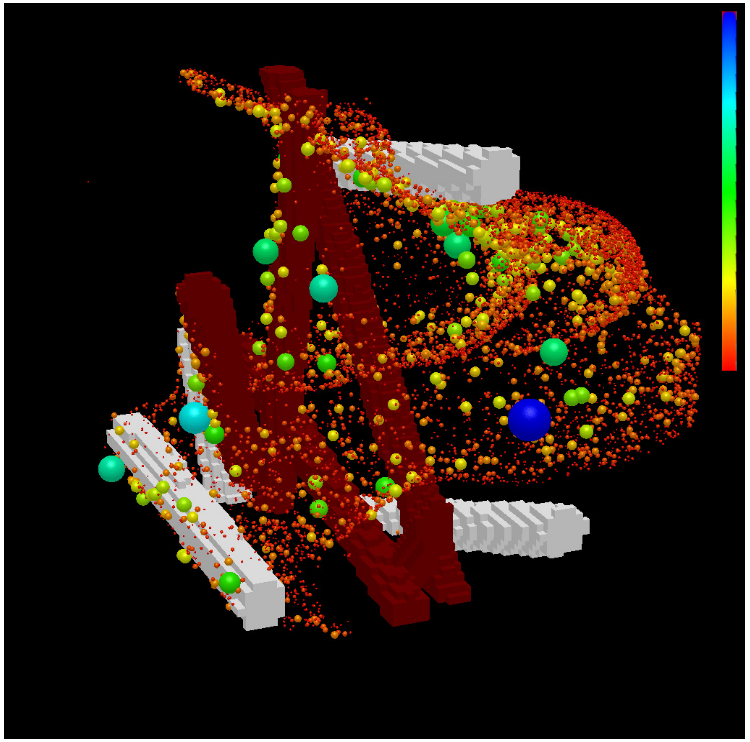
# Virtual Material Design and Air Filtration Simulation Techniques inside GeoDict and FilterDict



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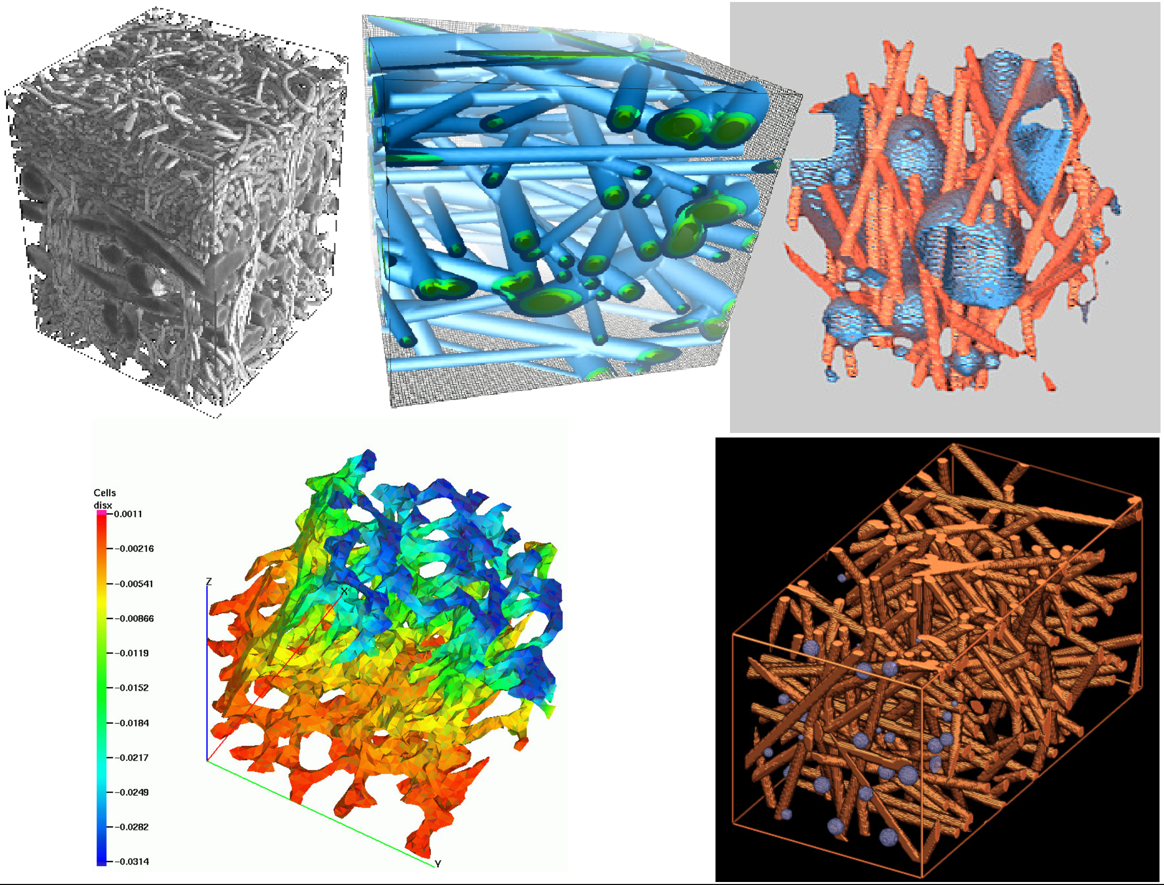
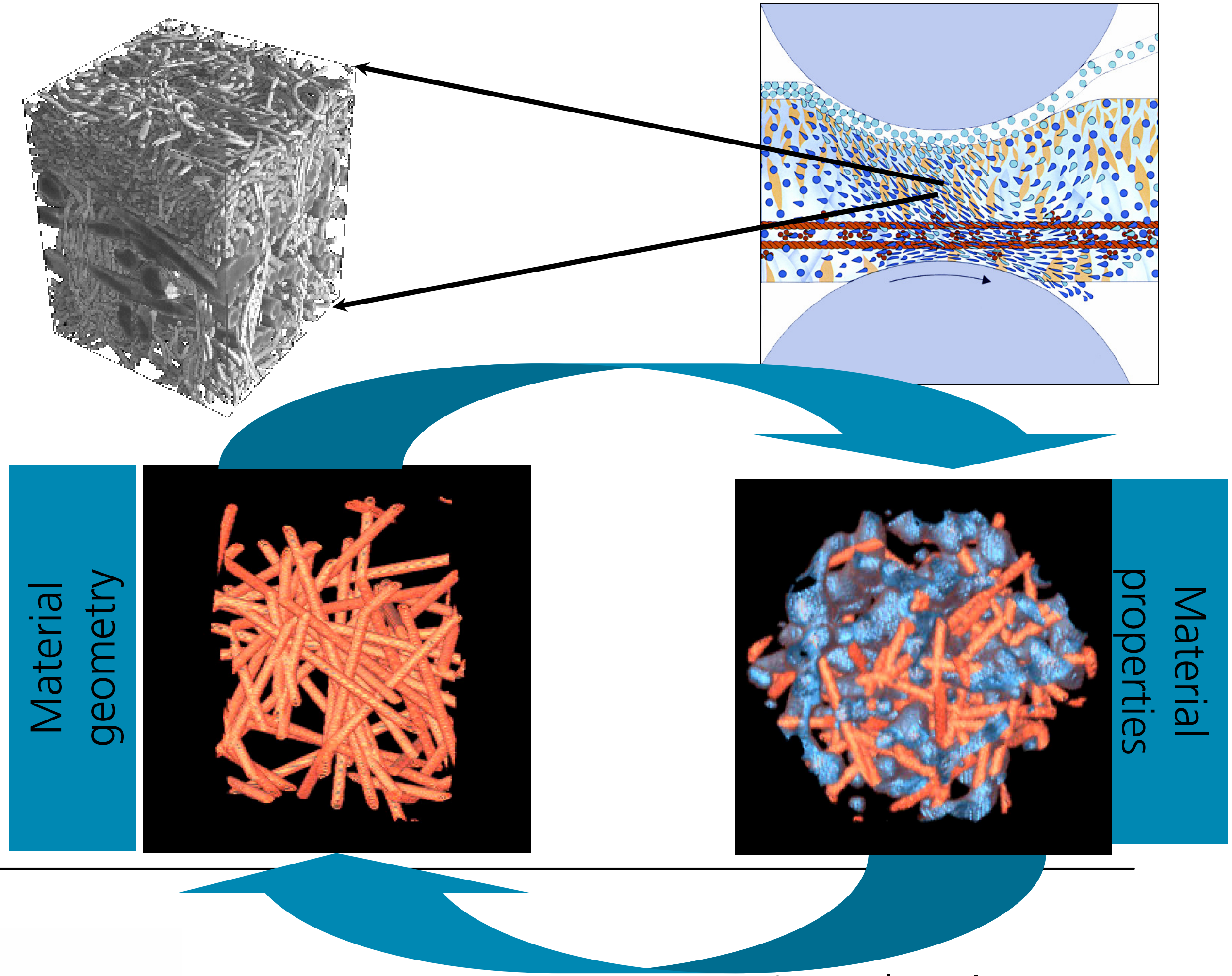
# Micro Structure Simulation and Virtual Material Design

- Structure generator + property simulator GeoDict / FilterDict
- Virtual three dimensional nonwoven models
- Computation of material properties
  - flow resistivity
  - permeability, capillary pressure
  - particle filtration, filter efficiency
  - filter lifetime
  - acoustic absorption
  - effective elasticity properties
- Sequences of simulations to optimize material geometry

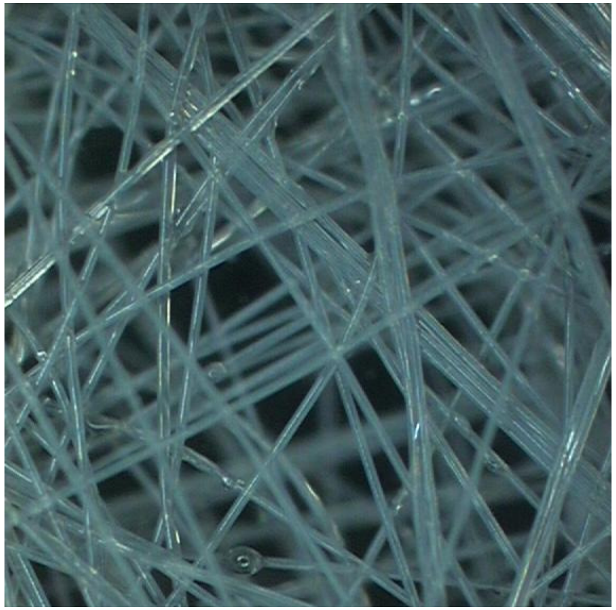


# The Virtual Material Design Cycle

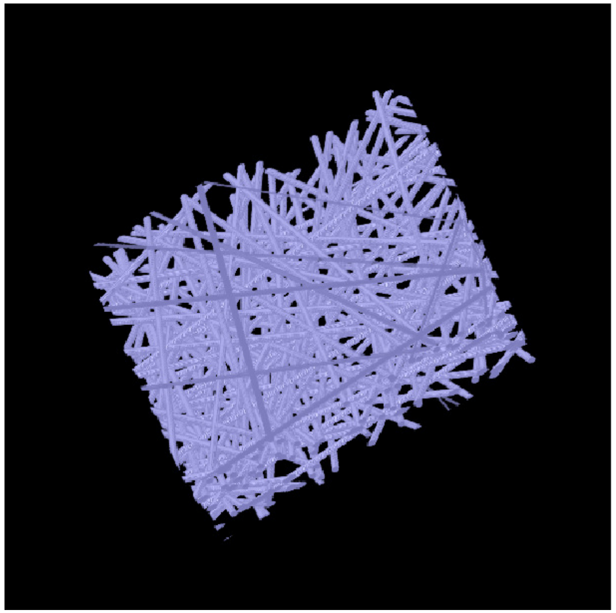
1. Identify parameters for real, existing material
2. Generate 3d geometry for parameters
3. Solve Stokes equations in 3d geometry
4. Compute filter efficiency in 3d geometry
5. Modify material parameters
6. Go back to 2.



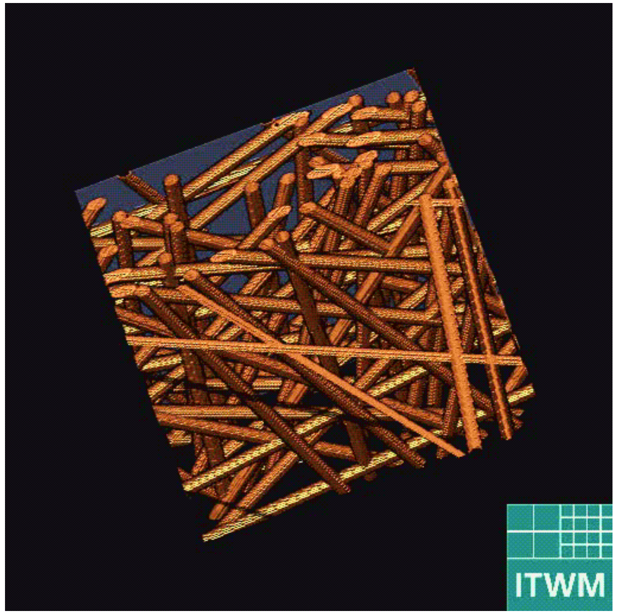
# The Geometric Nonwoven Model



Microscopy



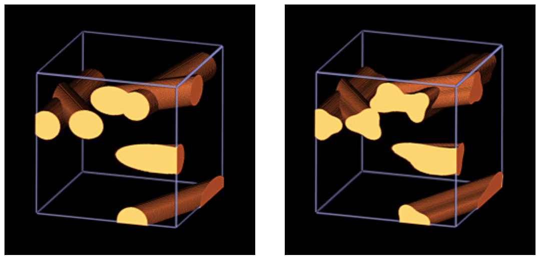
Fiber model



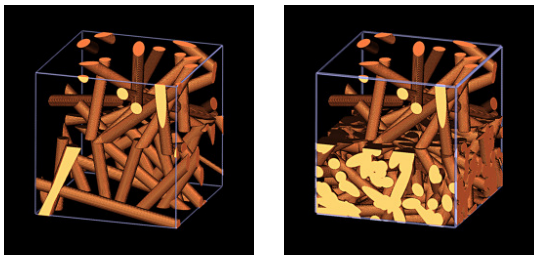

Flow simulation in the model

Possible variations:  for example

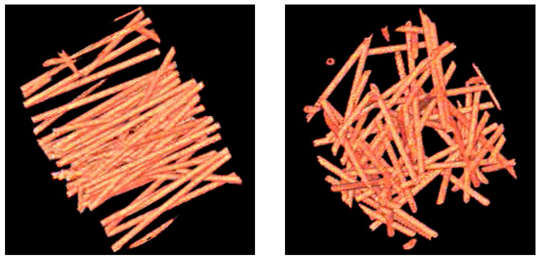
- Cross sections



- Layers

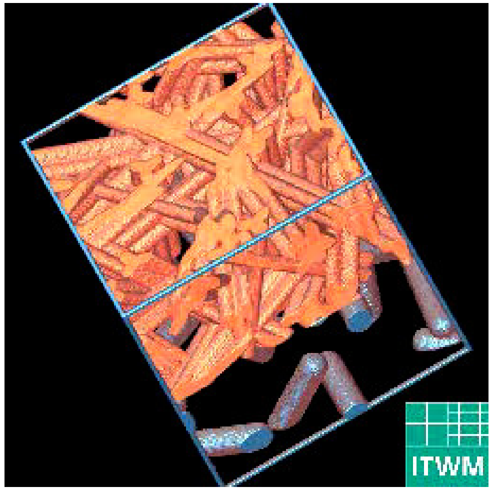


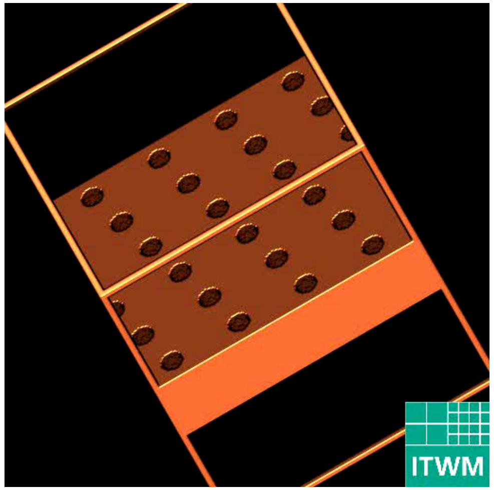
- Anisotropy

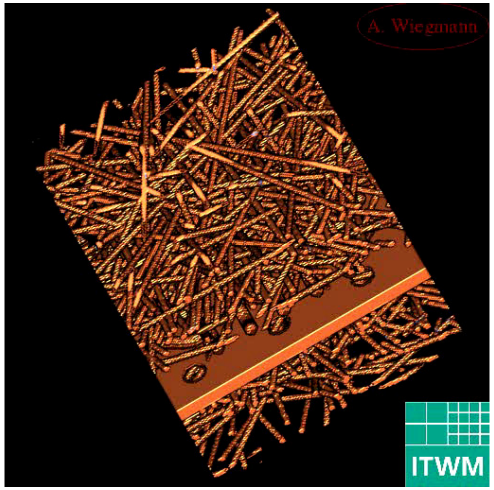


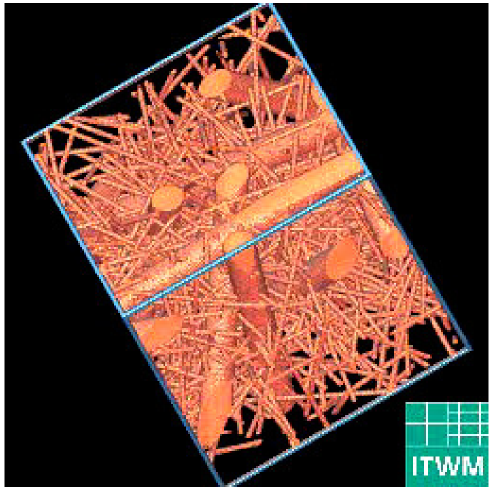
# Design Parameters for Nonwoven Filter Media

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









# Transverse Isotrope Fiber Orientation Probability and Nonwoven Material Density

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

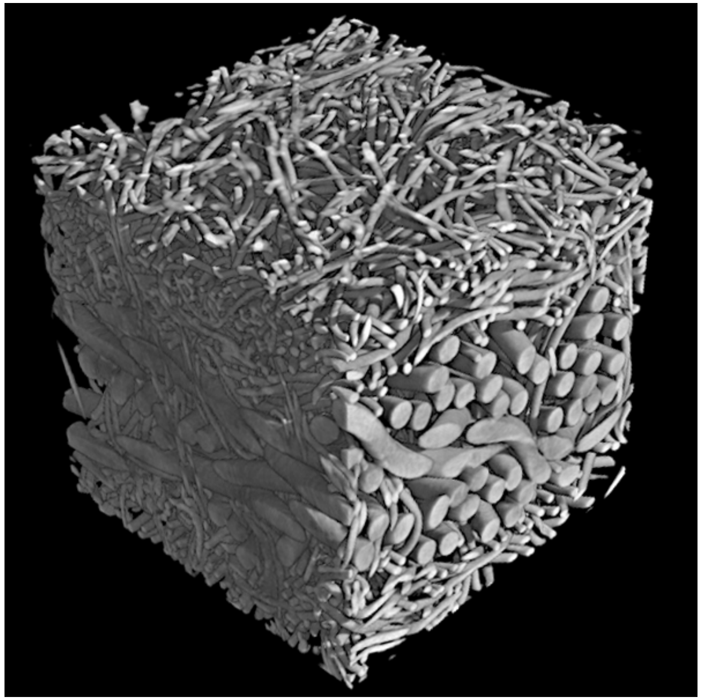
$$p(\vartheta,\varphi)=\frac{1}{4\pi}\frac{\beta\sin\vartheta}{(1+(\beta^2-1)\cos^2\vartheta)^{3/2}} \quad , \qquad \vartheta\in[0,\pi),\varphi\in[0,2\pi)$$

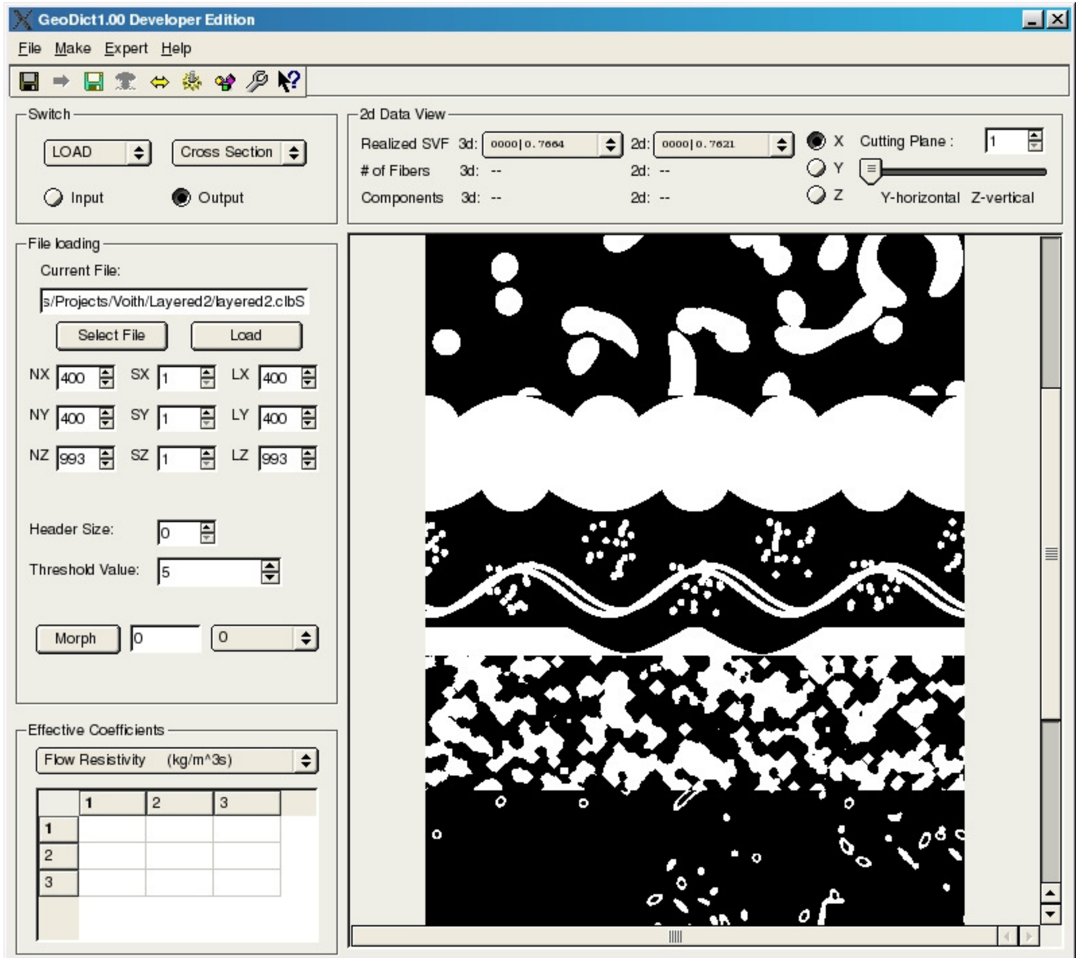
- For two fiber types with probability $0 \leq p \leq 1$ and $1-p$, generate random number $n$ between 0 and 1 and select first type if $n \leq p$ and second type if $n>p$.

- 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.

# Real and Generated Three Dimensional Images






Synchrotron image vs. generated structure (paper dewatering felt)

# Eulerian Description of Stationary Stokes Flow

$$\mu\, \Delta\vec{u} + \vec{f} = \nabla p \quad : \text{ momentum balance}$$

$$div\, \vec{u} = 0 \quad : \text{ incompressible conservation of mass}$$

$$\vec{u} = 0 \text{ on } \Gamma \quad : \text{ no-slip on fiber surfaces}$$

- $\vec{f}$ : force in direction of the flow,
- $\vec{u}$ : 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.

# Filter Efficiency Model

**A) Testdust:**
Sphere radii
Specific weight
Electrostatic charges

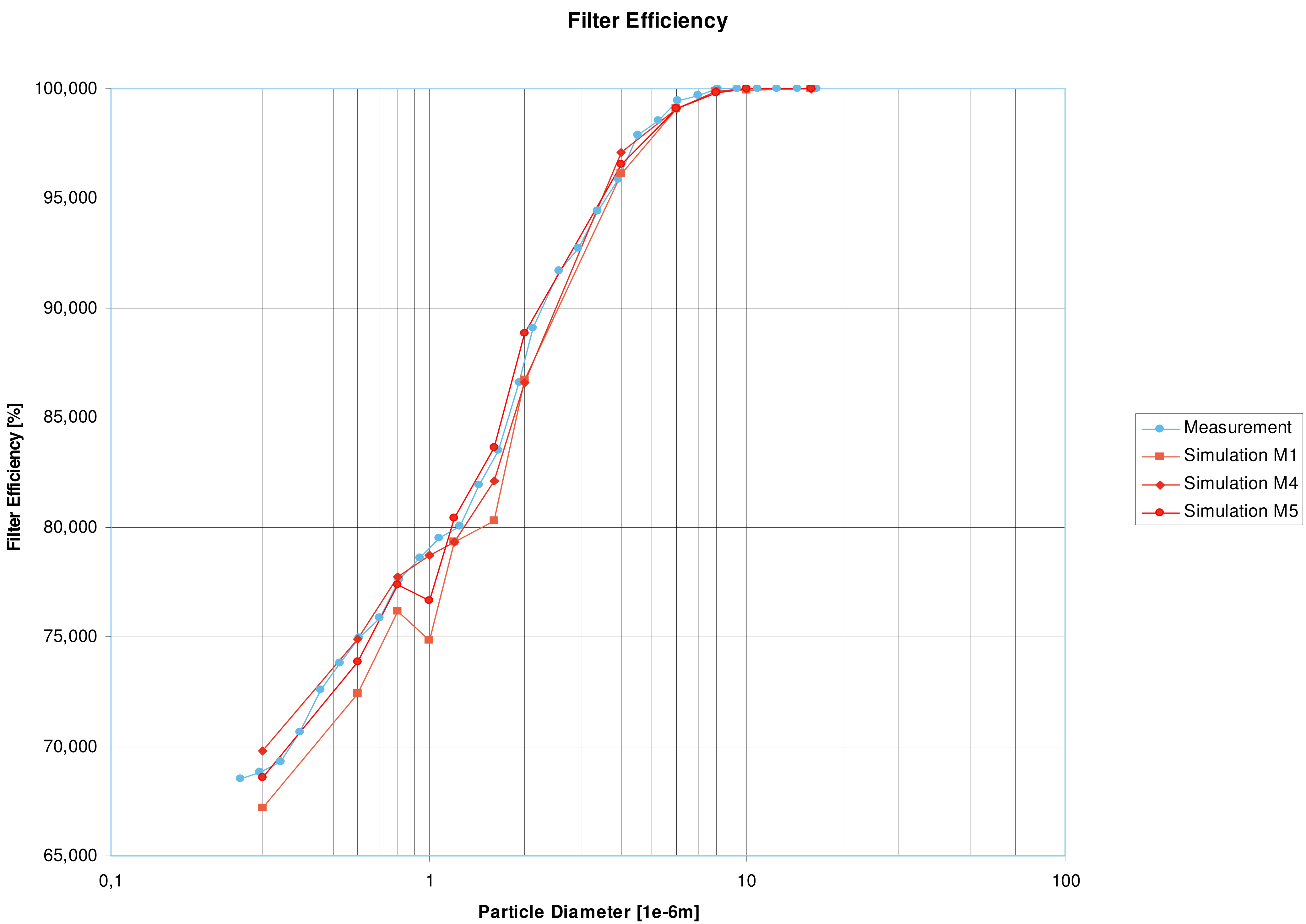
**B) Fluid:**
Viscosity
Density
Temperature
Mean flow velocity

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

**D) Interaction:**

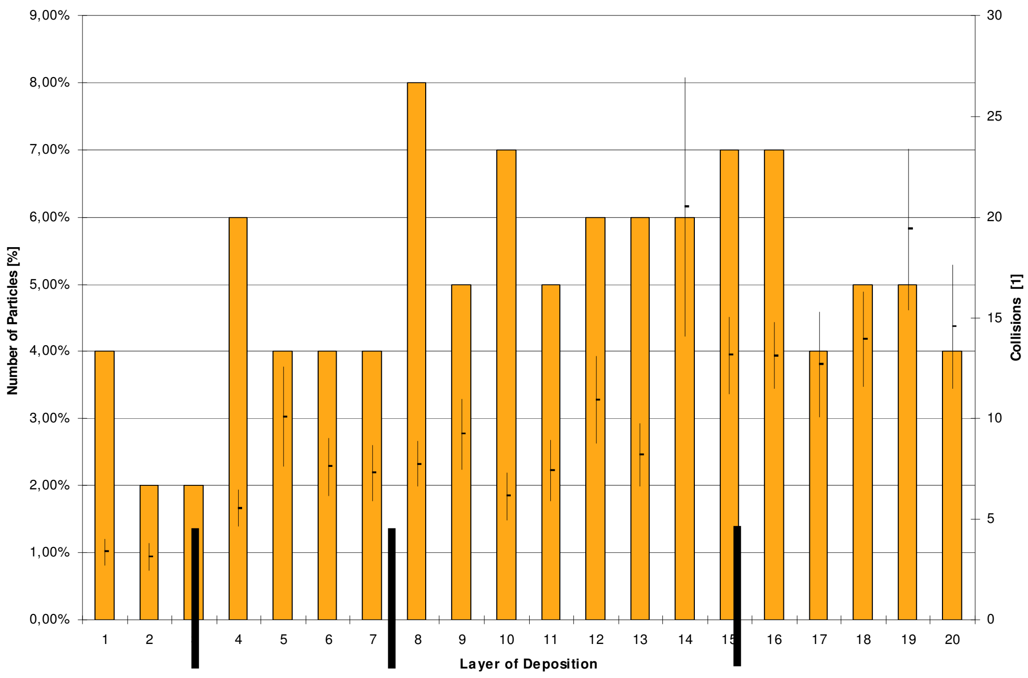
| | |
|---|---|
| Flow & pressure drop : | B & C |
| Electrostatic field: | C |
| Friction: | A & B |
| Diffusion: | A & B |
| Collision: | A & C |
| Adhesion: | A & C |
| Electrostatic attraction: | A & C |
| Particle Paths: | A,B & C |

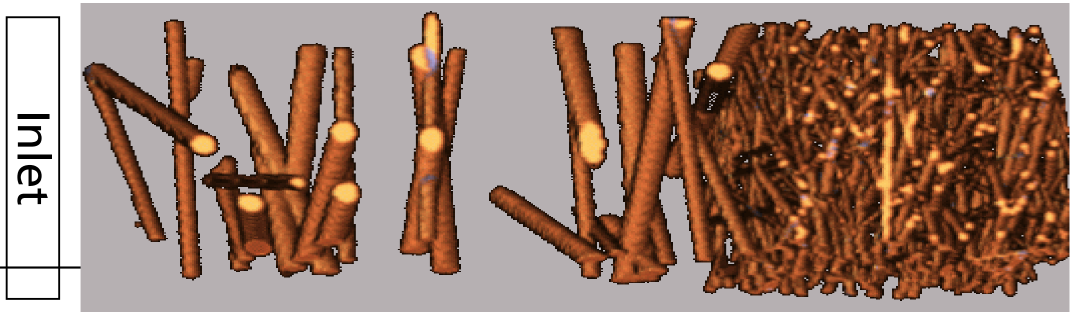
**E) Deposition due to:**
Inertial impact + adhesion
Diffusion + adhesion
Electrostatic attraction +adhesion
Sieving

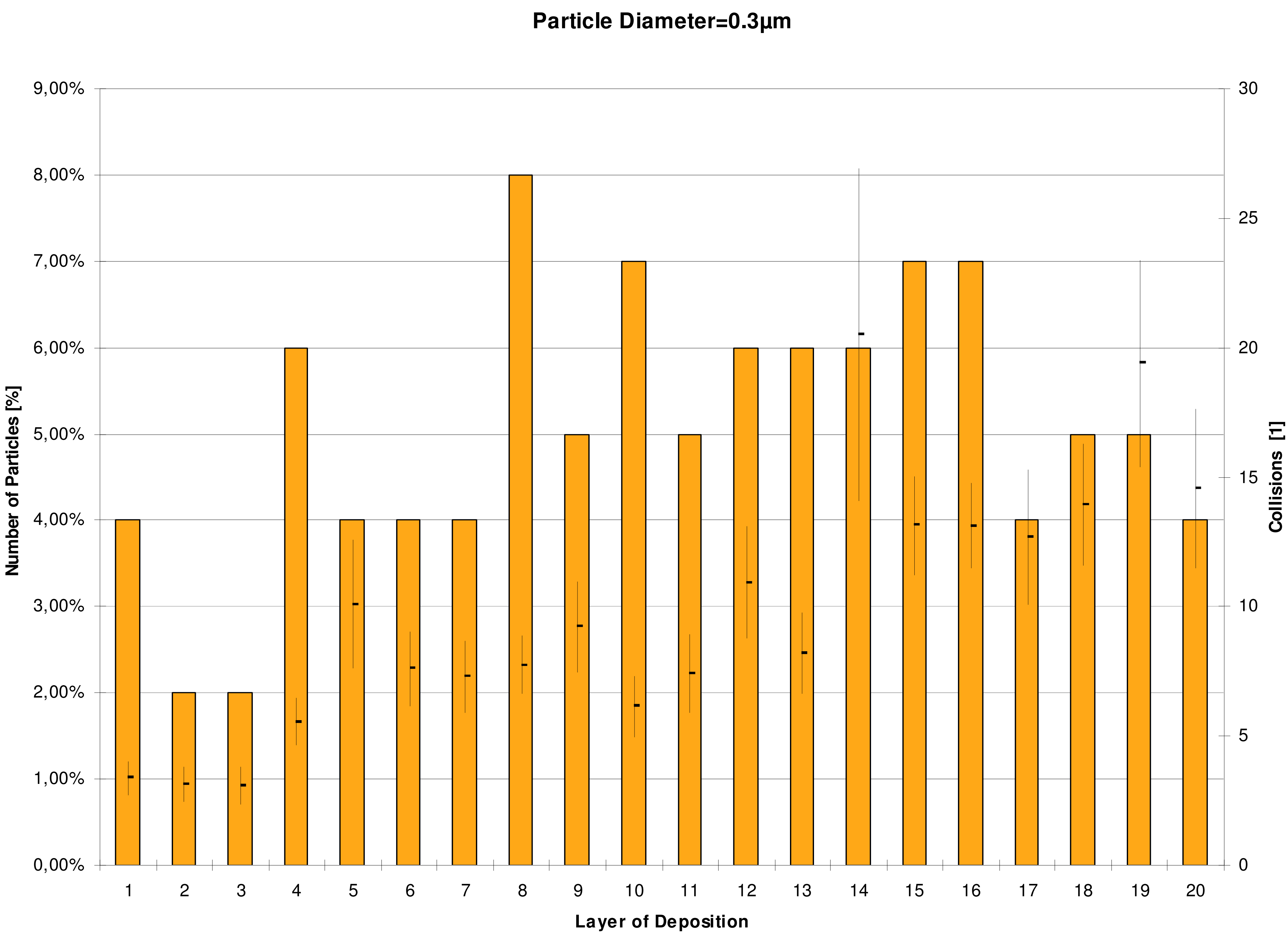

Filter Efficiency
100,000
95,000
90,000
85,000
80,000
75,000
70,000
65,000
Filter Efficiency [%]
0,1
1
10
100
Particle Diameter [1e-6m]
Measurement
Simulation M1
Simulation M4
Simulation M5

# Deposition Diagram

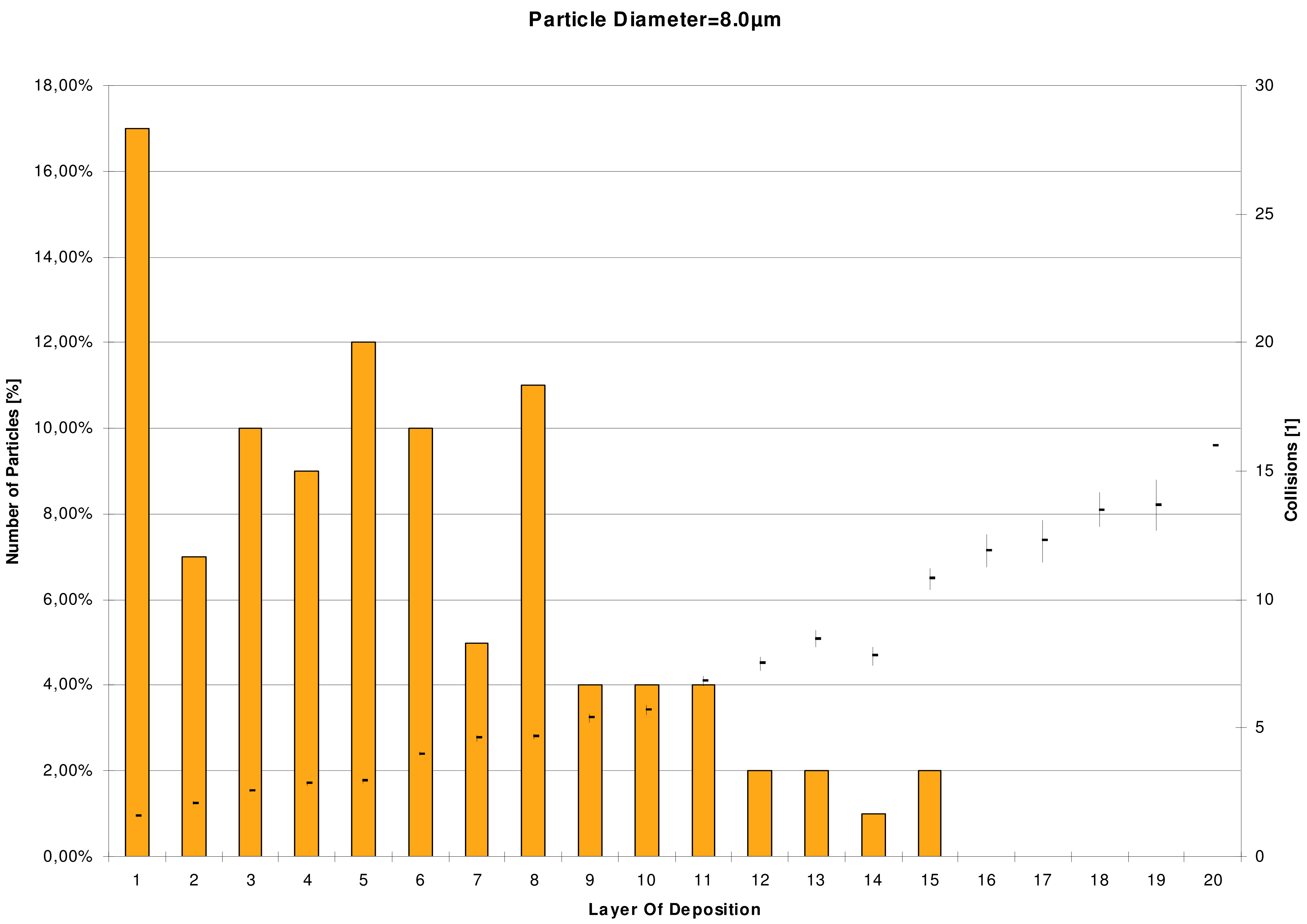
- Deposition locations are 20 64µm layers.
- Orange: particle numbers
- Lines: mean value and standard deviation of number of collisions
- Example: Layer 15 contains 7% of the filtered particles. Those had on average 13.15 collisions with standard deviation 1.9
- 4 layers of gradient material indicated by thick black lines:





Particle Diameter=0.3µm
Number of Particles [%]
Collisions [1]
Layer of Deposition
9,00%
8,00%
7,00%
6,00%
5,00%
4,00%
3,00%
2,00%
1,00%
0,00%
30
25
20
15
10
5
0
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20


Particle Diameter=8.0µm
Number of Particles [%]
Collisions [1]
Layer Of Deposition
18,00%
16,00%
14,00%
12,00%
10,00%
8,00%
6,00%
4,00%
2,00%
0,00%
30
25
20
15
10
5
0
1
2
3
4
5
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7
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11
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13
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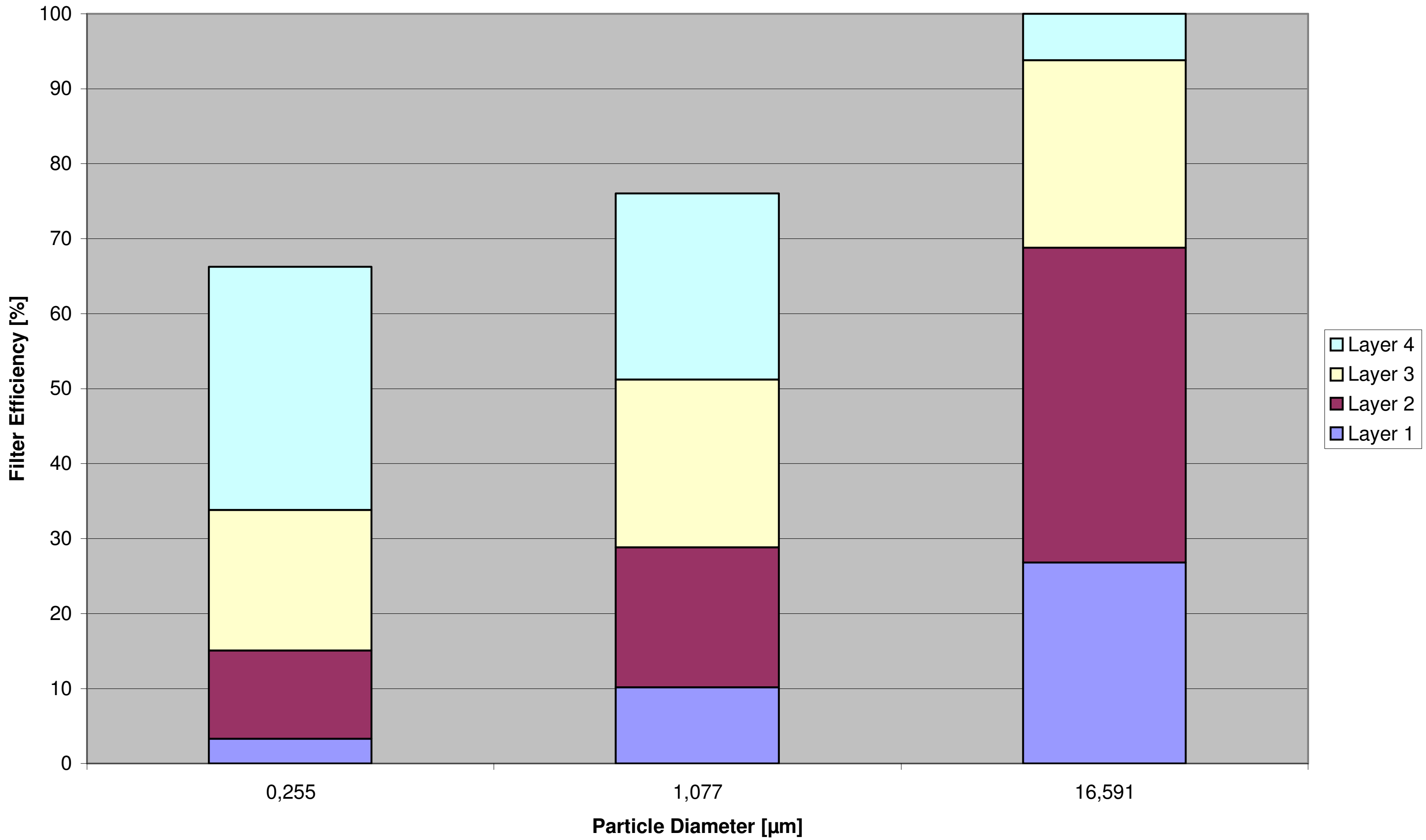
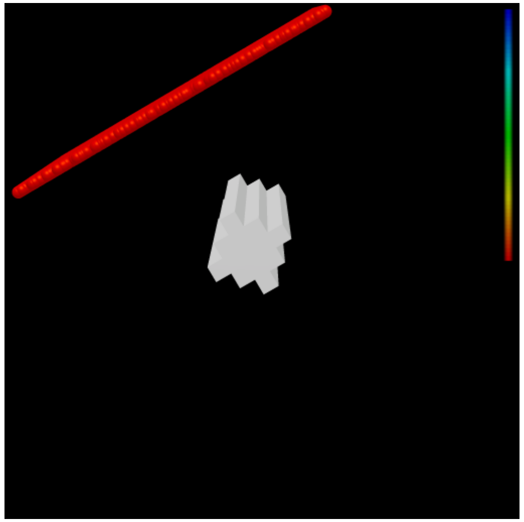
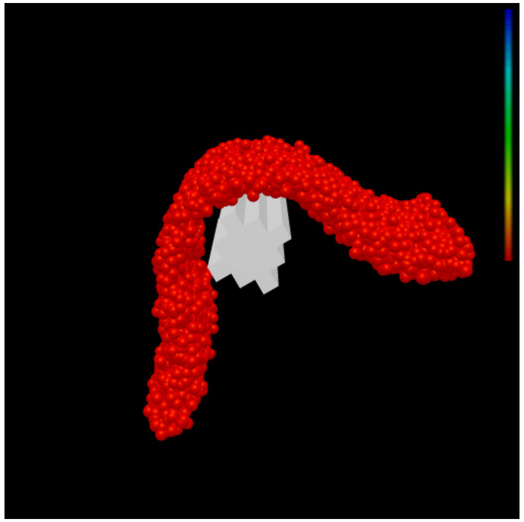
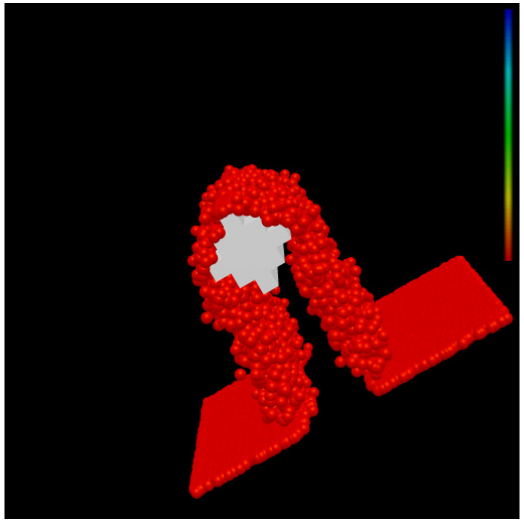
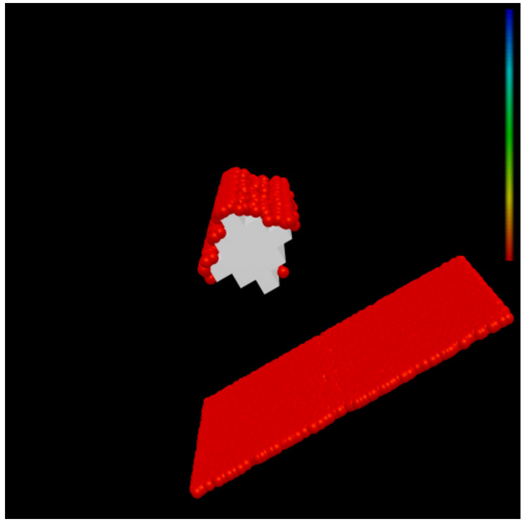
15
16
17
18
19
20

# Deposition of Different Sized Particles in the Different Layers

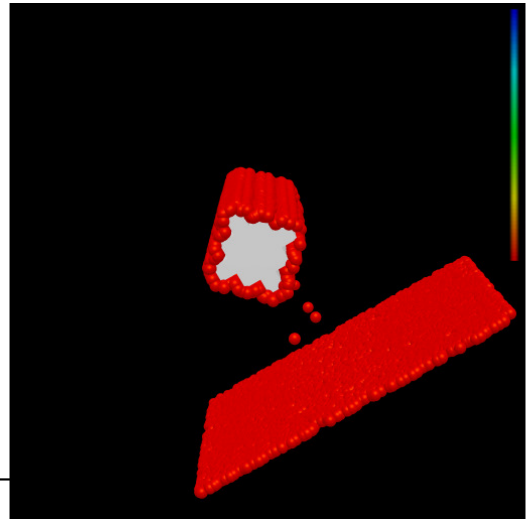


# Influence of Electrostatic Surface Charges

**Deposition of uniform sized particles on a single fiber in the absence and in the presence of an electric field:**

- **deposition rate doubles,**
- **particles also stick to the „back“ of the fiber.**



# 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 |
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| Friction: | A & B |
| Diffusion: | A & B |
| Collision: | A & C |
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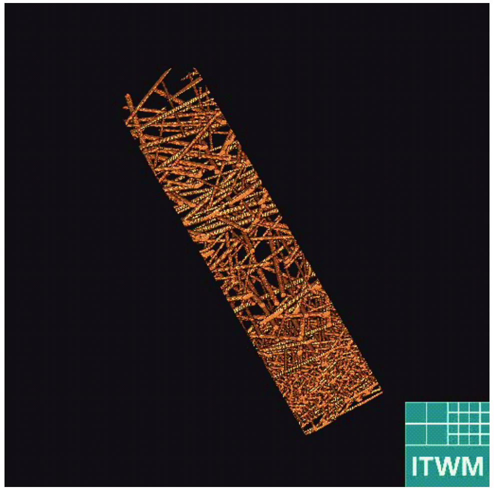
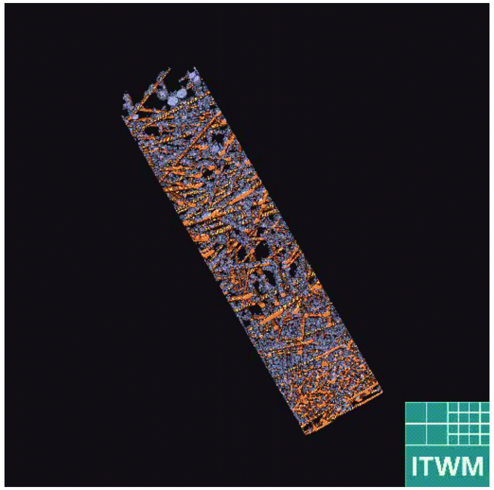
| Particle Paths: | A, B & C |

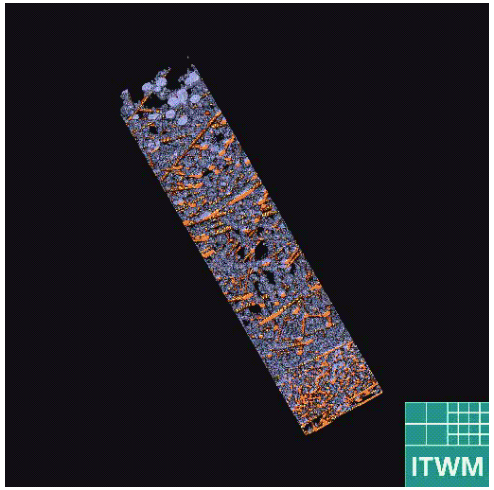
**E) Deposition due to:**
Inertial impact + adhesion
Diffusion + adhesion
E-static attraction +adhesion
Sieving

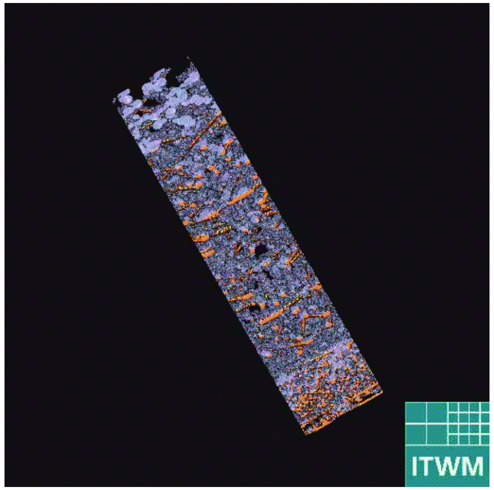
**F) Clogging:**
Deposited particles determine new geometry model, including permeable voxels

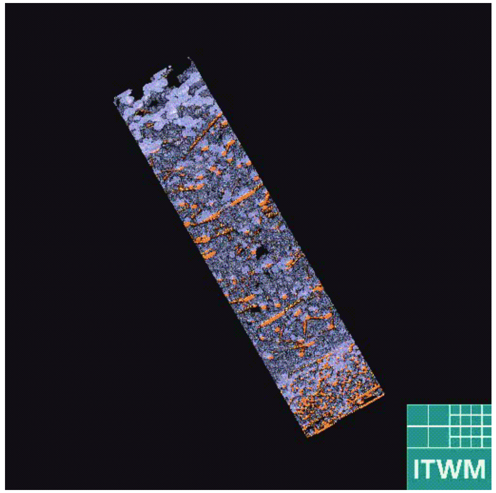
# Filter Lifetime Simulation: from Clean to End-of-Life

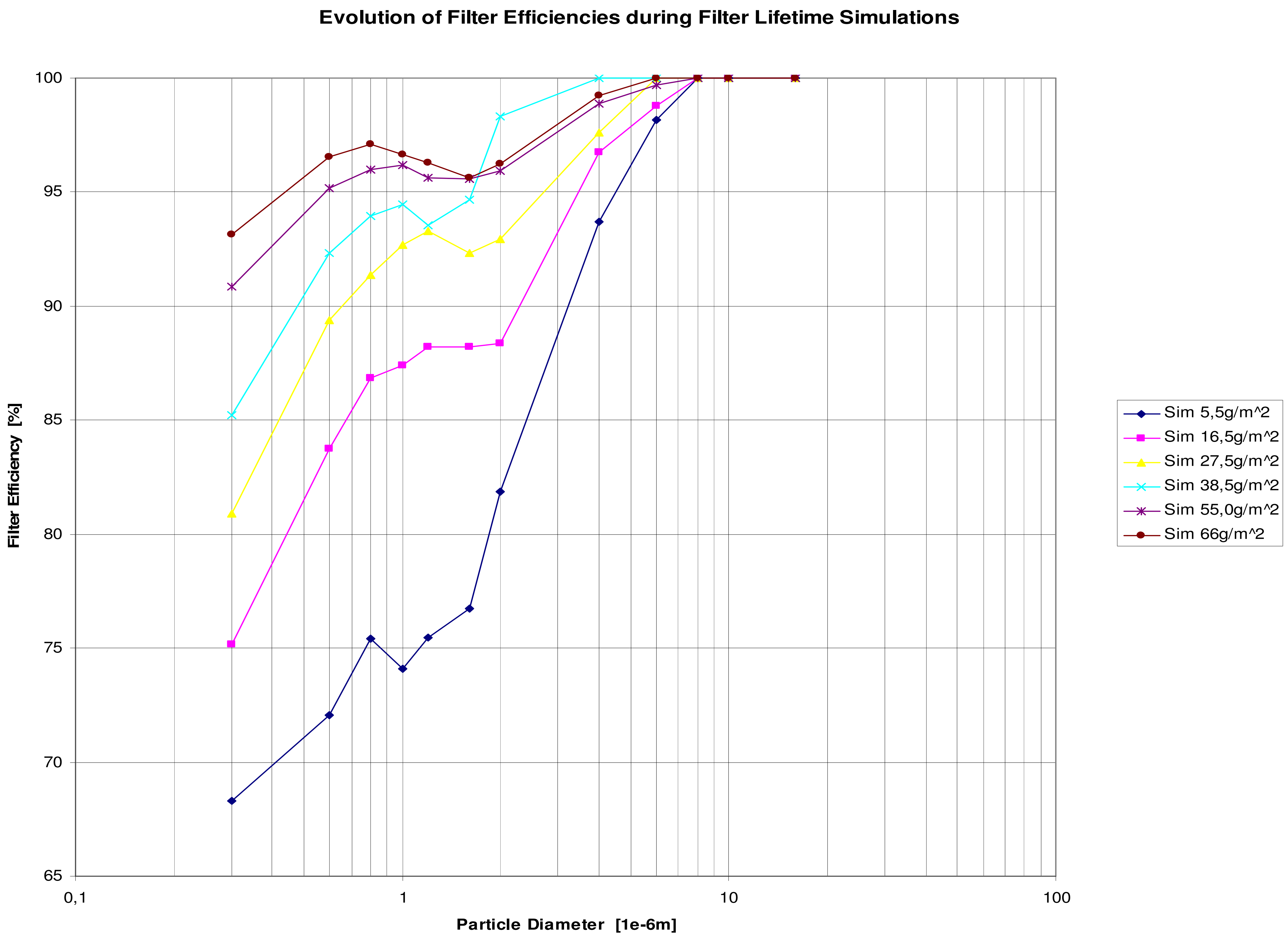


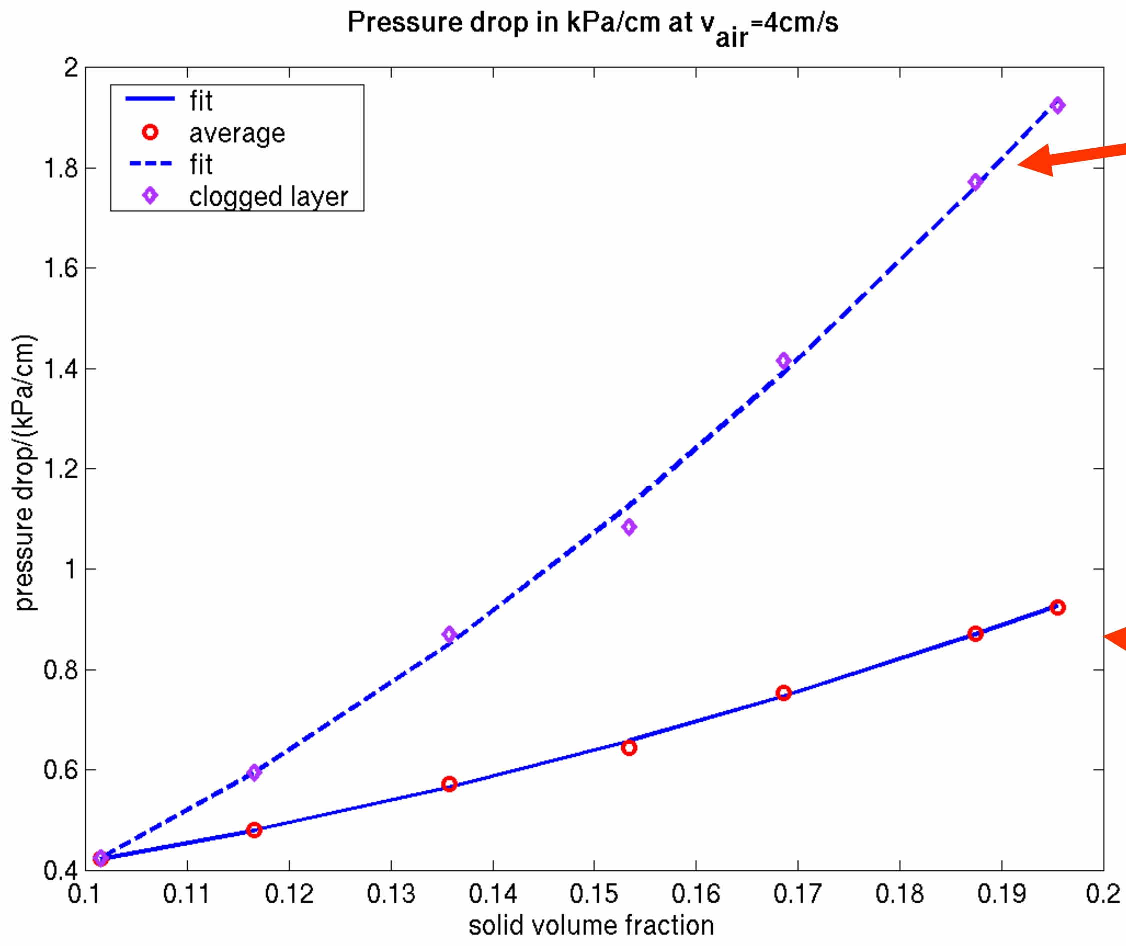





Evolution of Filter Efficiencies during Filter Lifetime Simulations
Filter Efficiency [%]
100
95
90
85
80
75
70
65
0,1
1
10
100
Particle Diameter [1e-6m]
Sim 5,5g/m^2
Sim 16,5g/m^2
Sim 27,5g/m^2
Sim 38,5g/m^2
Sim 55,0g/m^2
Sim 66g/m^2

# Time Dependent Pressure Drop




in the loaded portion of the media

on average over the whole media

# Summary

Filtration properties of filter media can be computed and optimized

1. 3d geometry from tomography or mathematical model
2. Model media, fluid flow and the dirt as well as their interactions
3. MPPS: small particles filtered by diffusion, large ones by sieving
4. Layered materials give more uniform clogging, can have multiple properties
5. Study of electrostatic effects on filtration is on its way
6. Study of subvoxel effects is on its way
7. Virtual filter material design is possible!

# GeoDict and FilterDict: Contributors from ITWM

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