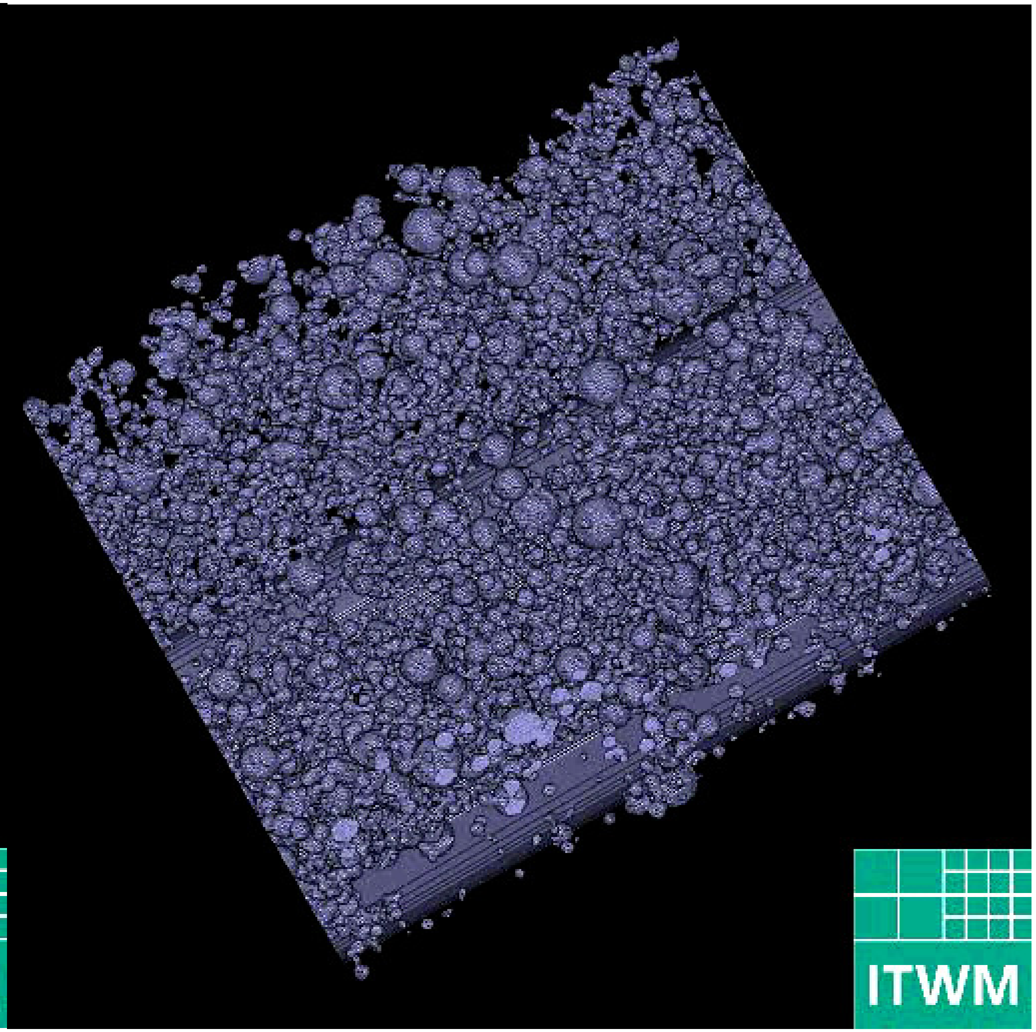
Nano Simulations of Soot Deposition

1.67cm/sec



10.0cm/sec



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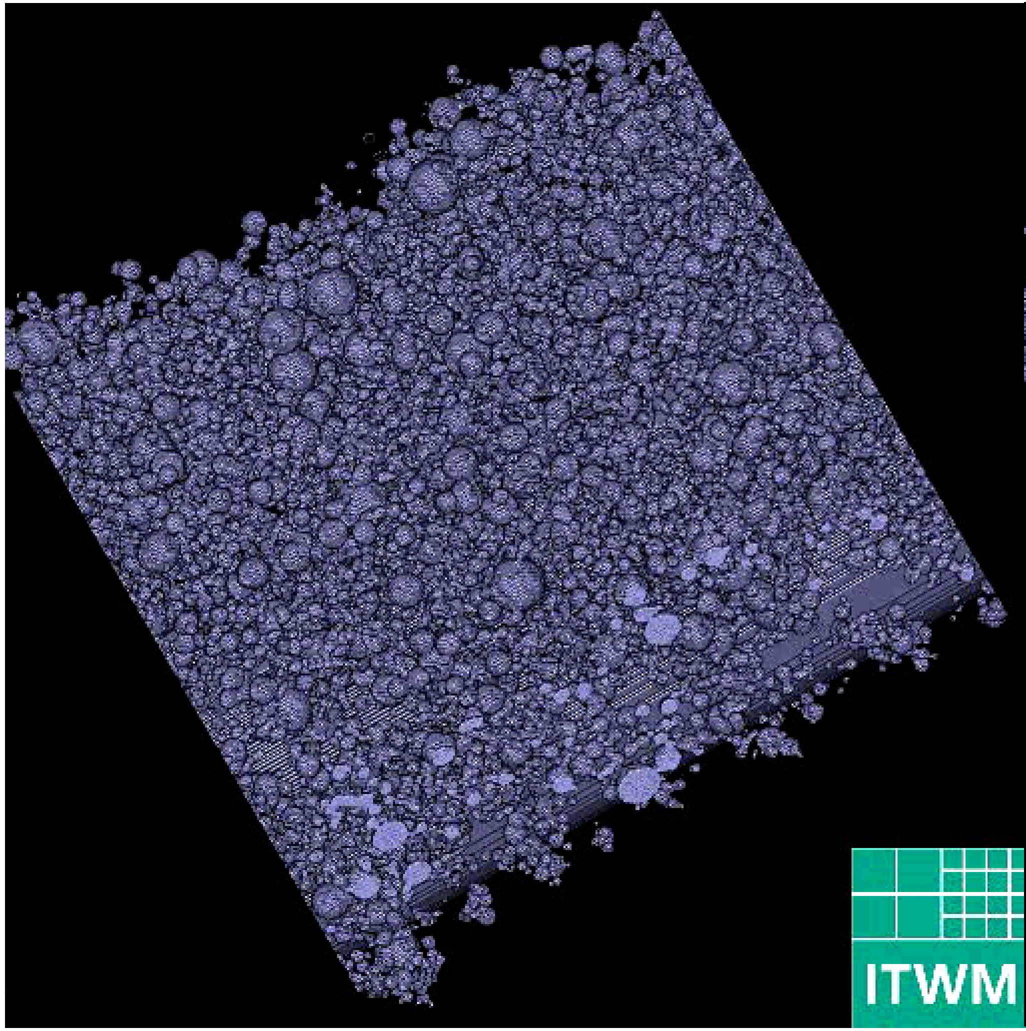
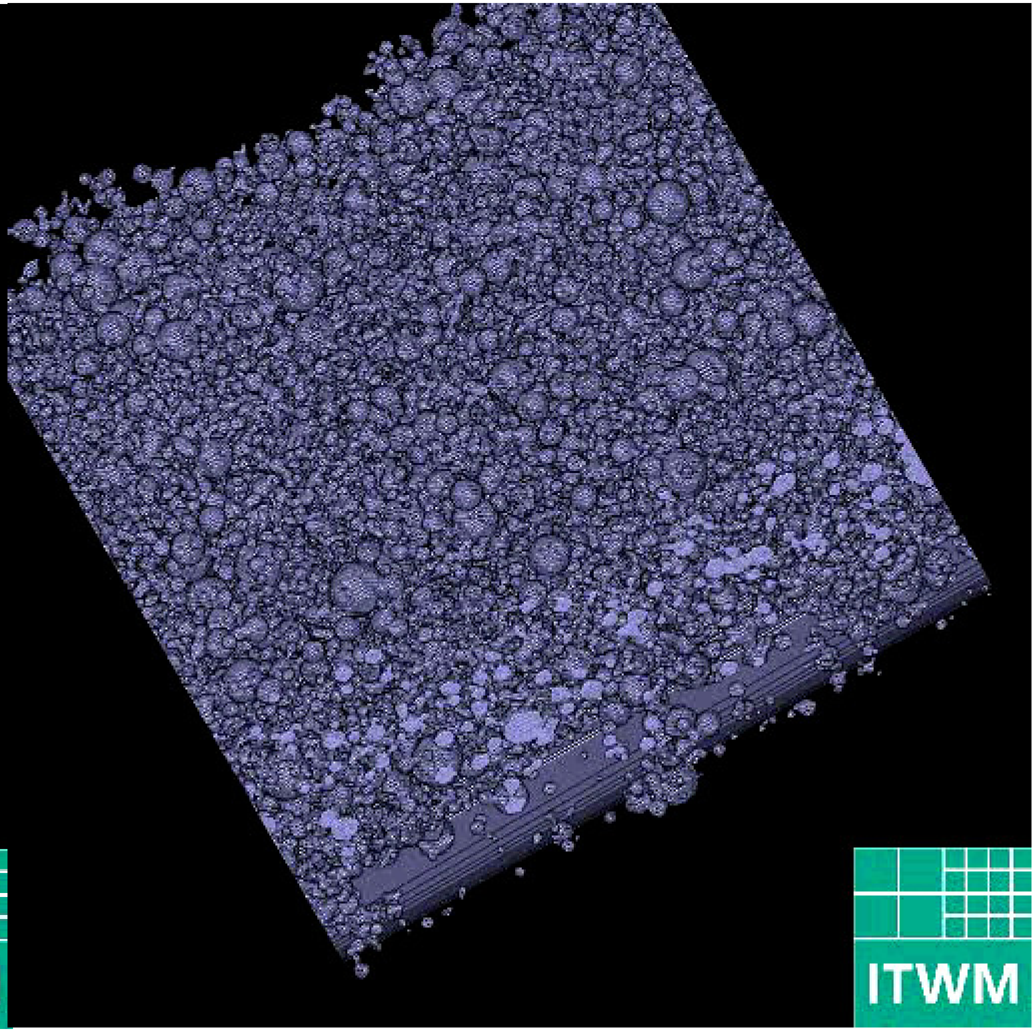
Nano Simulations of Soot Deposition

1.67cm/sec	10.0cm/sec
	

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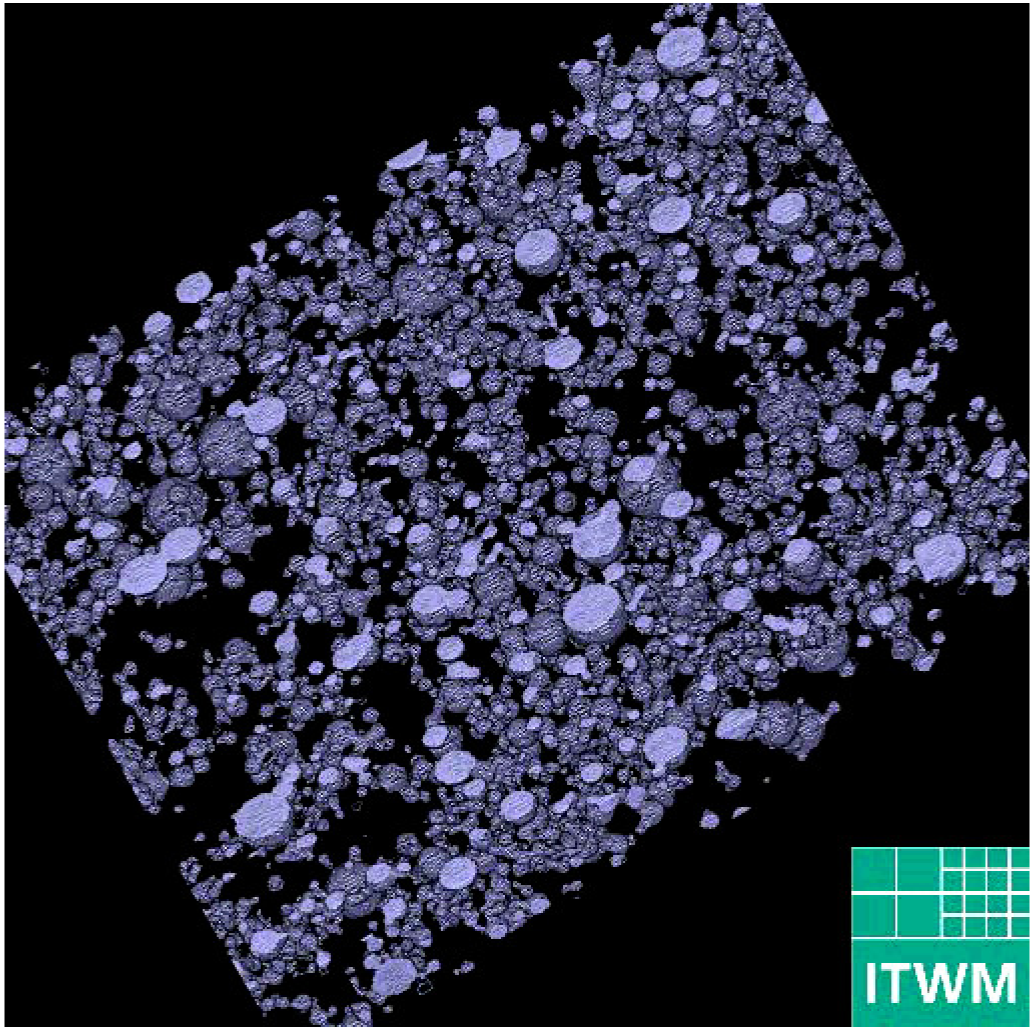
Nano Simulations of Soot Deposition

- Dendritic growth can be well observed especially at the beginning
- Deposition patterns depend on far field velocity
- Porosity of soot layers depend on far field velocity

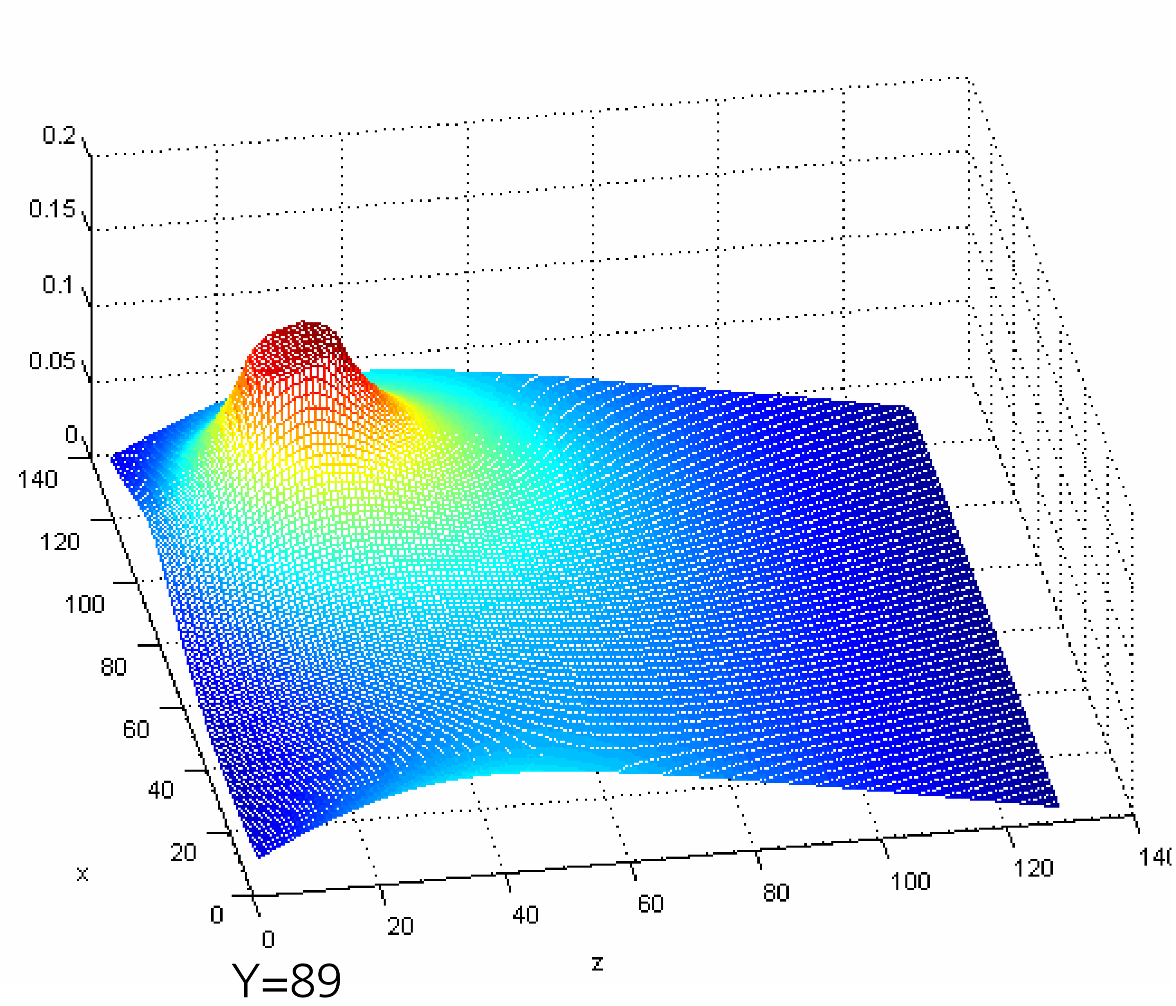
Result:

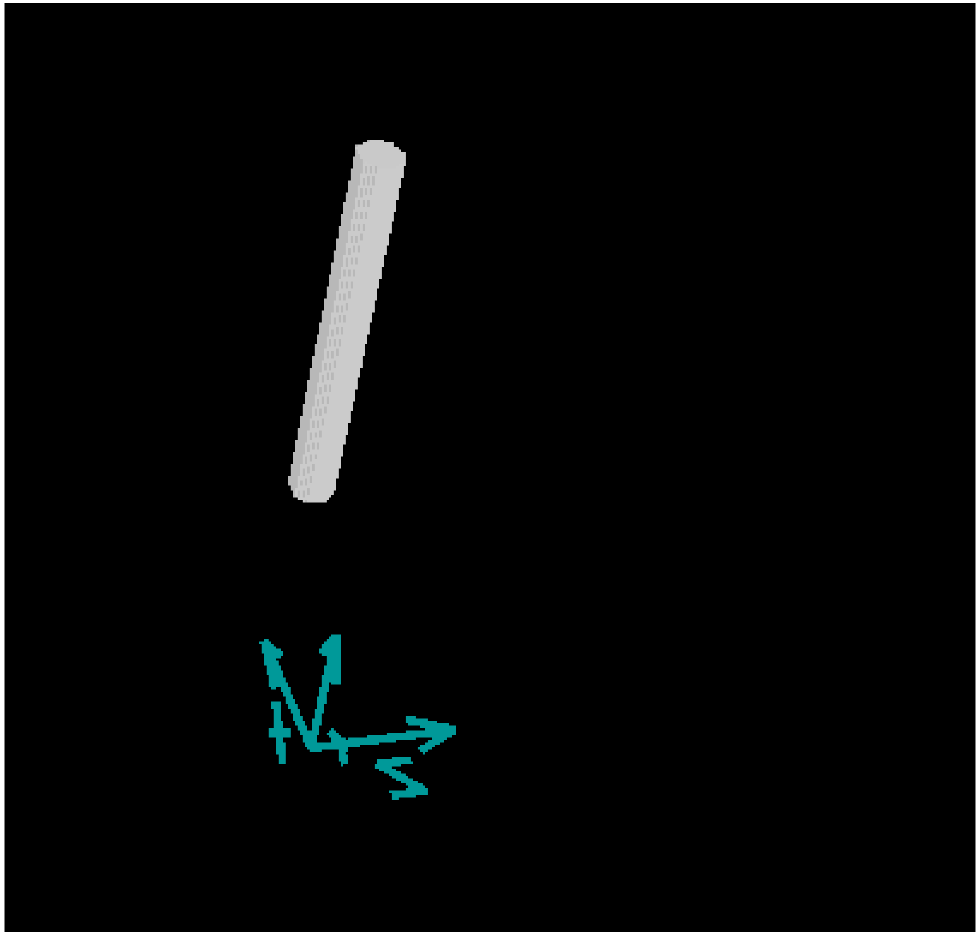
- Need porosity and permeability of the soot layers for subvoxel model
- Derivation by cut-outs of filled single fiber geometries



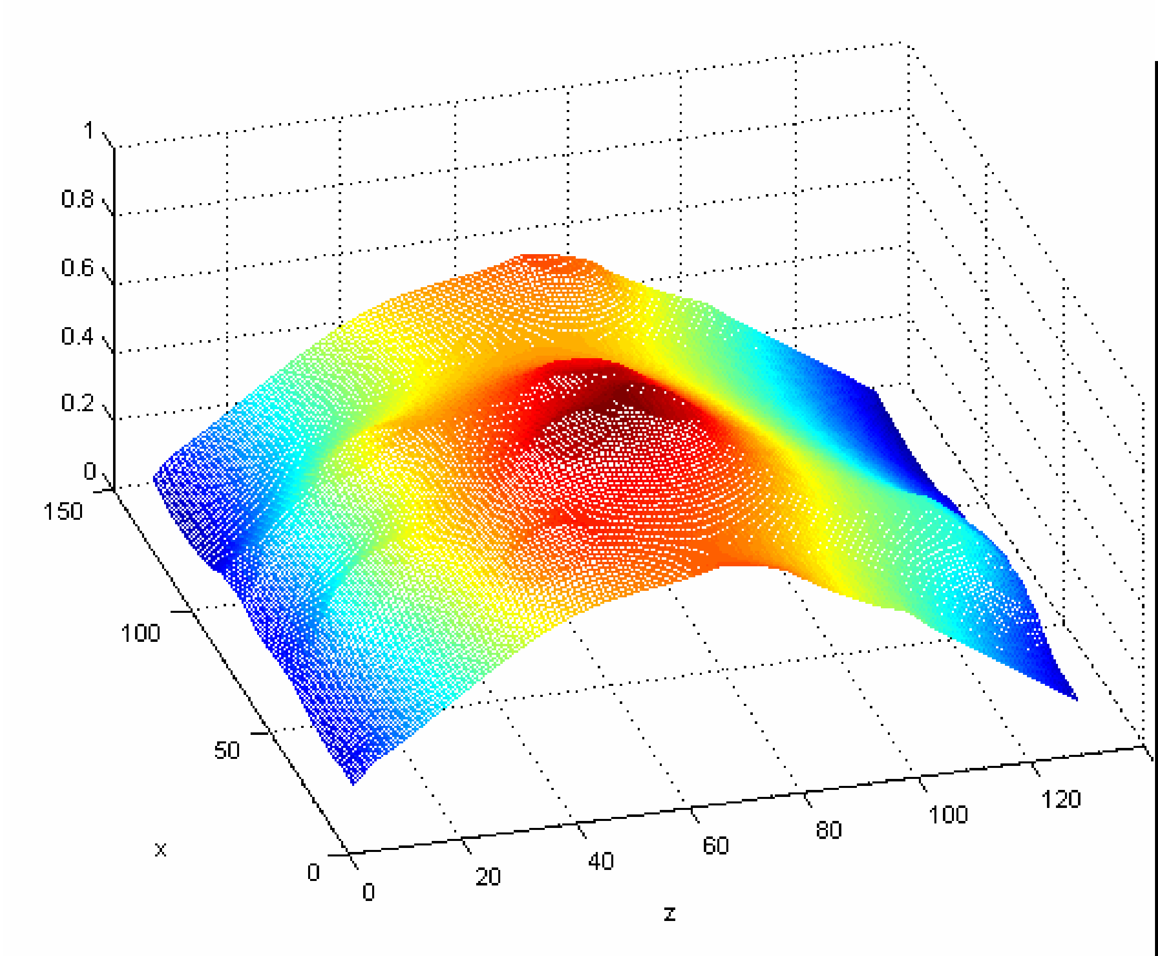
Soot Layer Cut-Out

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

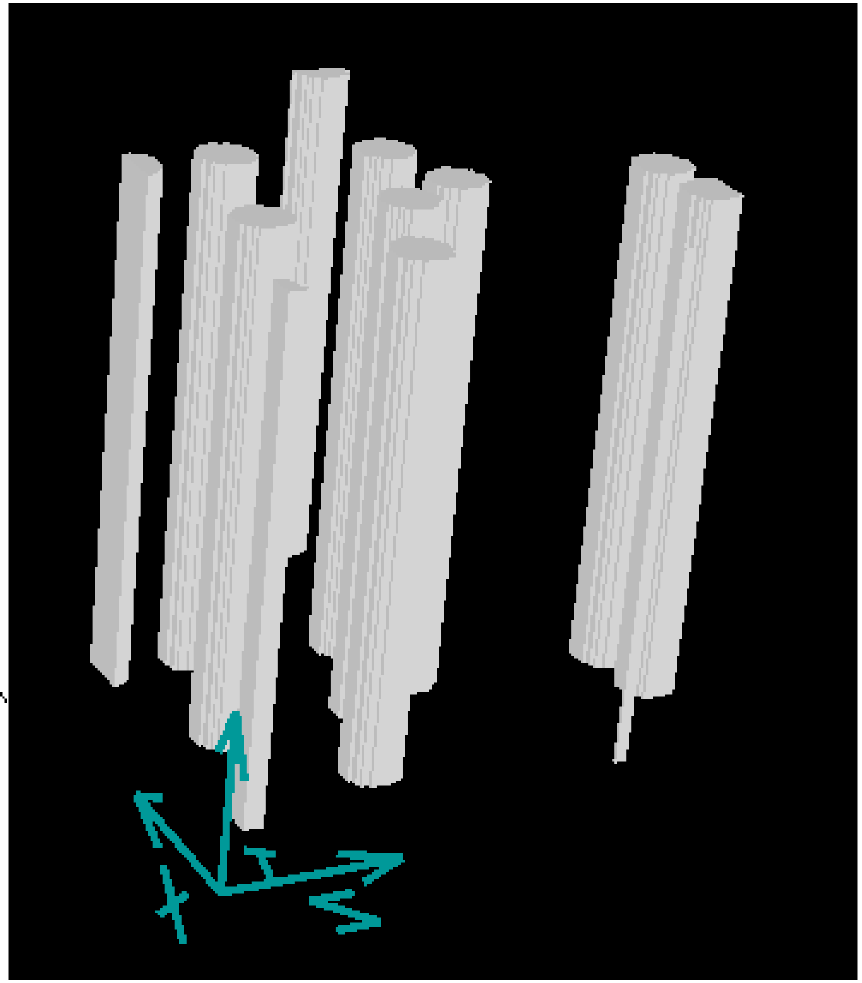




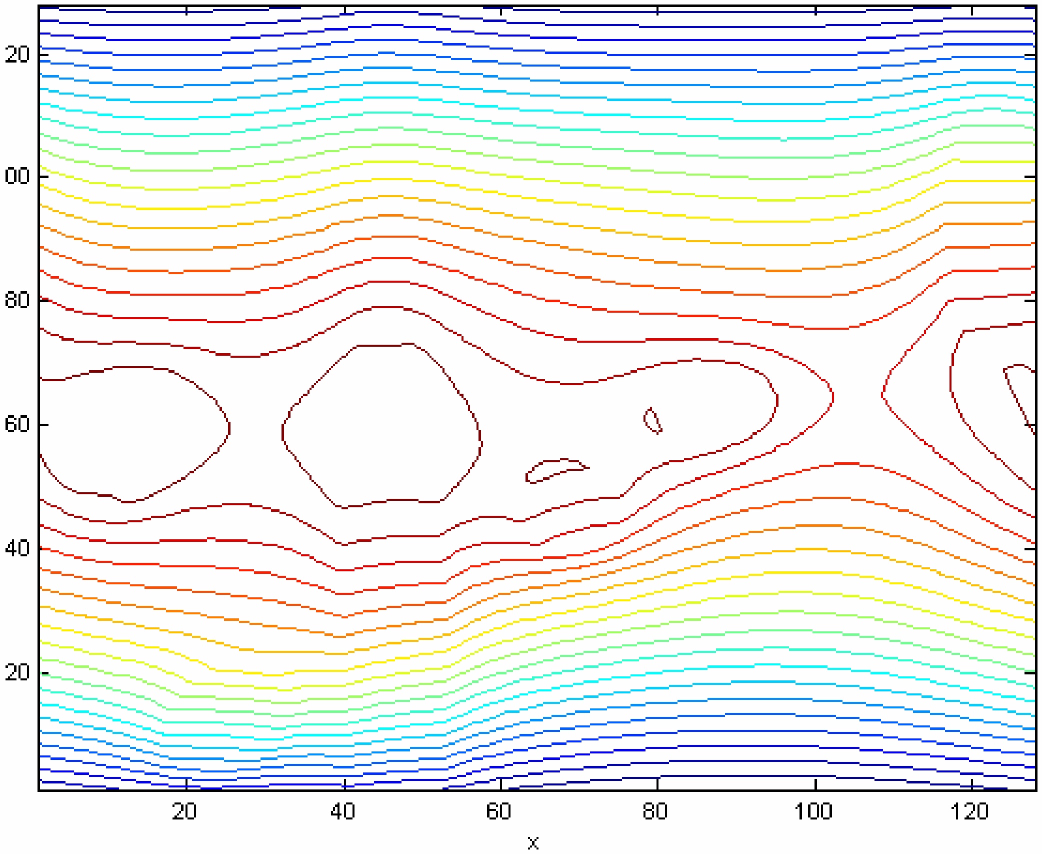
Electric potential (cross section Y=89) for 10 parallel fibers



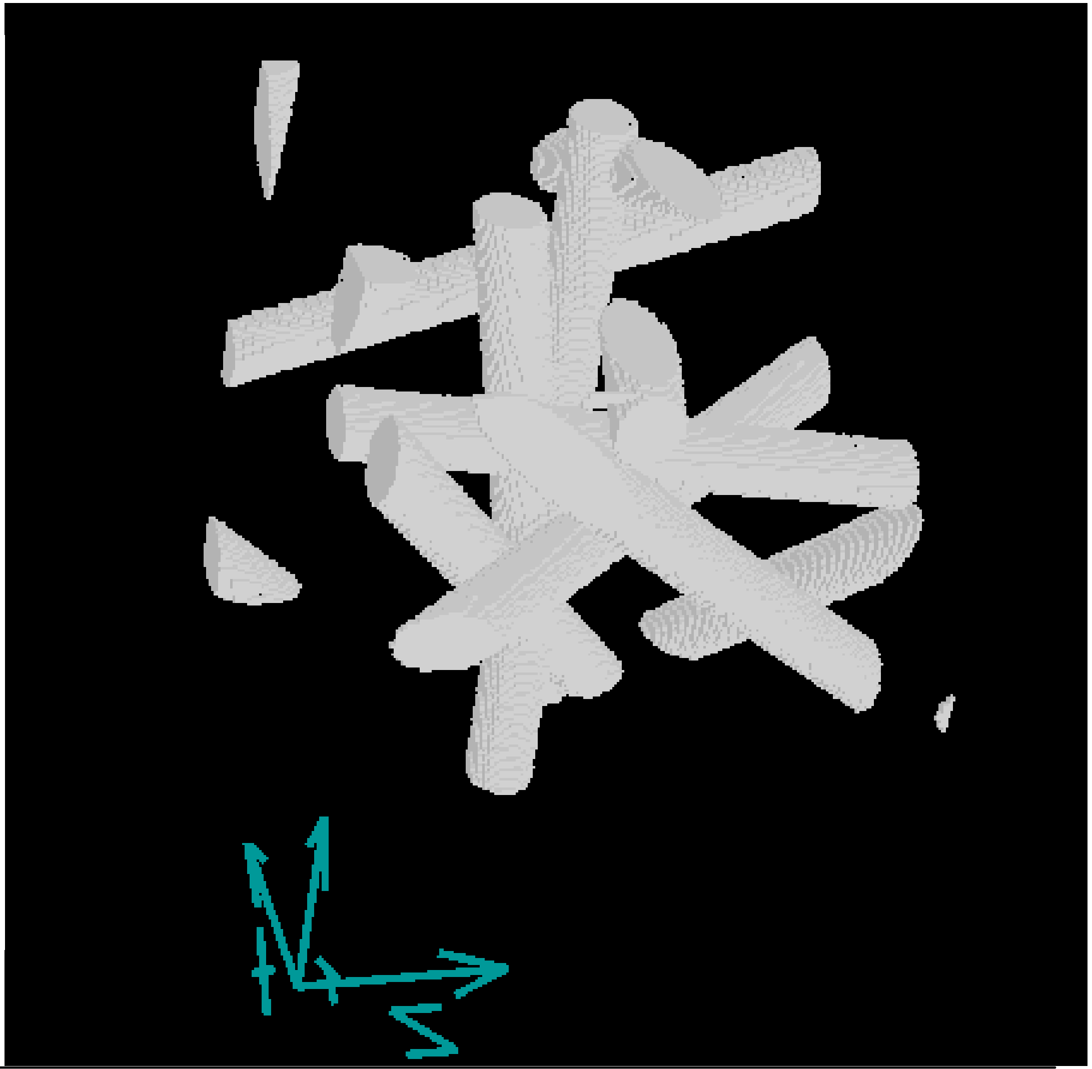
Y=89



Electgric potential (contour Y=89) for random fibers



Y=89



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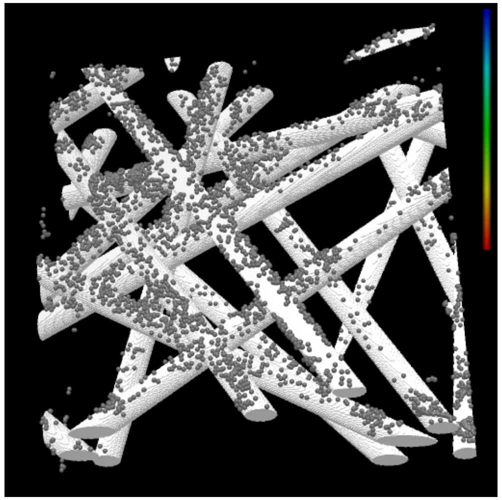
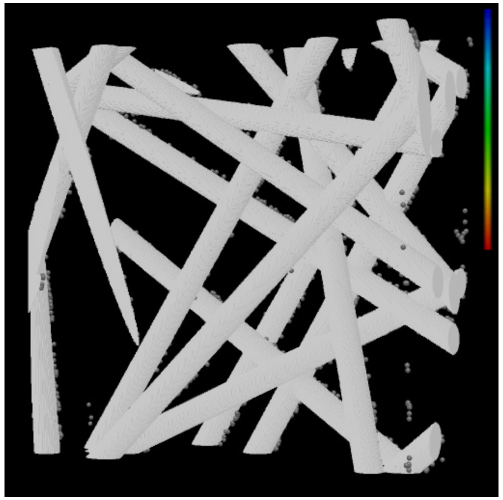
Simulation results with(out) electric surface charge

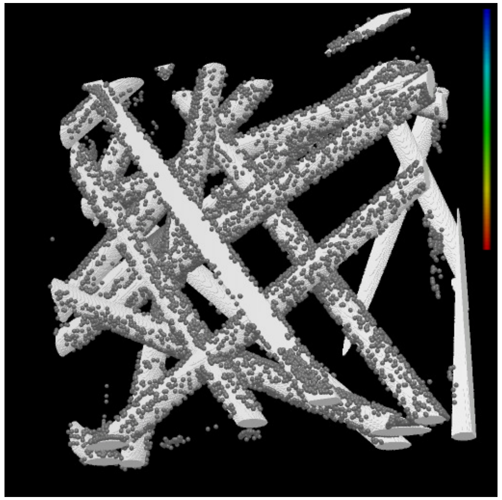


Simulation result without the influence of electric surface charges on the fibers.

Front view

back view



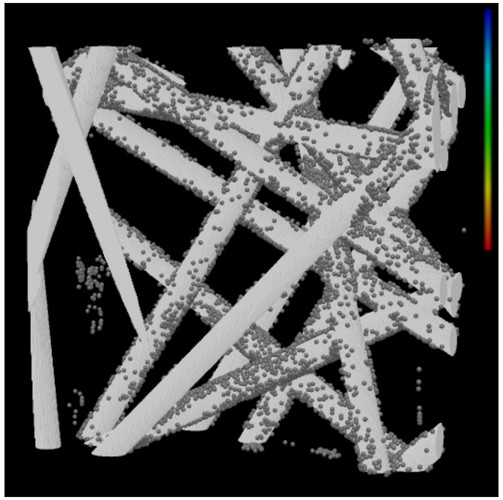


Simulation result under the influence of electric surface charges on the fibers.

Retention rate increased by about 50%!

Front view

back view



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Summary

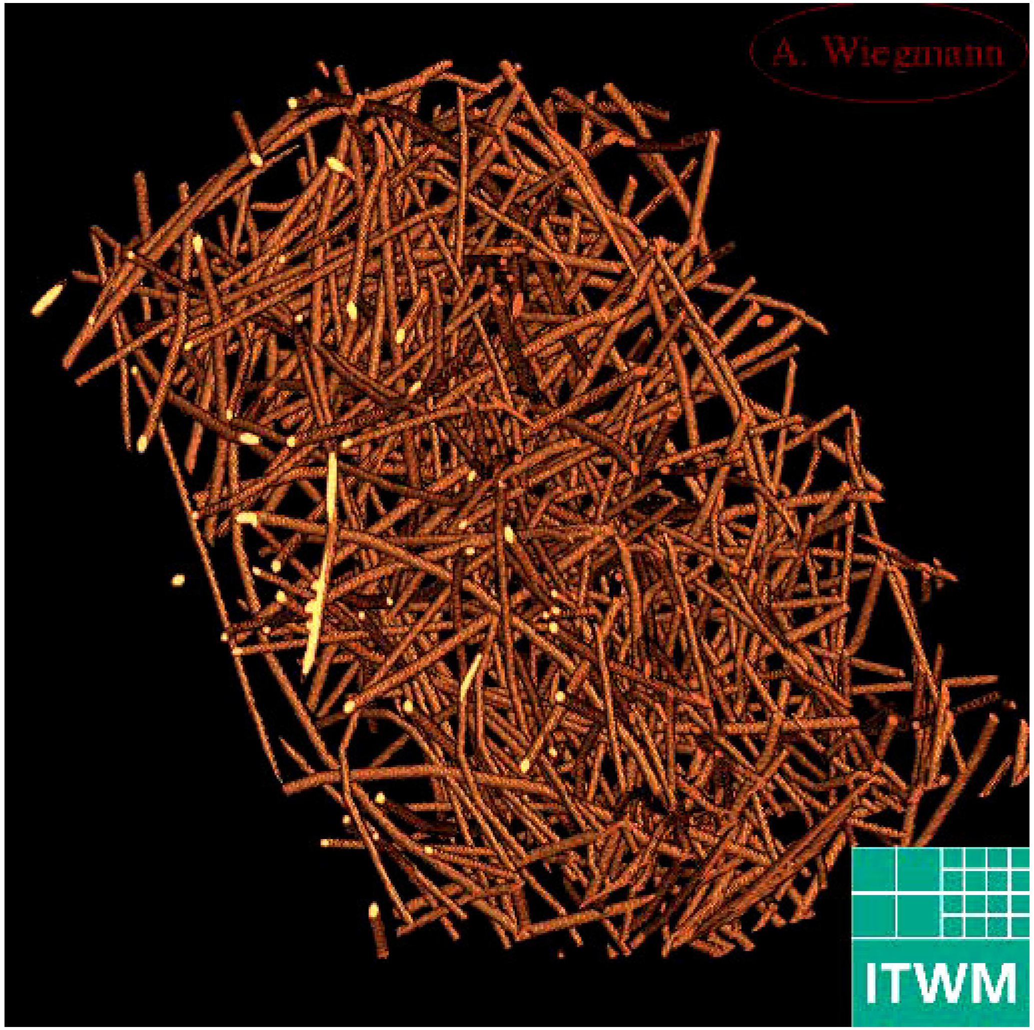
<u>Have added porous voxels to account for subvoxel sized particles depositing</u>

- Find dendritic growth by nano-scale simulations on simple configurations
- Determine parameters like permeability from porosity by nano-scale simulations on simple configurations
- Soot modelling is still difficult: particle shapes, densities, ...

<u>Have added electrostatic field to air filtrations</u>

- Front and back of media behave like front and back of a fiber
- Find dramatic increase in filtraton efficiency
- Do not know exactly what the charges on the fibers nor particles should be

Outlook: Compression of fibrous media – needed by oil filtration simulation???



GeoDict and FilterDict: Contributors from ITWM

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Arnulf Latz
Andreas Wiegmann
Stephan Nowatschin
Christian Wagner
Rolf Westerteiger

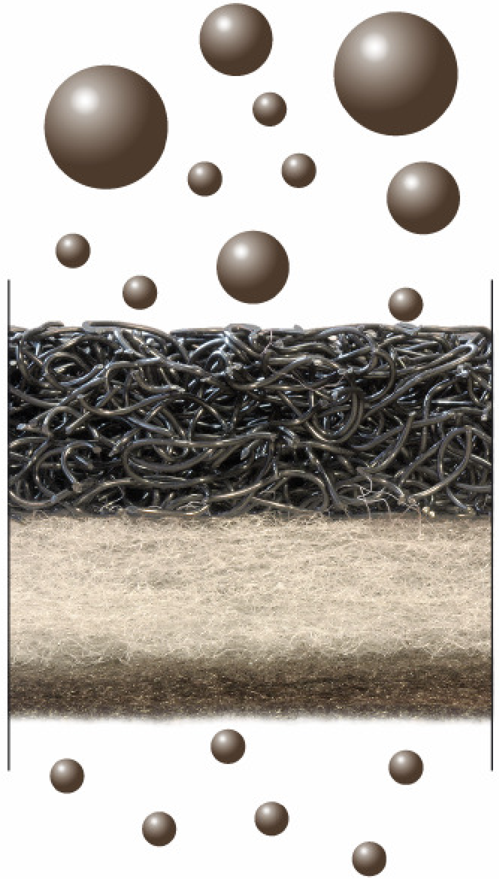
The Volume Rendering Team

Carsten Lojewski

You are friendly invited to

Visit us at booth E 7!

Workshop



Microstructure Simulation
and
Virtual Material Design

Kaiserslautern,
January 26th to 27th, 2006
Fraunhofer ITWM, Fraunhofer-Platz 1

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