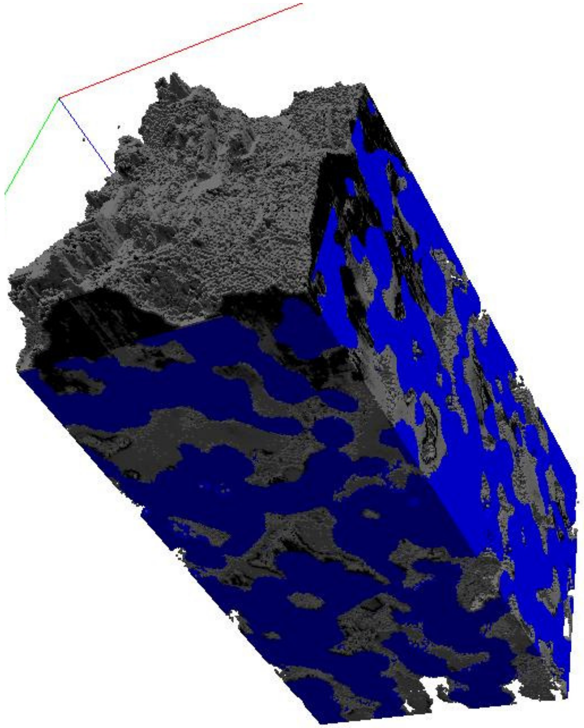
Virtual Diesel Particulate Filters: Simulation of the Structure, Exhaust Gas Flow and Particle Deposition



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3rd AFS Conference "Emission Solutions in Transportations"

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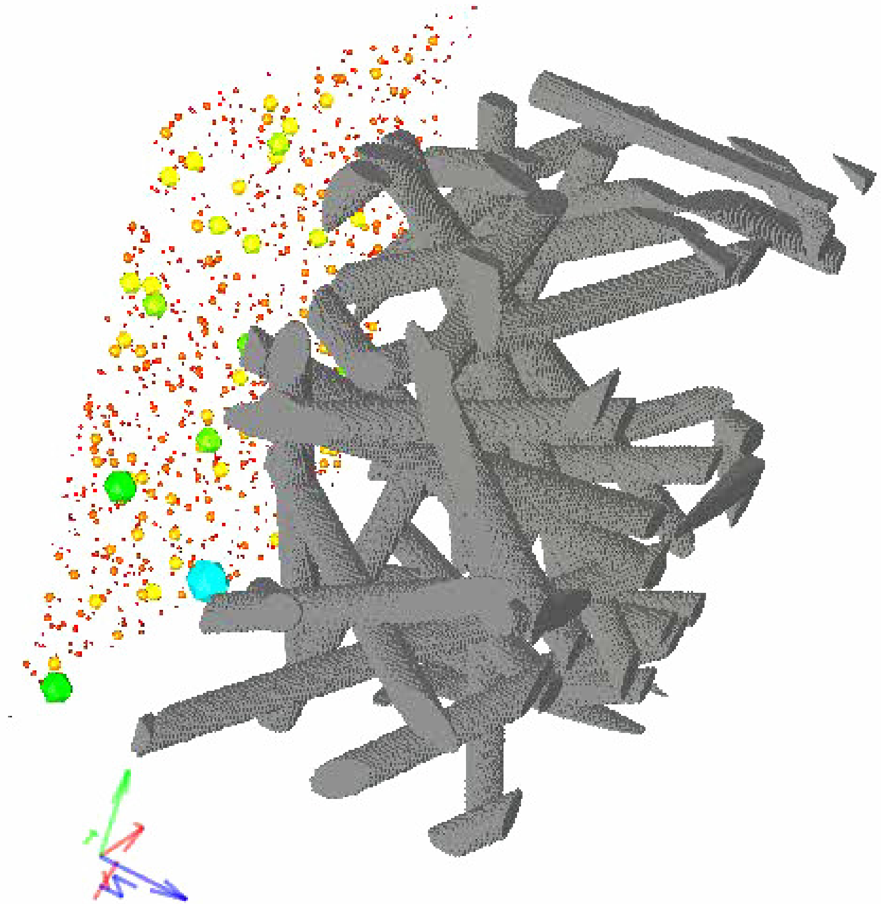
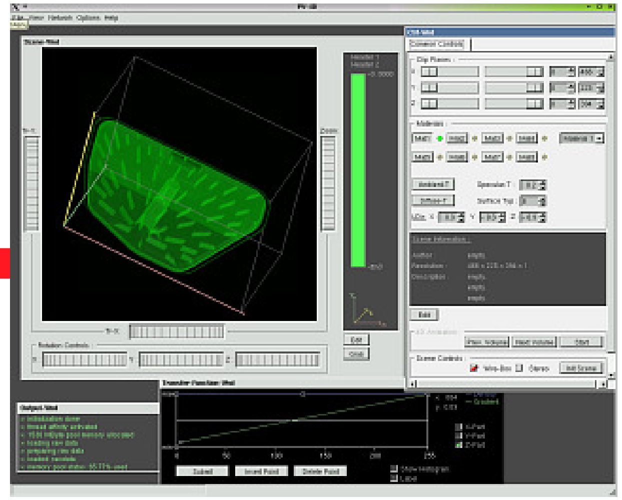
Overview

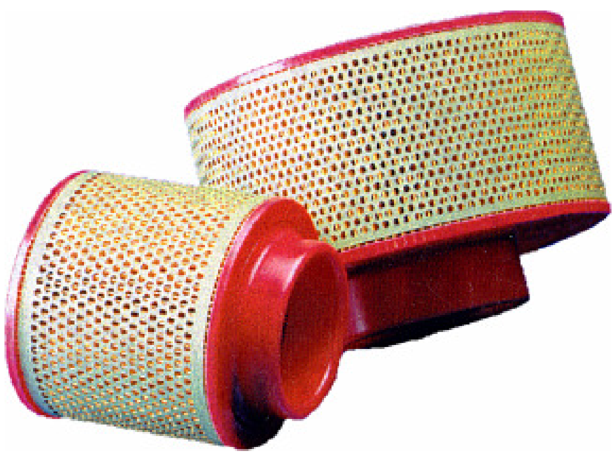
1. Virtual Material Design Cycle
2. Virtual Filter Geometries
3. Simulation of Filtration Processes
   a) Modeling
   b) Simulation Results
   c) Software Tools
4. Summary and Future Developments



1. Virtual Material Design Cycle

Property Requirements Fulfilled?

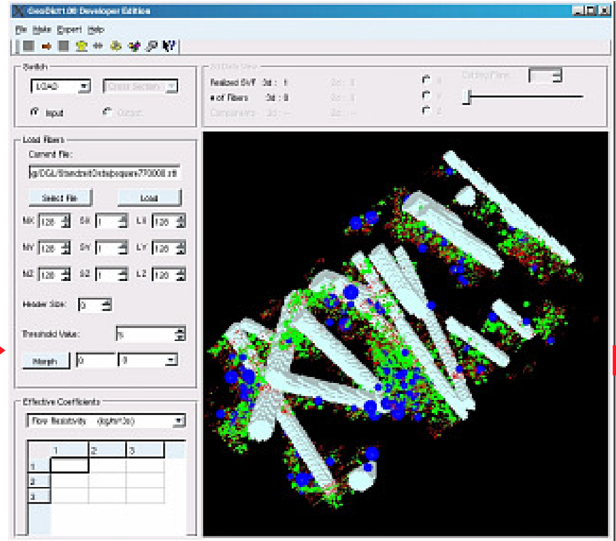




Virtual Design Cycle

Selection of Media Types, Dimensions, etc.

Computation of Macroscopic Properties of the Filter



Computation of Microscopic Properties of the Filter Medium

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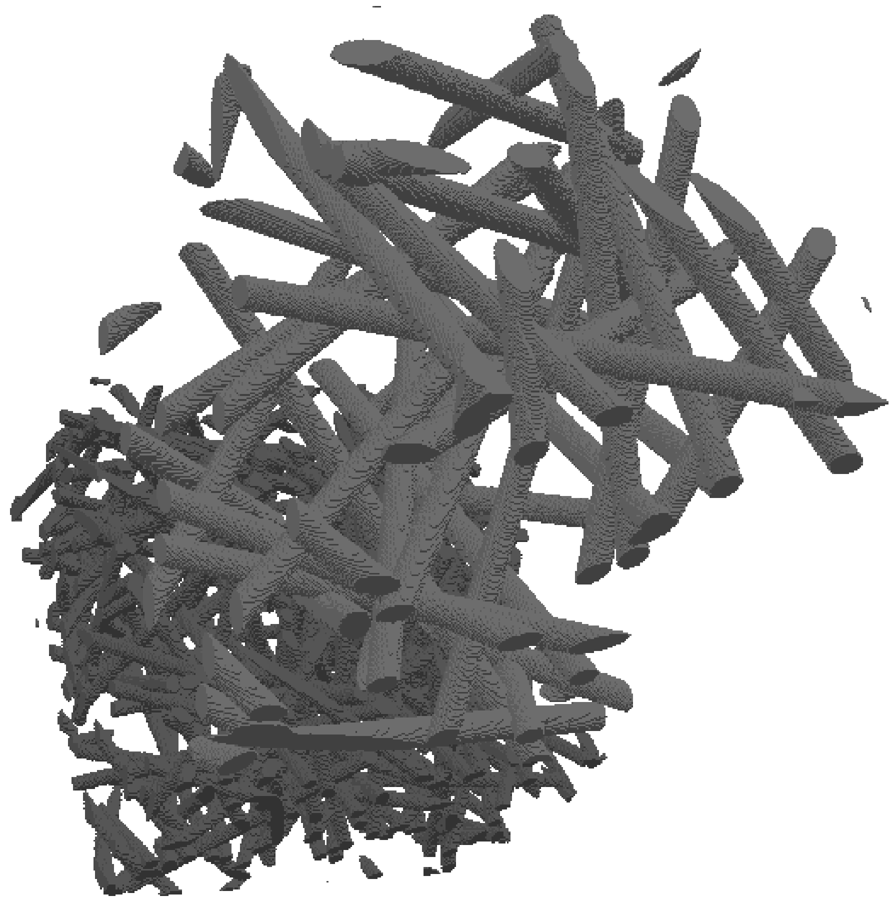
2. Virtual Filter Geometries

Multilayer Virtual Nonwoven

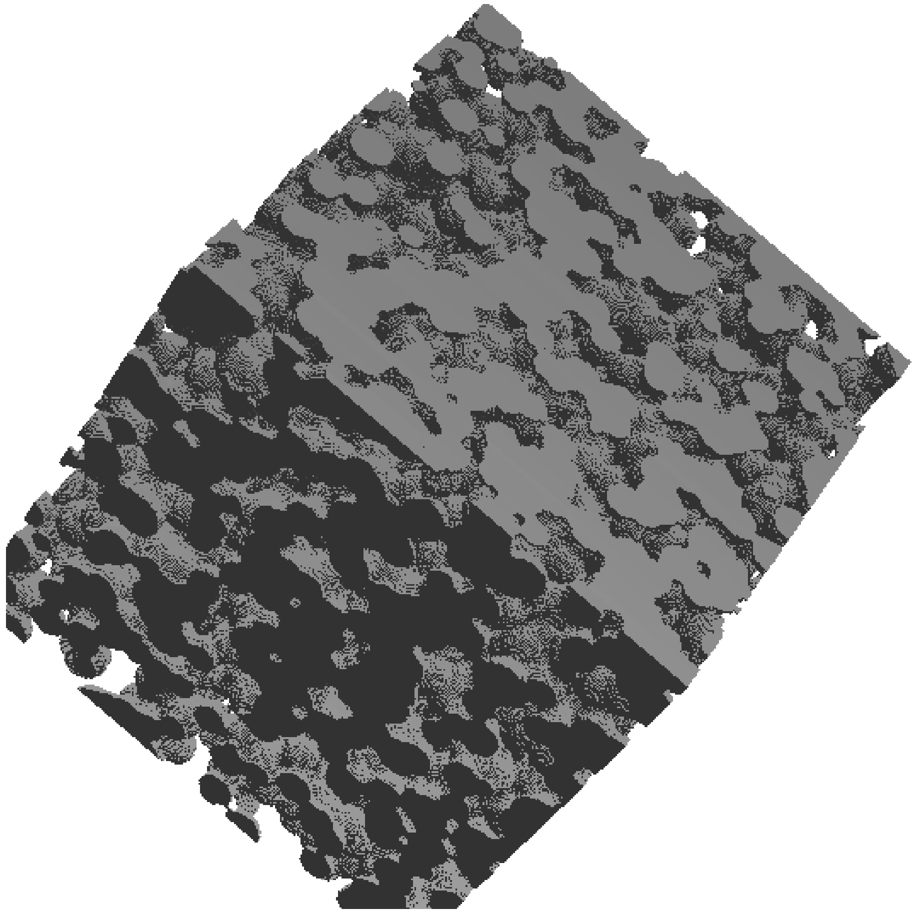
- Stochastic generation of the structure with guaranteed adjustable properties, e.g.
  - Distribution of fiber diameters and cross sections
  - Fiber orientation
  - Porosity
  - Layer thickness
  - …
- Stacking of layers with different parameters
- Use of highly flexible voxel meshes



2. Virtual Filter Geometries

Virtual Sinter Structure I

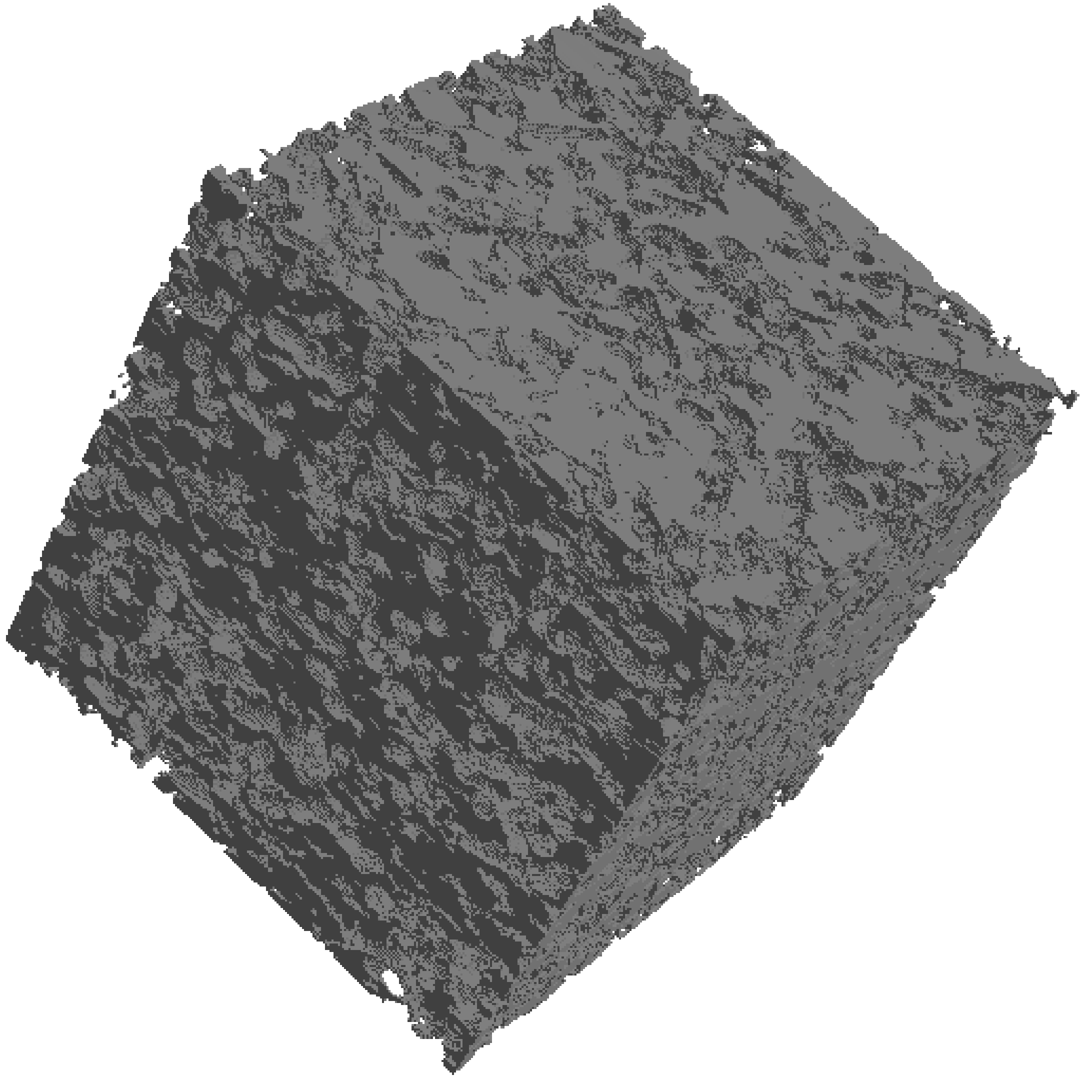
- Stochastic generation based on
  - Packings of spheres
  - Morphological operations (to generate sinter necks)
- Packings of spheres selected to match the initial grain size distribution of the sinter process
- Approach was applied in an industrial project when no tomographies were available due to
  - Too coarse resolution
  - Difficult preprocessing of samples



2. Virtual Filter Geometries

SEM image

Virtual Reconstruction



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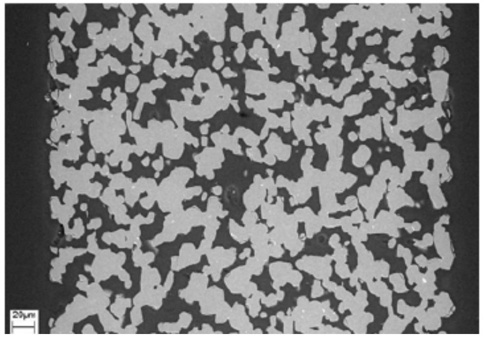
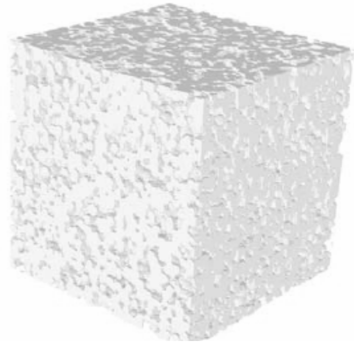
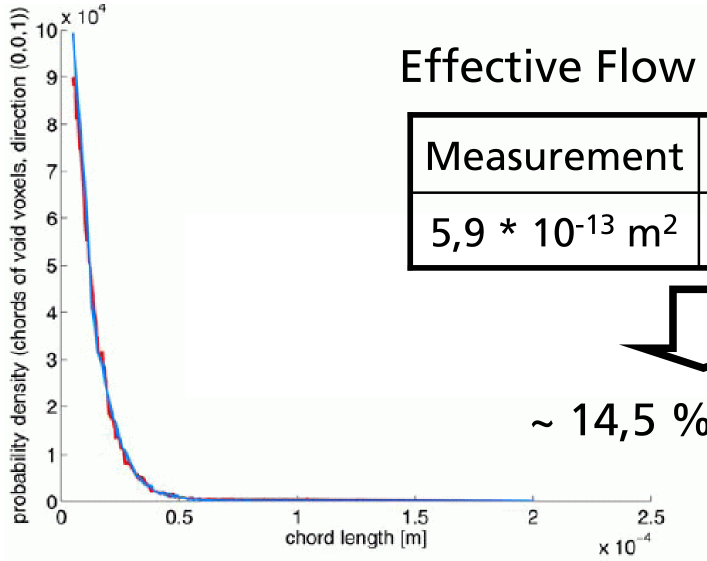
2. Virtual Filter Geometries

Quality Measures for Virtual Structures

- "The Eye"
- Porosity
- Cord length distributions: Virtual vs. real SEM cross sections
- Pore size analysis
- Flow properties, e.g. effective permeability or flow resistivity
- Filtration properties
- …







Effective Flow Permeability

Measurement	Simulation
$5{,}9 * 10^{-13}\ m^2$	$5{,}1 * 10^{-13}\ m^2$

~ 14,5 % deviation !

3. Simulation of Filtration Processes

A) Modeling

- Flow
- Particle Transport
- Particle Deposition

B) Simulation Results

- Design of Diesel Particulate Filters

C) Software Tools

- GeoDict
- FilterDict

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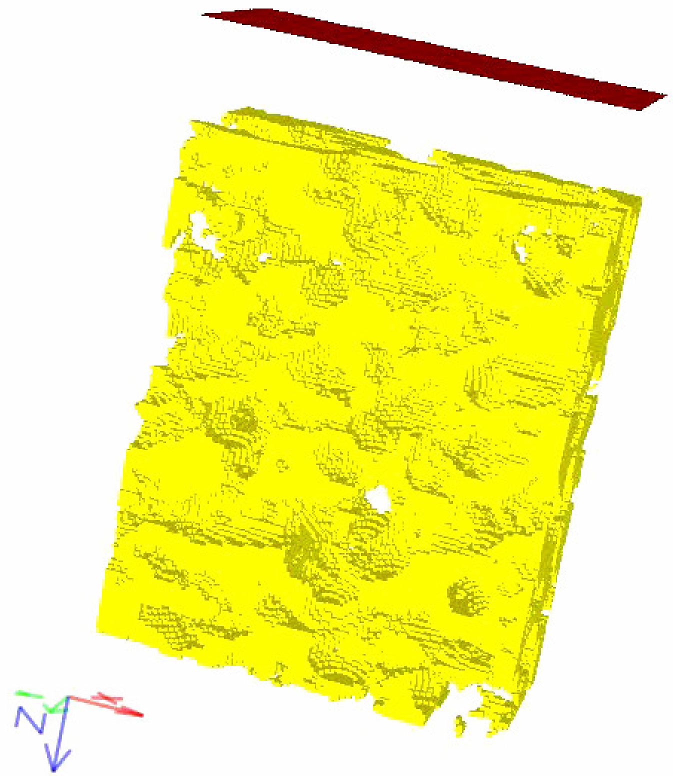
3. Simulation of Filtration Processes - Modeling



Flow simulation is based on Navier-Stokes-Brinkmann equations

$$
\begin{aligned}
-\mu\Delta\vec{u} + \nabla\vec{u}\cdot\vec{u} + \kappa^{-1}\vec{u} + \nabla p &= \vec{\mathbf{f}}, \qquad \text{(momentum balance)} \\
\nabla\cdot\vec{u} &= 0, \qquad \text{(continuity)}
\end{aligned}
$$

$+$ boundary conditions,

$\vec{u}$: velocity

p : pressure

$\vec{\mathbf{f}}$: force (density)

μ : fluid viscosity

κ : permeability of porous voxel

Remark

- convective term optional -> fast flow
- Brinkmann term optional -> subgrid particle deposition and effective porous media

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3. Simulation of Filtration Processes - Modeling

Lagrangian Particle Transport

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

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

Particle Deposition

- Collision handling
- Adhesion model

Modification of Geometry

- Solid deposition model (particles resolved by voxels)
- Porous deposition model (small particles)

3. Simulation of Filtration Processes - Modeling

Model inherent filtration mechanisms

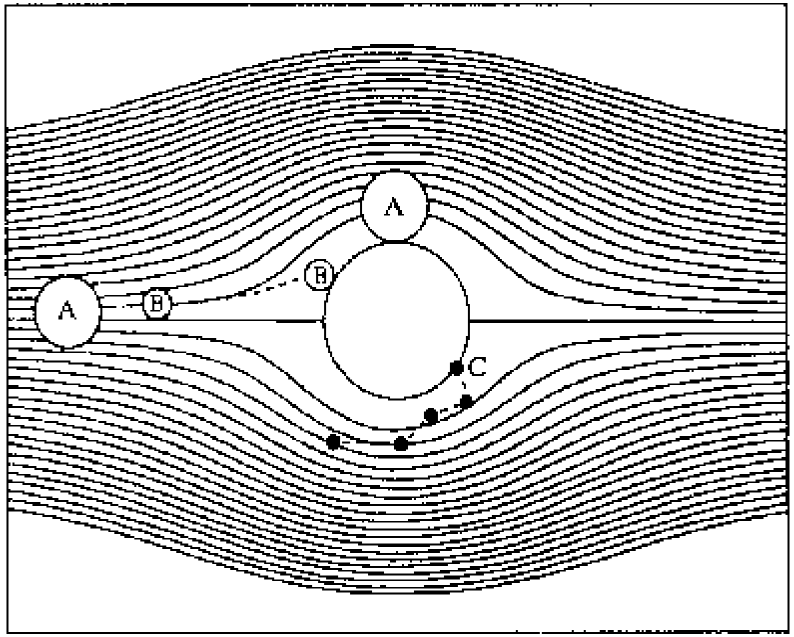
A) Barrier effect

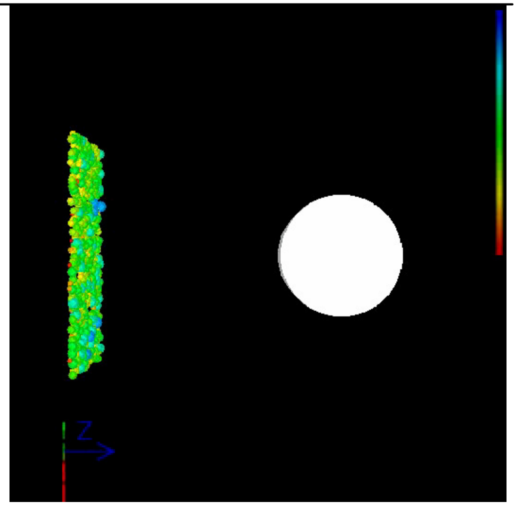
B) Inertia effect

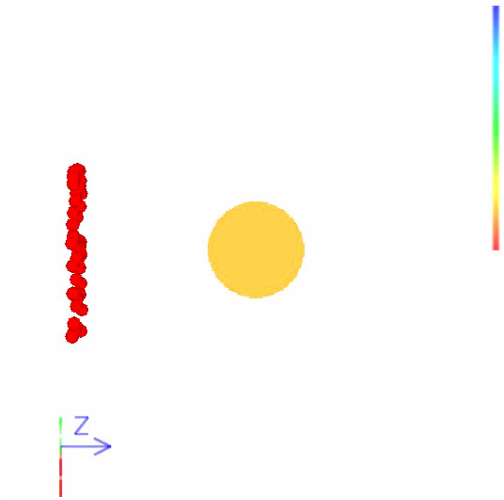
C) Diffusion effect (Brownian motion)

D) Sieving

E) Electrostatic attraction







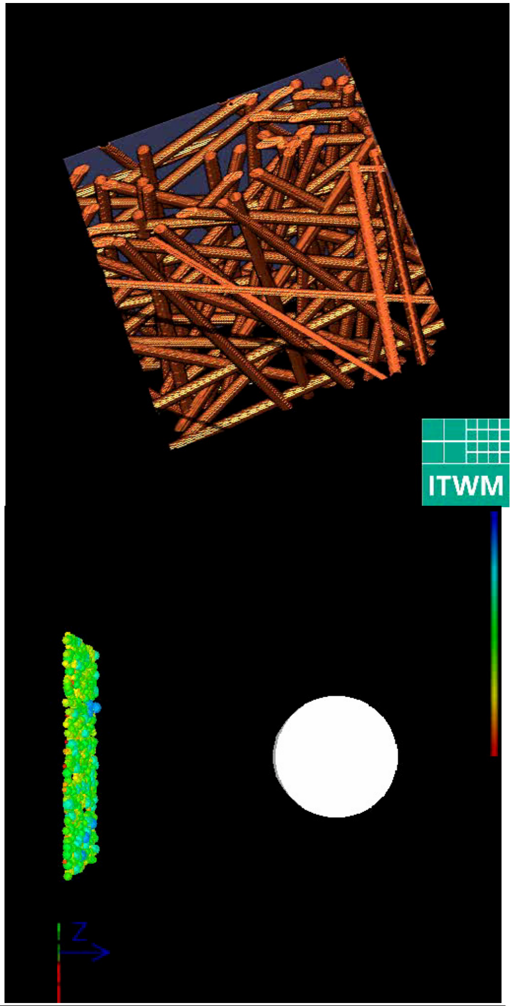
3. Simulation of Filtration Processes - Modeling

OPTIMIZATION

1. Determine parameters of the real filter
2. Generate 3d virtual structure
3. Compute flow field
4. Compute particle transport and deposition
5. Modify geometry
6. Compute filter efficiency, pressure drop, lifetime
7. New material parameters

ITERATION

Flow

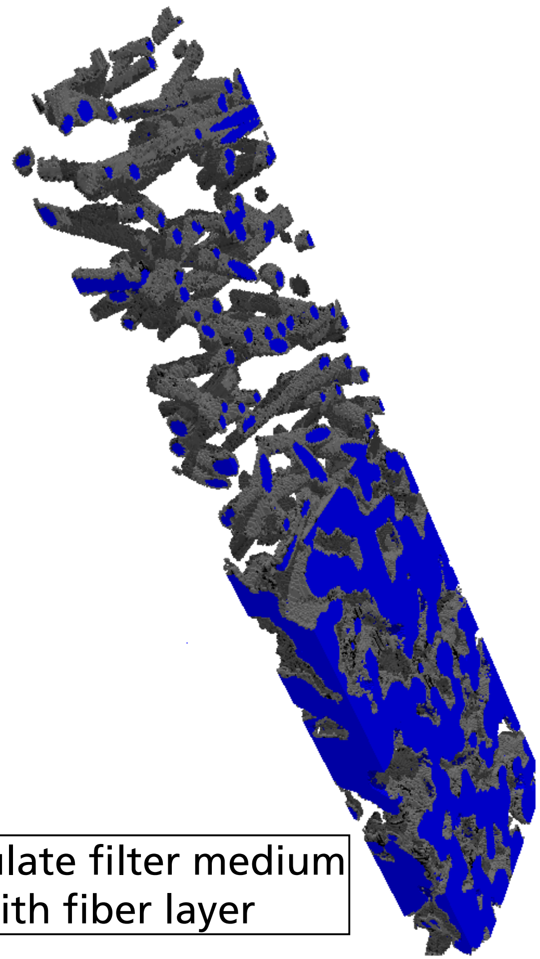


Single Fiber Simulation

3. Simulation of Filtration Processes - Simulation Results

Design study of a Diesel particulate filter

- What is the effect of an additional fibrous layer on top of a sintered substrate ?
- Soot particles (~80nm) are much smaller than voxels (1µm) -> porous deposition model
- Navier-Stokes-Brinkmann model to handle free and porous flow
- Permeability and maximum degree of filling of porous voxels are determined by high resolution single fiber experiments
- Some hundreds of millions of particles are needed for a lifetime computation



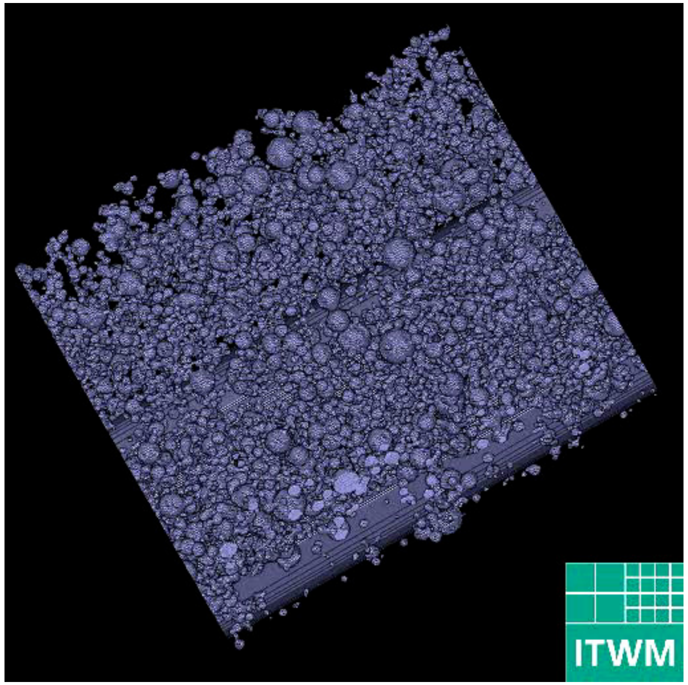
Particulate filter medium with fiber layer

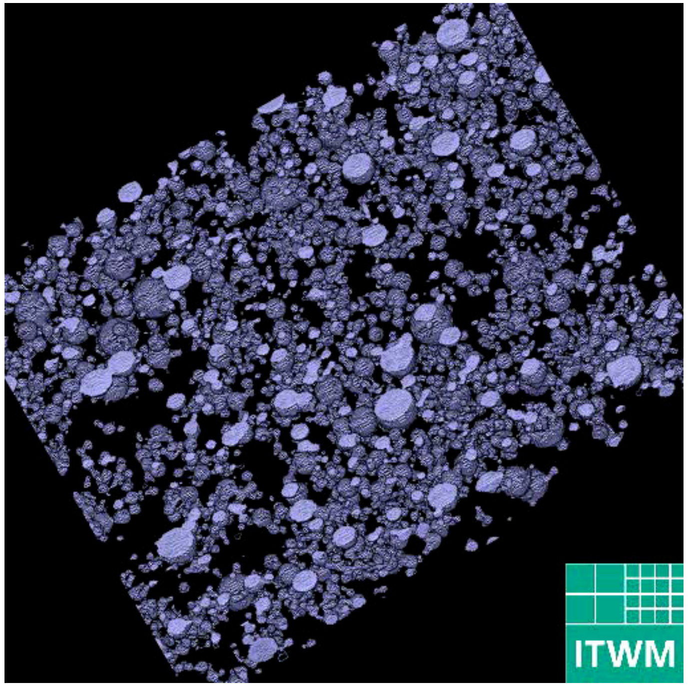
3. Simulation of Filtration Processes – Simulation Results

Single Fiber Nanosimulation

Soot Layer Cut-Out

Effective Microproperties

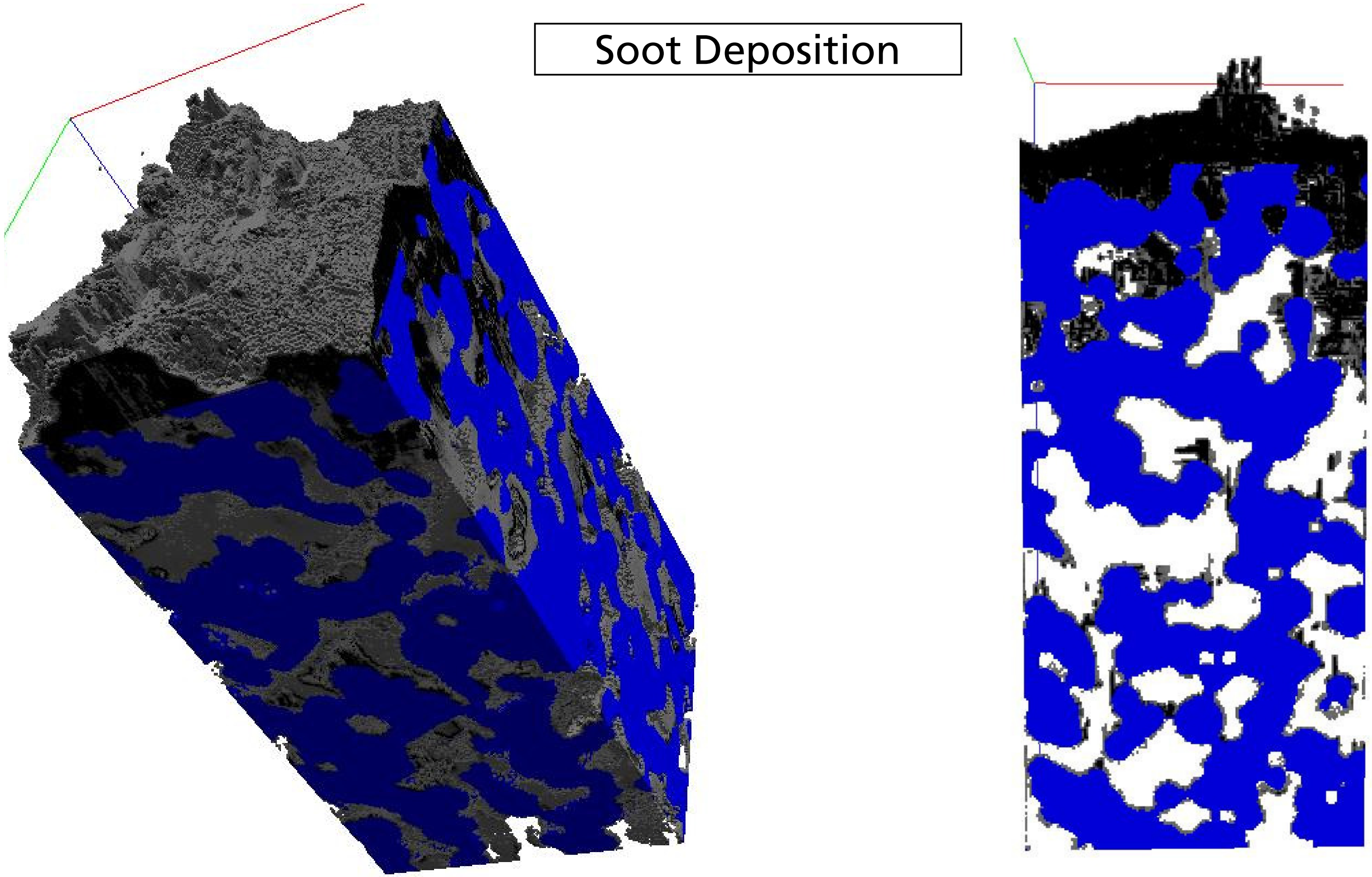




- Porosity = 85 %
- Permeability = 1e-15 m^2

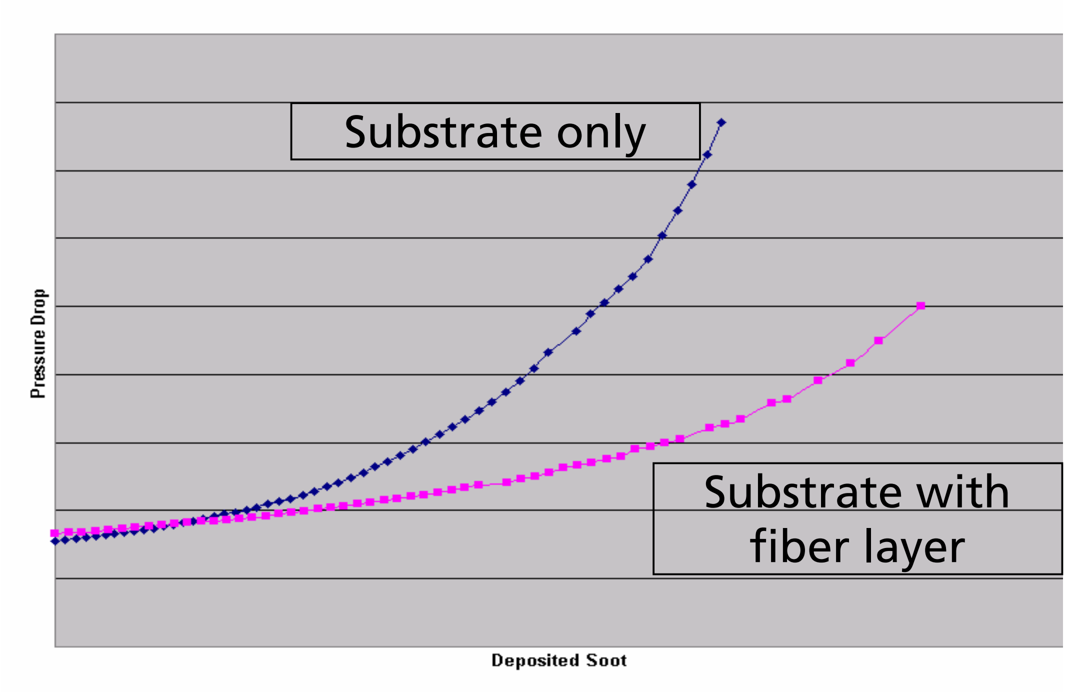
3. Simulation of Filtration Processes - Simulation Results

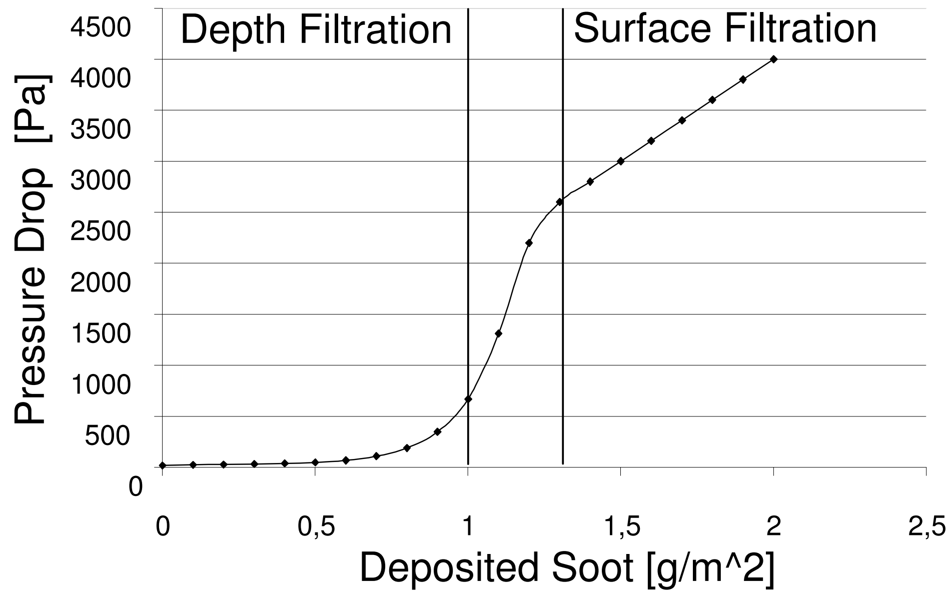
Soot Deposition



3. Simulation of Filtration Processes - Simulation Results

Pressure Drop Evolution





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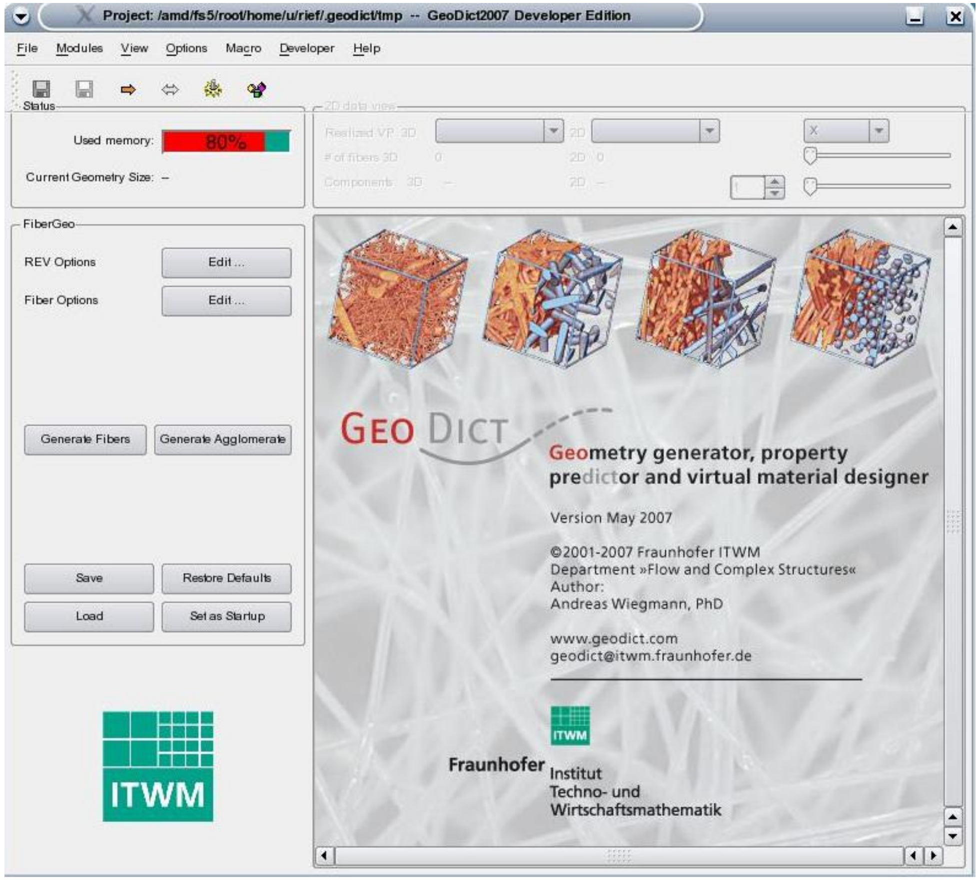
3. Simulation of Filtration Processes – Simulation Tools

- Software Tool GEO DICT

  - GeoFiber: Nonwoven generator
  - GeoSinter: Sinter structure generator
  - GeoProcess / GeoLayer: structure processing
  - FilterDict: Particle filtration
  - SatuDict: pressure-saturation relations
  - PoroDict: Pore size distributions



4. Summary and Future Developments

Today

- Virtual structure generation
- Effective flow properties
- Filter efficiencies
- Filter lifetime
- Coupling of scales
- All methods are available by software tools

GEO DICT

FILTER DICT

Tomorrow (DPF related)

- Extending virtual structure generation
- Coupling of length scales
- General particle shapes
- Fractional Slip Phenomena

Tomorrow (in general)

- Standard Tests
- Particle re-entry into fluid flow
- Electrostatic effects
- Particle-particle interaction
- Fluid-structure interaction

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GeoDict development teams

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Software for Generation, Simulation, Visualization:

GEO DICT

www.geodict.com

Thank you for attending this presentation.

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