# **Concepts for Modelling Filter Media and Simulating Filtration Processes**

Andreas Wiegmann CEO, Math2Market GmbH April 11<sup>th</sup>, 2017







# Thanks to collaborators at Math2Market, Fraunhofer ITWM, and elsewhere

#### Math2Market:

Mehdi Azimian, Jürgen Becker, Liping Cheng, Erik Glatt, Barbara Planas, Christian Wagner, Rolf Westerteiger.

#### ITWM:

Heiko Andrä, Oleg Iliev, Mathias Kabel, Ralf Kirsch, Peter Klein, Sven Linden, Stefan Rief, Katja Schladitz, Konrad Steiner, Aivars Zemitis.

#### **Formerly** at ITWM:

D. Elvikis, I. Ginzburg, D. Kehrwald, Z. Lakdawala, A. Latz, J. Ohser, D. Reinel-Bitzer, V. Rutka, K. Schmidt, A. Kumar Vaikuntam, Q. Zhang.

#### Others:

- Martin Lehmann, Alexander Killian & Friedemann Hahn of MANN+HUMMEL GmbH
- Markus Knefel, Engelbert Wegenke & Dominik Herper of GKD
- Friedrich Edelmeier, Frank Meyer, Mirko Theiß & Alexander Mantler of Haver & Boecker
- Graham Rideal, Whitehouse Scientific
- Andreas Schindelin, then of Argo-Hytos GmbH
- Jörg Adler, Uwe Petasch & Lars Mammitsch of Fraunhofer IKTS
- S. Jaganathan & H. Tafreshi, then at Nonwoven Cooperative Research Center, NC
- Nathalie Bardin-Monnier & Pierre-Colin Gervais, then at Nancy University





# Math2Market GmbH and its GeoDict software Some background information

- Math2Market creates & markets software to analyze/design porous & composite materials based on the material's geometric inhomogeneity
- M2Ms software is called GeoDict, the Digital Material Laboratory
- GeoDict works on μCT-based, FIB-SEM-based and intrinsic models
   in all cases, the computer representation consists of 3-D images
- M2M was spun off in 2011 from Fraunhofer Institute for Industrial Mathematics
- M2M is based in Kaiserslautern, Germany, and privately owned
- M2M has more than 150 clients from around the world





# Math2Market GmbH Location and contact



Stiftsplatz 5 67655 Kaiserslautern

Germany

Phone + 49 631 / 205 605 0 Fax + 49 631 / 205 605 99

www.geodict.com







# **Math2**Market GmbH Promoted Industries

**Filtration** 

Mostly automotive, filter media & filters for water, sludge, oil, air and fuel

Electrochemistry

Fuel cell media & battery materials, catalyst materials

Composites

CFRP, GFRP, mostly automotive, lightweight materials

Oil and Gas

**GEODICT** 

Digital rock physics, digital sand control



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#### About the need for modelling and simulation

- The function of porous and composite materials results from the choice of raw materials and their micro structure, i.e. the distribution of the constituents, e.g. fibers, in space.
- The power of simple models to predict the effects of the micro structure is limited.
- μCT and FIB-SEM provide 3D images of existing materials with unprecedented resolution.
- From these, one can compute the material's properties to match measured properties.
- Models also convert into 3D images. From these, material properties can be determined without the need to manufacture the new materials first.
- Instead of letting universities or institutes develop next generation materials, companies keep this knowledge in-house, by letting their own employees run the digital experiments.
- The Difficulty of the Math & Software Know-How is such that even the largest companies cannot do it all by themselves.
- 10 of the top 100 market capitalized companies are M2M clients, including Shell and P&G, who introduced the concept of open innovation about 2 decades ago.
- In the future, companies will need to be on top of their materials. The days of trial and error are coming to an end as powerful research tools deliver scientific data of unprecedented depth.

  [http://www.economist.com/technology-quarterly/2015-12-05/new-materials-formanufacturing]
- At M2M, we believe this is true in particular for filter media the future has already begun!

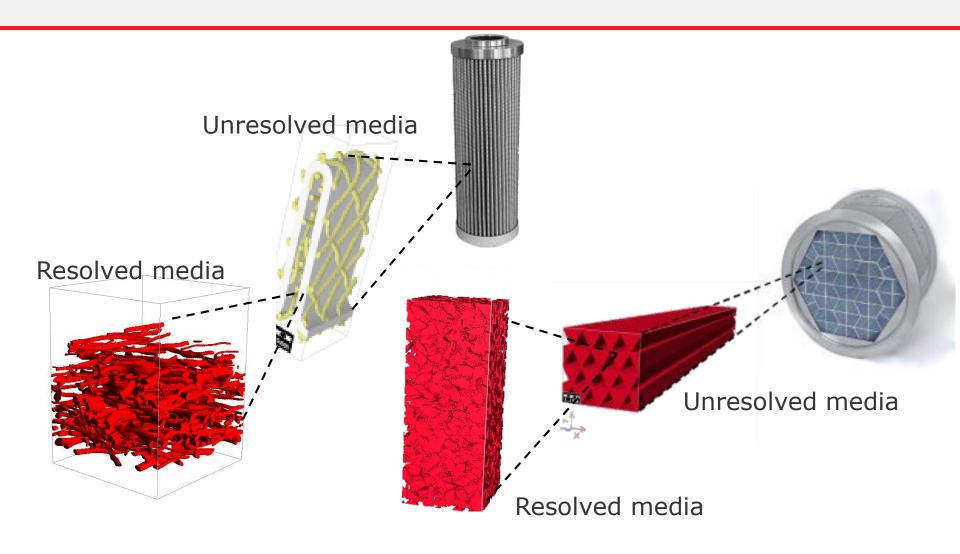




# Media models, pleat models and filter models



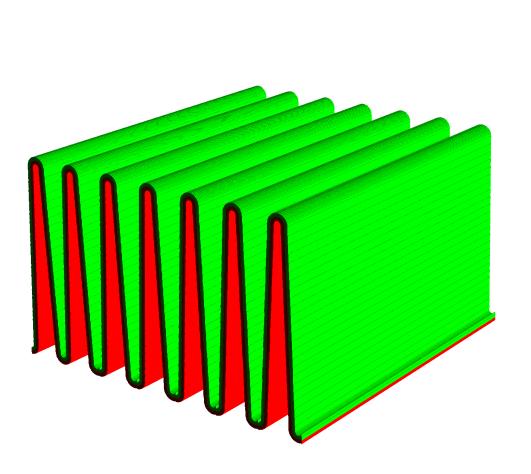
#### Simulate filtration at different scales

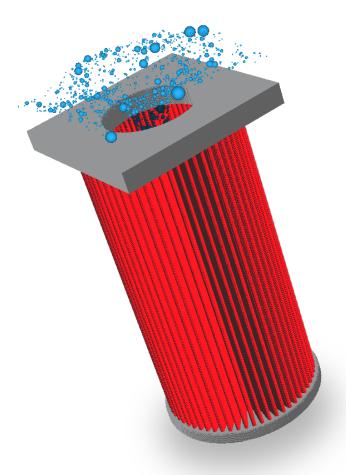






#### **Create Pleat scale and Element scale models**







## Simulate on µCT scans

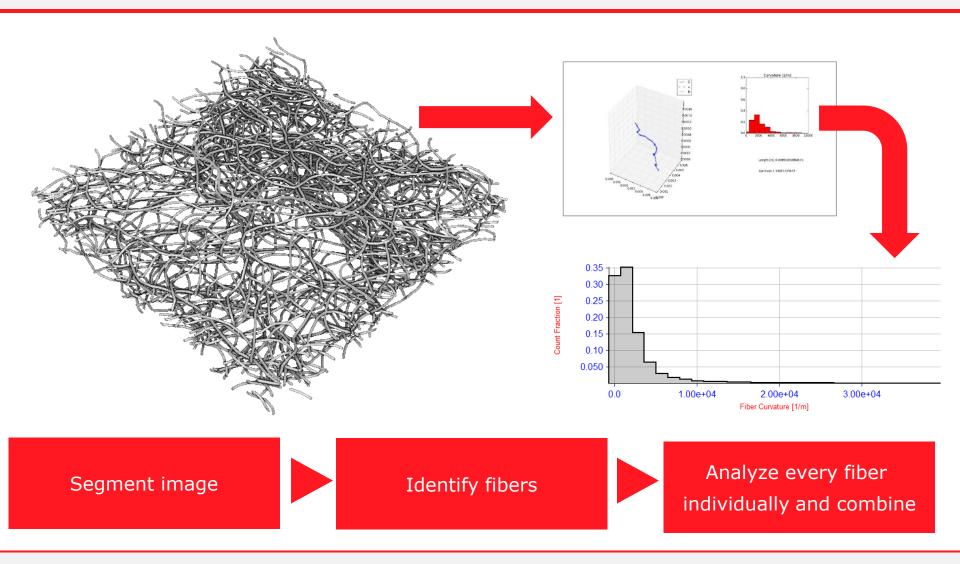
- (+) Allows simulations on real filter structures
- (-) Modifications of the filter structure are not possible

Aim: create a model that mimics the tomography first, then modify it to find structures with even better properties!





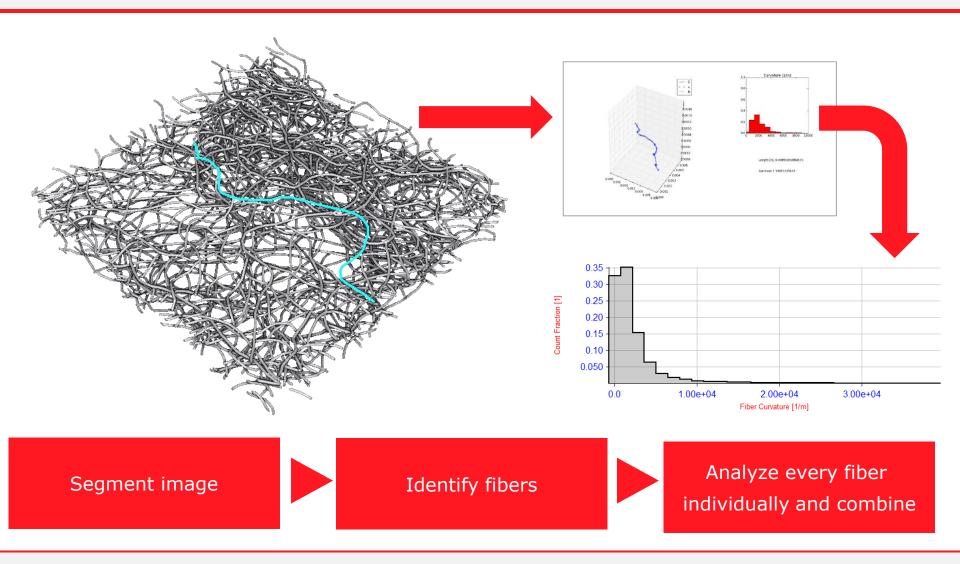
#### 3. Fiber Curvature







#### 3. Fiber Curvature



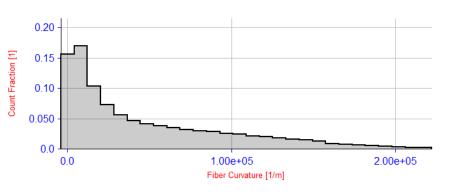


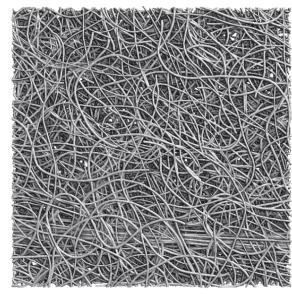


# Estimated parameters used to generate a model of the gas diffusion layer

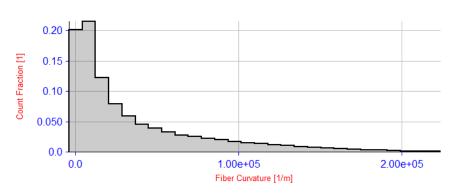


Original structure





Modeled structure





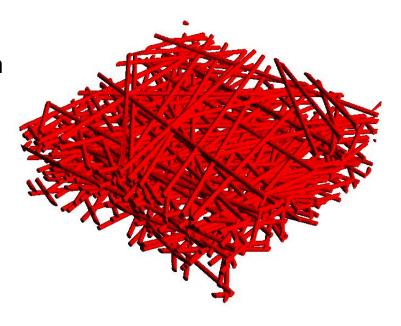
#### Create 3D structure models

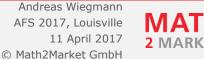
#### Input parameters needed (straight fibers):

- Porosity
- Fiber type: cross sectional shape, diameter, length
- Fiber orientation tensor
- Thickness (height) of the filter media

#### Parameters might be

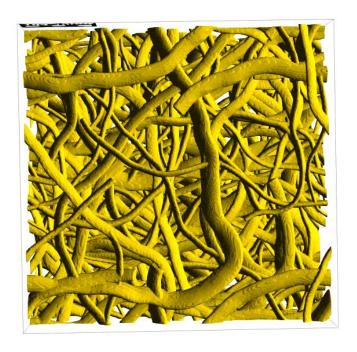
- known from manufacturing process
- measured experimentally
- measured from CT image





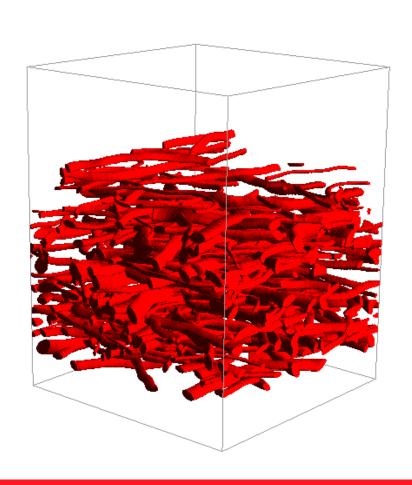
#### Create an oil filter model

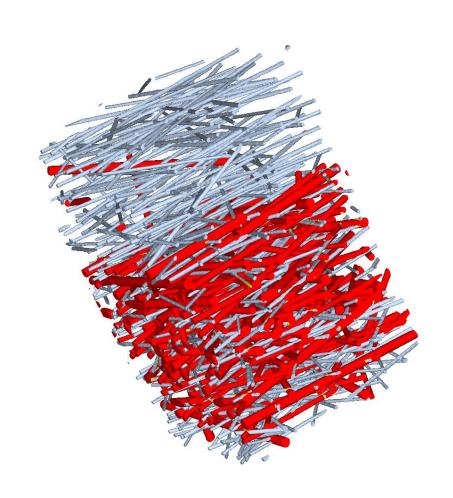
- Ellipsoidal cross section, diameter distribution
- Curved fibers
- Fibers oriented in xy-plane
- 500 x 500 x 650 grid cells,1 μm voxel length





#### Create cellulose and layered media scale models





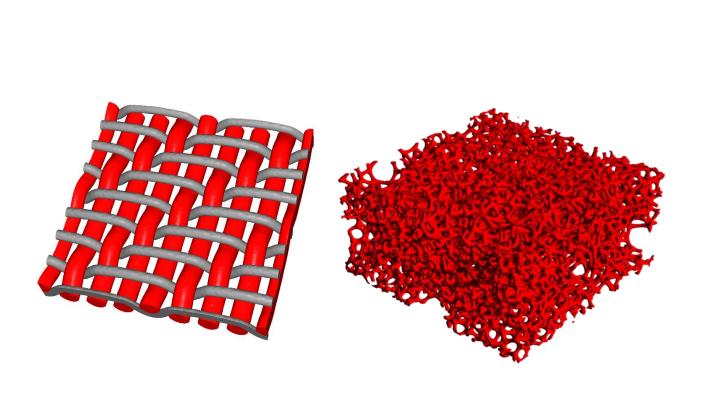
Cellulose nonwoven

Layered filter medium





#### Create woven, foam and sintered media scale models





Metal wire mesh

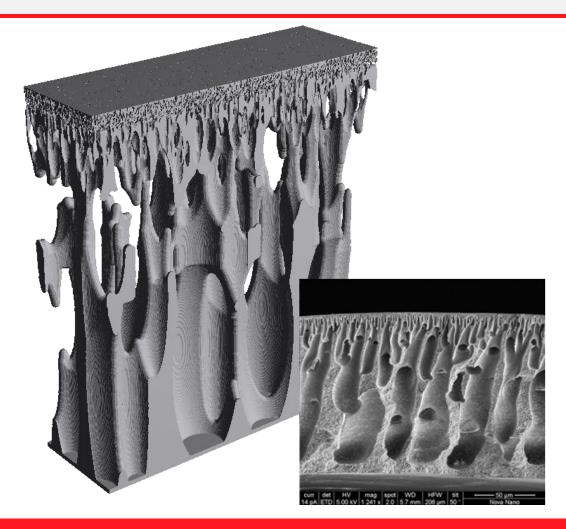
Open-cell foam

Sintered ceramics





#### Model a desalination membrane from a SEM image



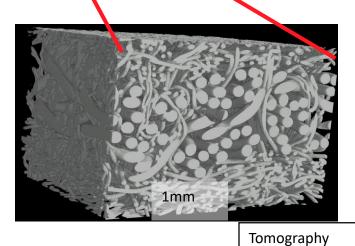
http://www.geodict.com/Showroom/structures.php

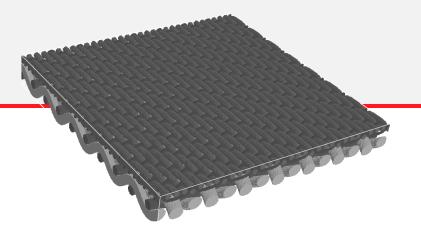




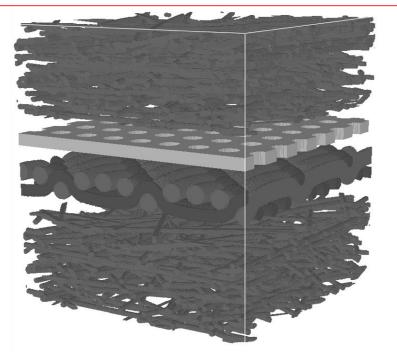
#### μCT scan and models of felts







Forming fabric and dewatering felt

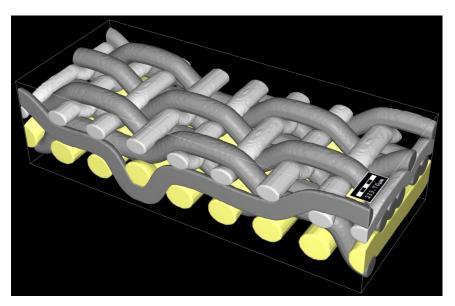


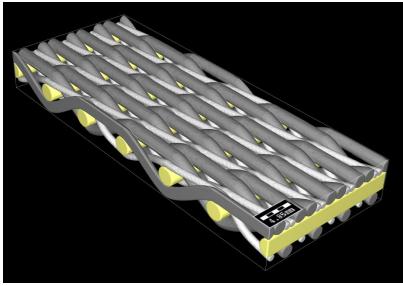






#### **Woven Metal Wire Meshes: Complex weave models**





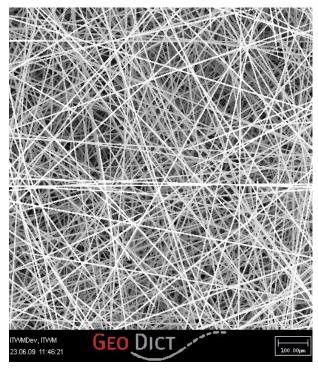
Left: Model of a two-layer weave based on a CT-scan. Right: Model of a complex one-layer twill Dutch-weave.



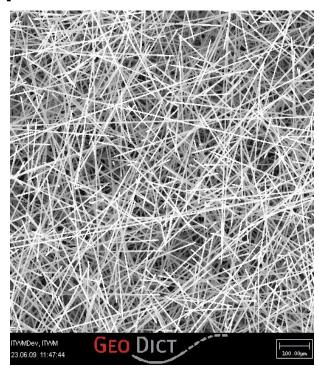


#### Glass fiber nonwoven

#### SEM visualization of 8 volume percent 5 micron fibers

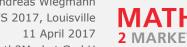


anisotropy 100

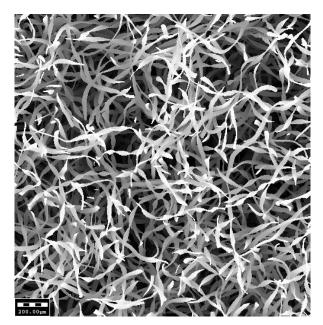


anisotropy 7

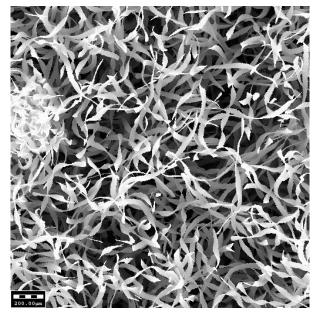




#### **Curled & inhomogeneous nonwoven**



20.00m

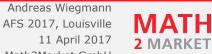


homogeneous model

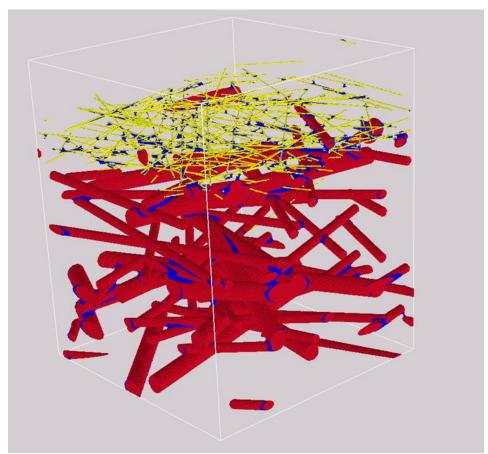
μCT scan

inhomogeneous model





#### Nonwoven with binder and layer of nano fibers



- 5.0 µm fibers (red)
- 2.5 µm fibers (red)
- 0.3 μm fibers (yellow)
- 2 vol % binder (blue)

L. Cheng et al., Filtech 2009.



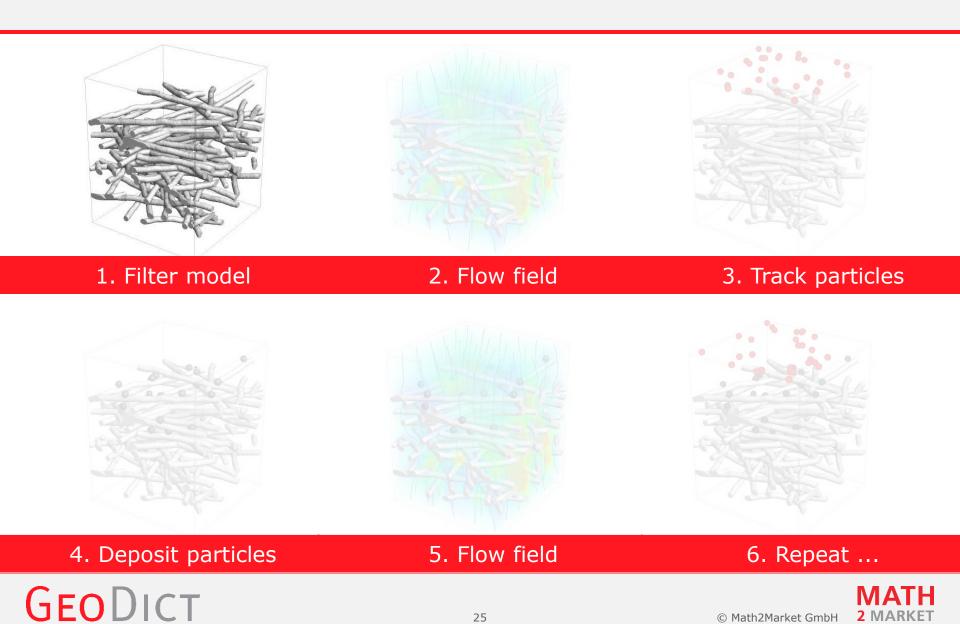


# Oil Filtration: Simulation of Filter Life Time and Dust Holding Capacity Improved Modeling of Filter Efficiency Simulations

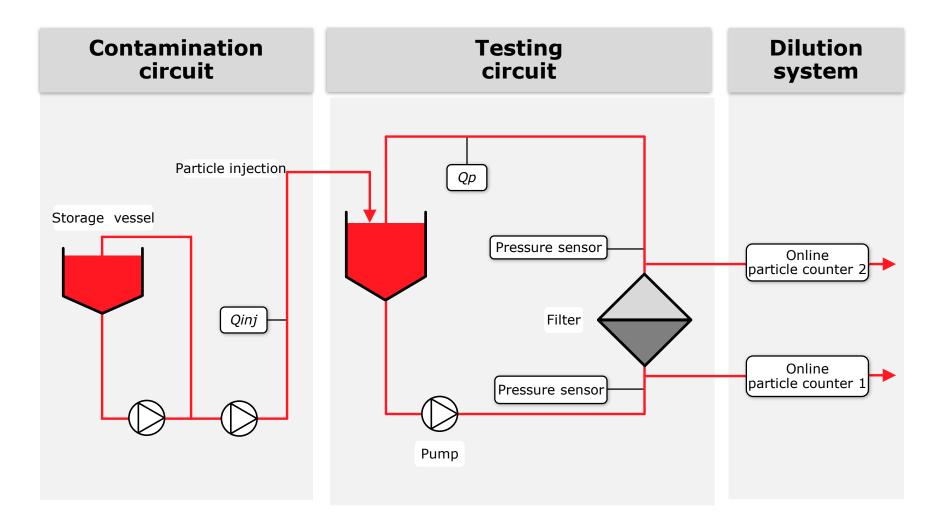
- Jürgen Becker, Andreas Wiegmann Math2Market GmbH, Kaiserslautern, Germany
- Friedemann Hahn, Martin J. Lehmann MANN+HUMMEL GMBH, Ludwigsburg, Germany
- Originally presented at Filtech



#### **Particulate flow simulations**



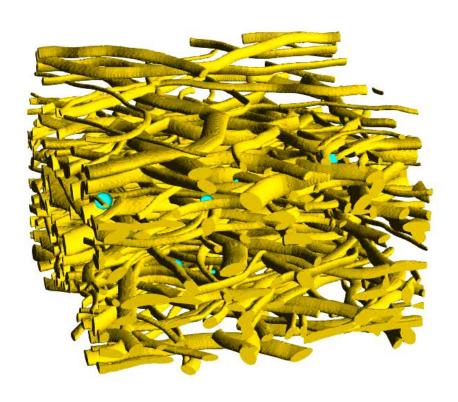
# The Multipass Test (ISO 4548)

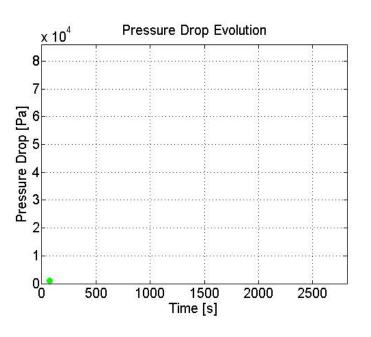






#### **Filter Capacity and Life Time**

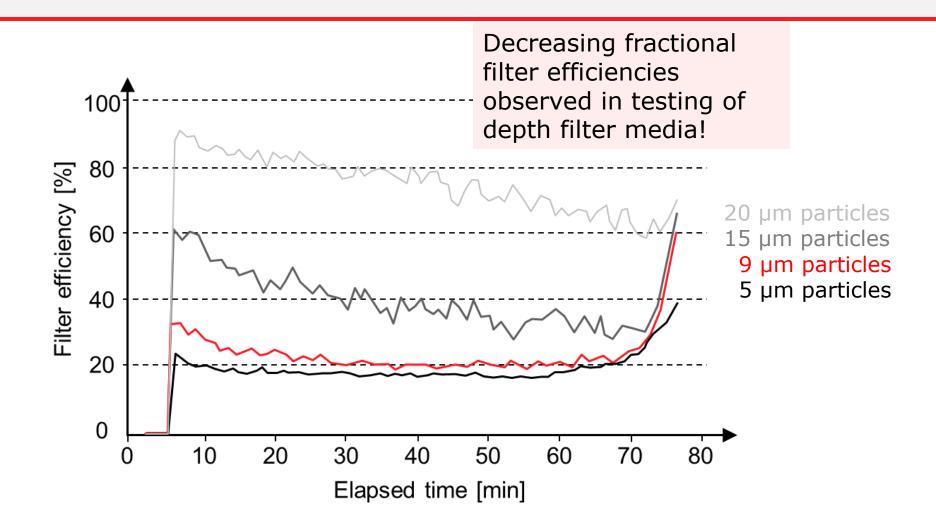




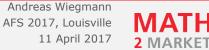




## The Multipass Test (ISO 4548)







#### Improvements to Filter Dict ....

- Global time concept: particles can continue to the next batch
  - allows lingering particles
  - needed for re-entrainment
- Enabled re-entrainment
  - Compare surface forces from adhesion and shear stress
- Previous particle tracking
  - flow solver uses staggered grid but writes cell-centered result file
  - particle tracking uses cell-centered file => accuracy lost (especially at no-slip boundary)
- New particle tracking (2013)
  - flow solver uses staggered grid and writes staggered grid result file
  - particle tracking uses staggered grid
- Introduction of ghost particles to decrease error bars for efficiency





# **Effect of Higher Accuracy: MPPS Simulation Example**

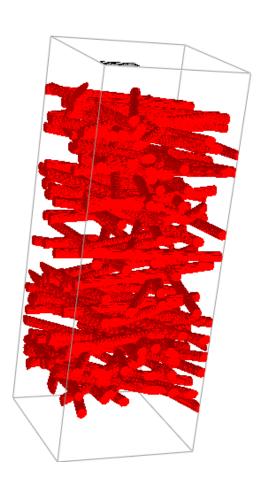
#### Structure:

- Fibers with diameter 20 μm
- Different porosities
- Different resolutions (voxel length 1 μm 4μm)

#### Simulation:

- Find efficiency for all particle diameters (caught on first touch, air filtration)
- Brownian Motion: on/off
- Inertia: on/off (by particle weight)
- Different flow velocities





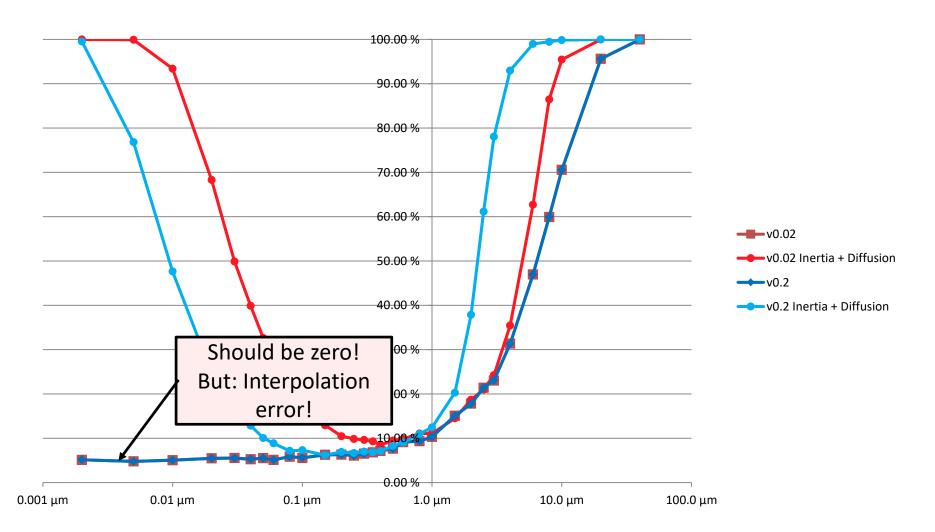






#### Fixed: Porosity 90%, Resolution 2 µm

**Vary: Velocity** 



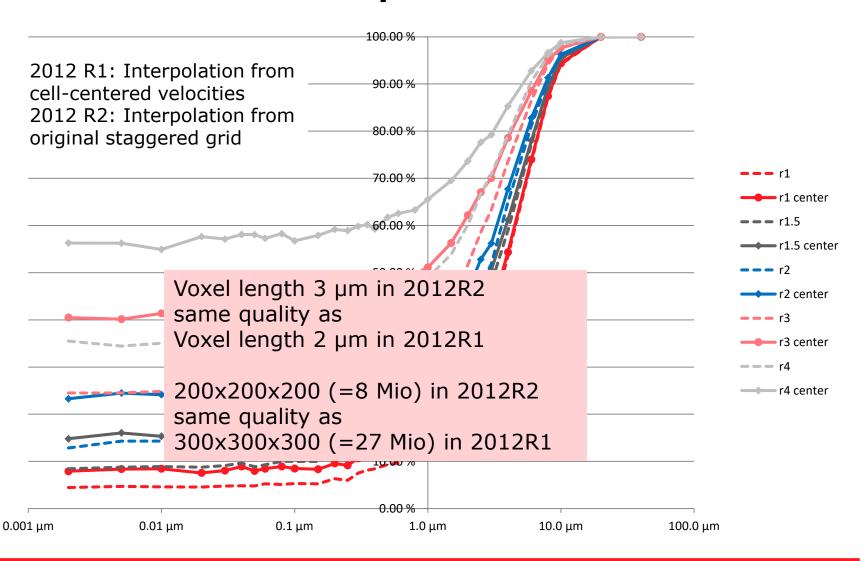








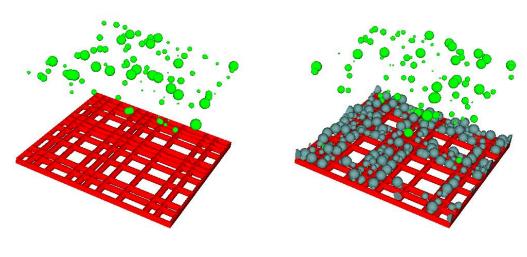
#### **Enhancement of Interpolation in 2012R2**

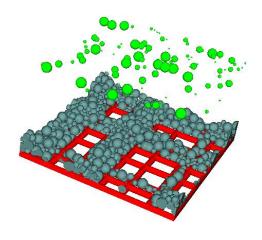




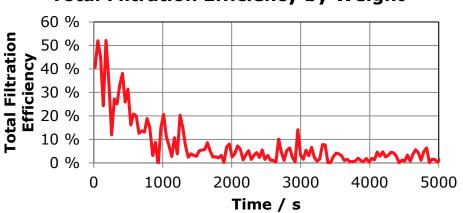


#### **Decreasing Efficiency by Changed Pathways**





#### **Total Filtration Efficiency by Weight**



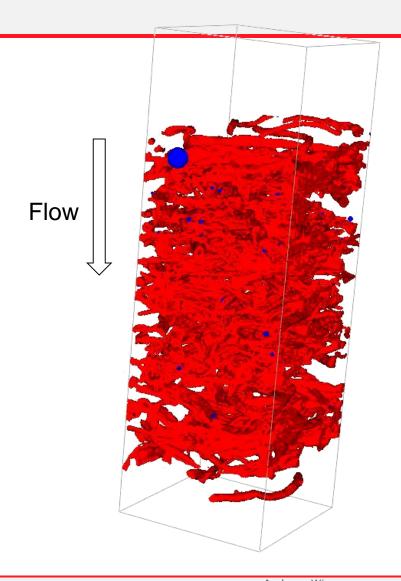
=> Effect can explain decreasing efficiencies!





#### Clogging simulation on µCT scan

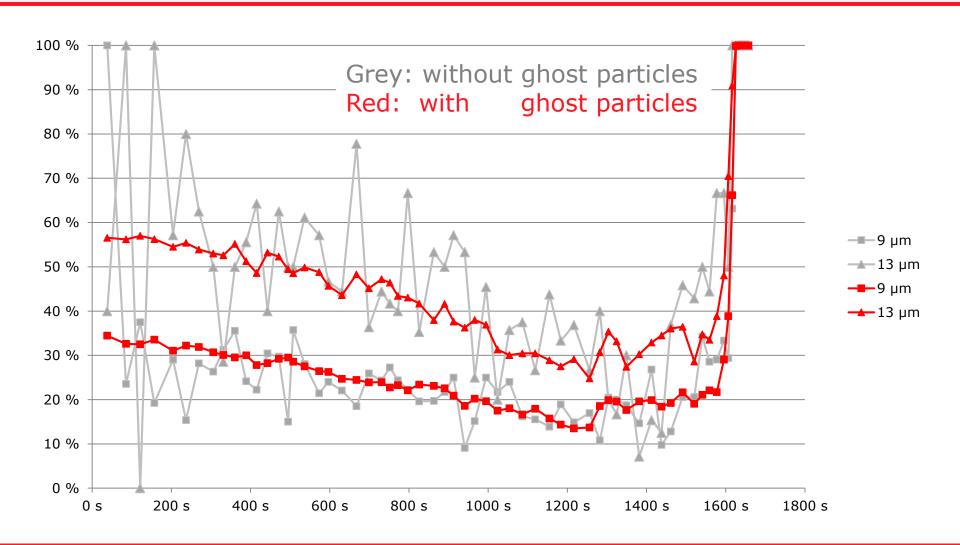
- Cut-out
- Oil filtration
- Particle size distribution from experiment



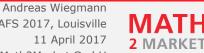




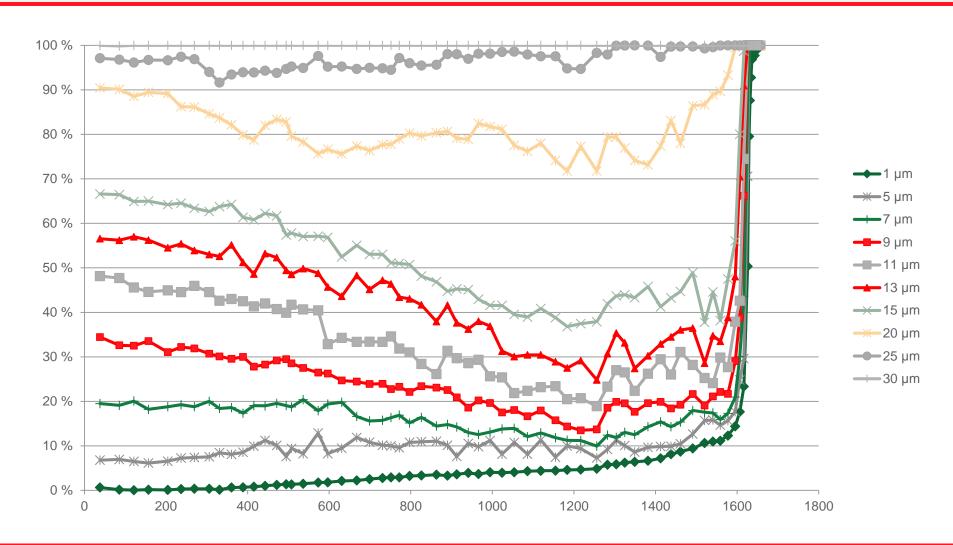
#### Simulated filter efficiency enhanced by ghost particles



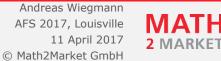




#### **Enhanced Simulated Fractional Efficiency**







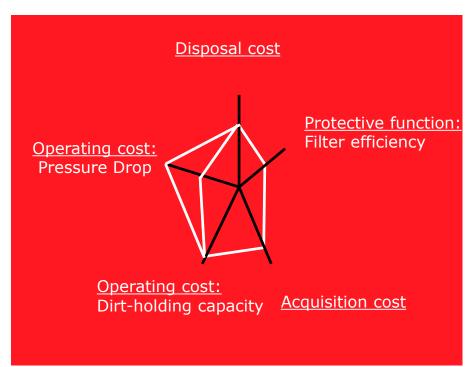
# Case Study: Pressure Drop improvement for a Hydraulic Filter (Patent granted to Argo-Hytos)

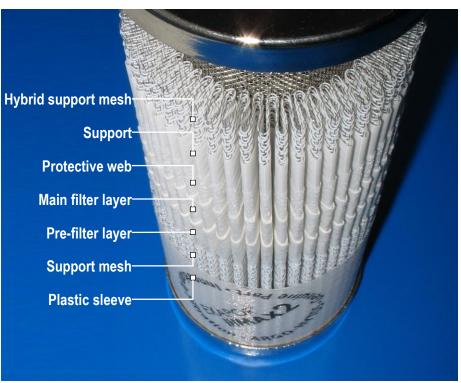
- Oleg Iliev & Andreas Wiegmann Fraunhofer ITWM, Kaiserslautern, Germany
- Andreas Schindelin, Argo-Hytos GmbH, Kraichgau, Germany
- Originally presented at CVTS Kaiserslautern



#### Parameters for a hydraulic filter element

- Oil flows from outside to inside
- Oil exits through perpendicular center region
- Oil passes through layered filter media
- Filter media removes dirt particles from oil

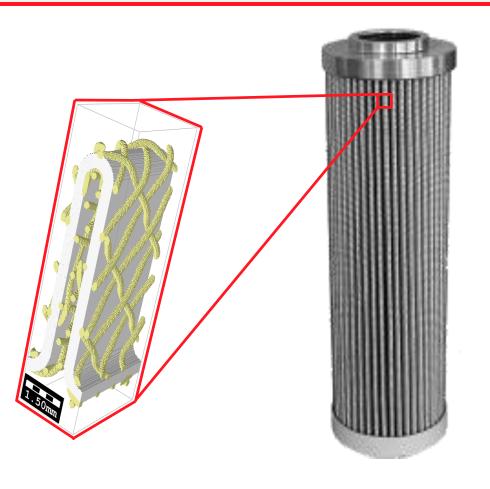






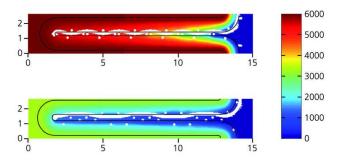


#### **Hydraulic filter with supported pleat**



Source: webpage ARGO HYTOS **Argo-Hytos** 





Two effects lead to pressure loss:

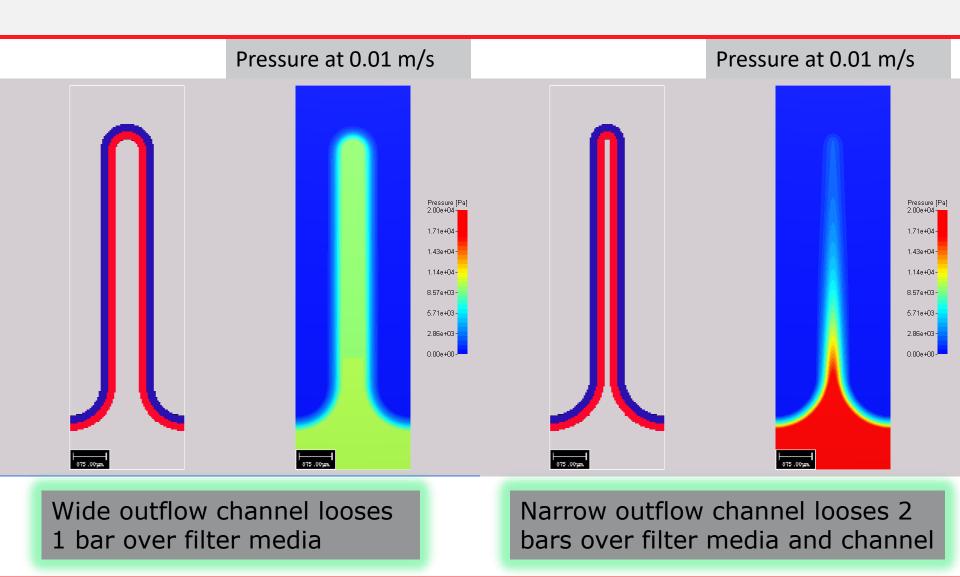
- 1. Across the filter media
- 2. Along the outflow channels

A support mesh prevents the collapse of the outflow channel





#### Pressure drop from media & capillary









#### **Optimized hydraulic filter**

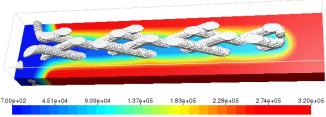
#### **FlowDict**

- Same pleat count
- Vary channel width by weave pattern & wire diameter

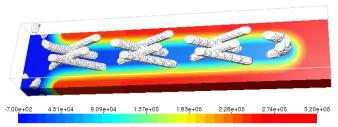
Trying different parameters, the pressure drop could be lowered by more than 35%, by reducing the pressure loss along the outflow channel.



Narrow Channel: 4 bar



Thick Wire: 3.1 bar



Thin Wire: 2.7 bar

Wiegmann, O. Iliev, and A. Schindelin, Computer Aided Engineering of Filter Materials and Pleated Filters, Global Guide of the Filtration and Separation Industry by E. von der Luehe. VDL - Verlag, 2010, pp 191-198.





#### The optimized filter element ...



A new design for hydraulic filter lowers the pressure drop by 40-50 % Patent granted to Argo-Hytos in 2009

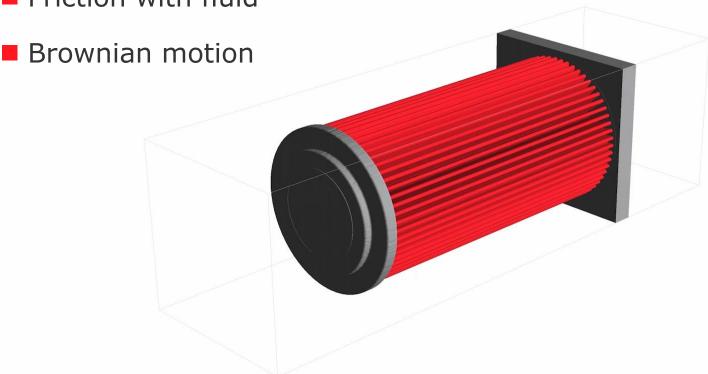




#### 2. Track Particles

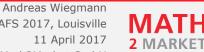
#### Movement of particles in fluid:

■ Friction with fluid

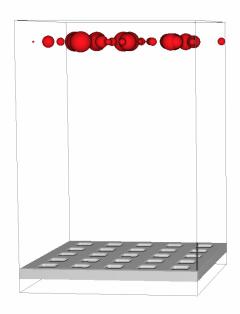


Particles enlarged for visualization



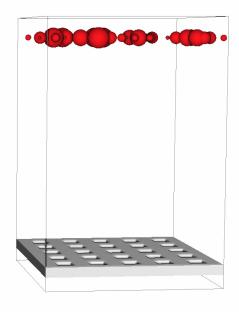


#### Caught on first touch (air filtration) & sieving collision model (oil filtration)



Caught on first touch

Filter cake with lower density & higher permeability, "dendrites"



Sieving

Filter cake with higher density & lower permeability, "dense packing"





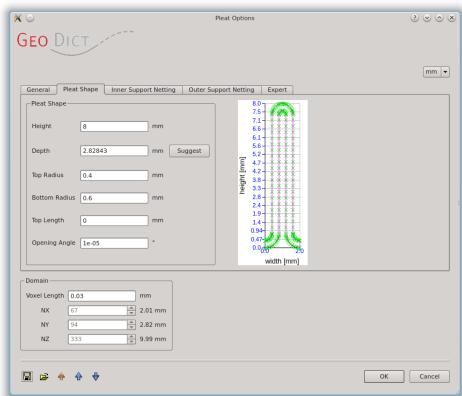
## Simulation of pleated air filter (for use in nuclear power plants)

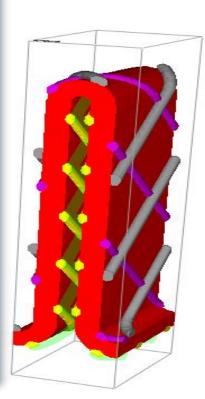
- Jürgen Becker, Liping Cheng, Andreas Wiegmann Math2Market GmbH, Kaiserslautern, Germany
- Nathalie Bardin-Monnier, Pierre-Colin Gervais Nancy University, France
- Originally presented at Filtech



#### **Pleat simulation**

- Pleat generator accounts for
  - Height
  - Width
  - Inner support
  - Outer support
  - Layered media
  - Angled pleats
  - etc

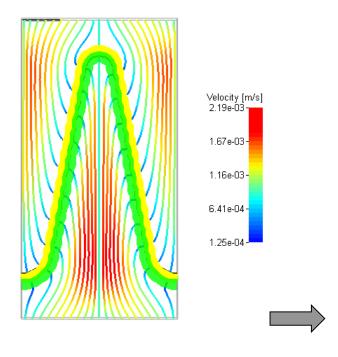




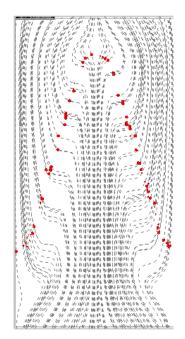




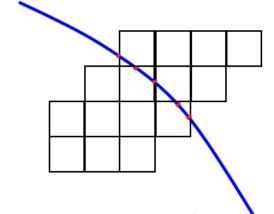
#### Pleat scale simulation



First, compute the flow in the pleat



Then, track the particles and find the trajectories following the flow field without obstacles.

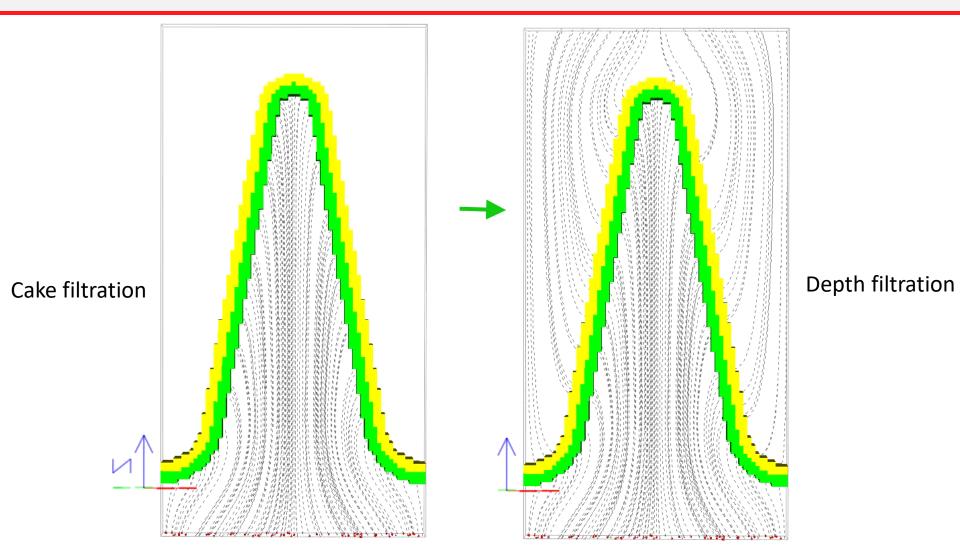


Locations where particles cross the media are found and the probability of particles being captured in the media is determined.





#### Simulate cake or depth filtration

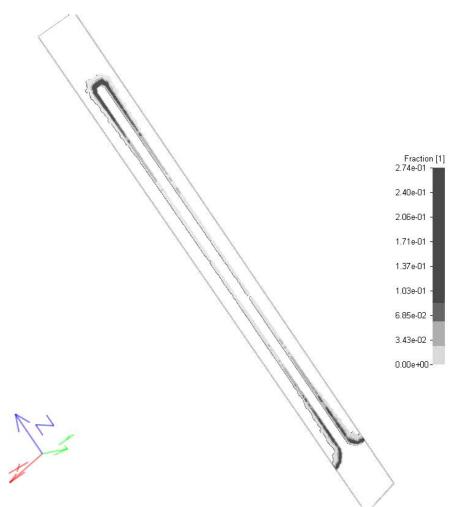


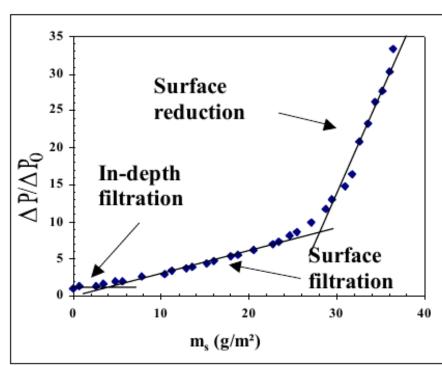
**GEODICT** 

Andreas Wiegmann AFS 2017, Louisville 11 April 2017 © Math2Market GmbH



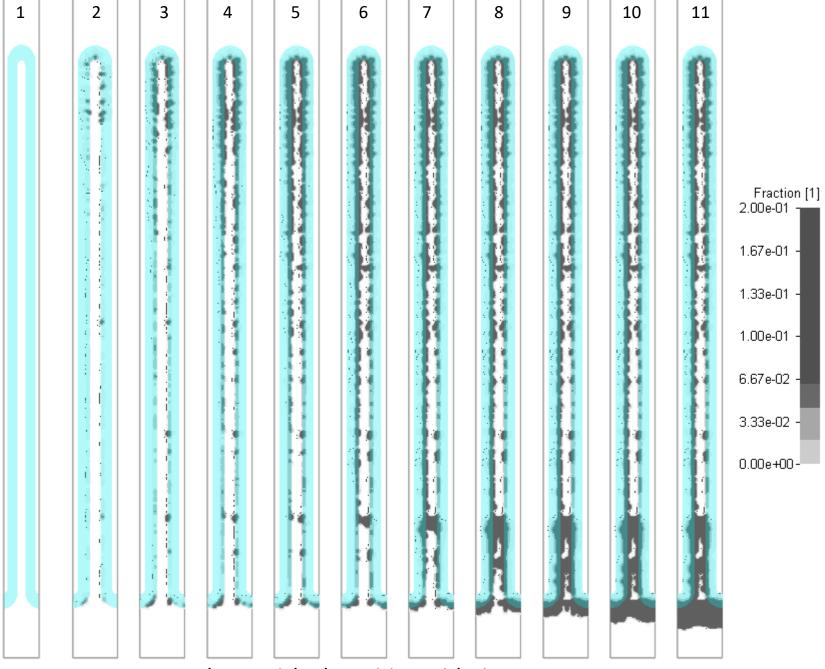
#### **Compare with experimental data**







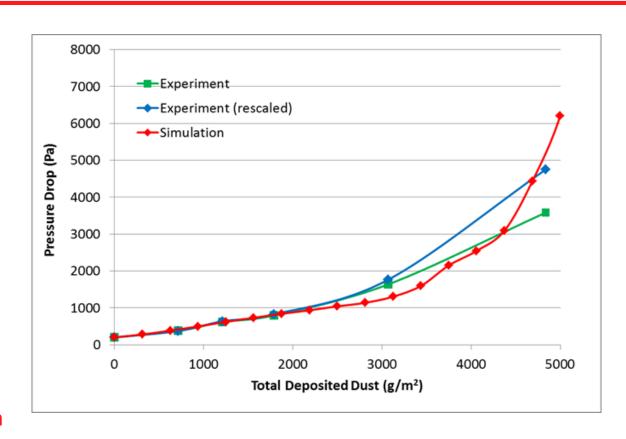




The particle deposition with time

#### Agreement with experimental data

- Pressure drop vs. load of a pleated filter
- Rescale to constant flow rate, what the pump was asked to do but did not do
- Simulation results compared with experimental measurements (rescaling done w.r.t. fluctuations in the volumetric flow rate)

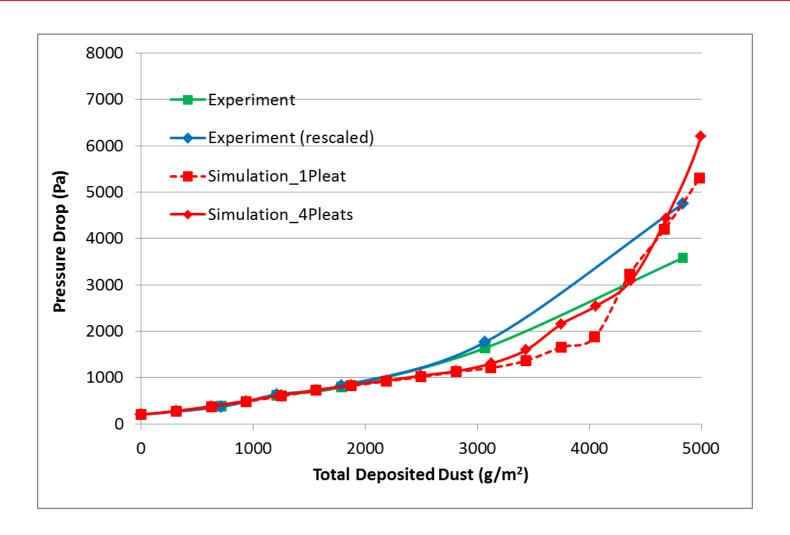


\*Pierre-Colin Gervais, Experimental and numerical study of clogging of pleated filters. PhD thesis, CNRS, LRGP, UMR 7274, Nancy, F-54000, France, 2013.





#### Agreement with experimental data





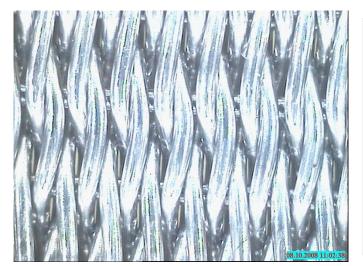


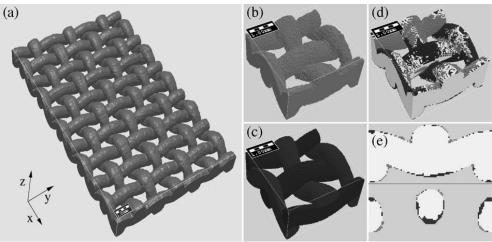
#### **Metal Wire Mesh**





#### **Reconstruction of Woven**







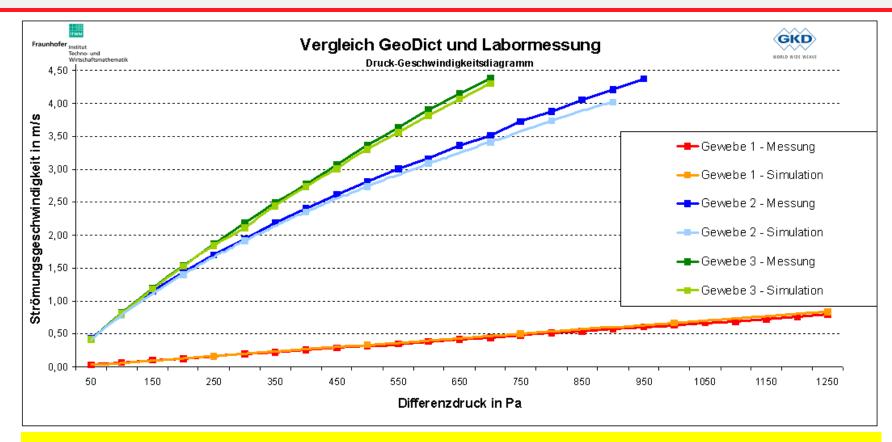
E. Glatt, S. Rief, A. Wiegmann, M. Knefel and E. Wegenke, *Structure and pressure drop of real and virtual metal wire meshes*, Bericht des Fraunhofer ITWM, Nr. 157, 2009.



**Andreas Wiegmann** 

AFS 2017, Louisville

#### Measured vs Simulated pressure drop for GKD meshes



E. Glatt, S. Rief, A. Wiegmann, M. Knefel and E. Wegenke, *Structure and pressure drop of real and virtual metal wire meshes*, Bericht des Fraunhofer ITWM, Nr. 157, 2009.

Deviation of simulation and experiment independently confirmed to lie within 3% over all differential pressures by A. Mantler and M. Theiß of Haver & Boecker, 2017.



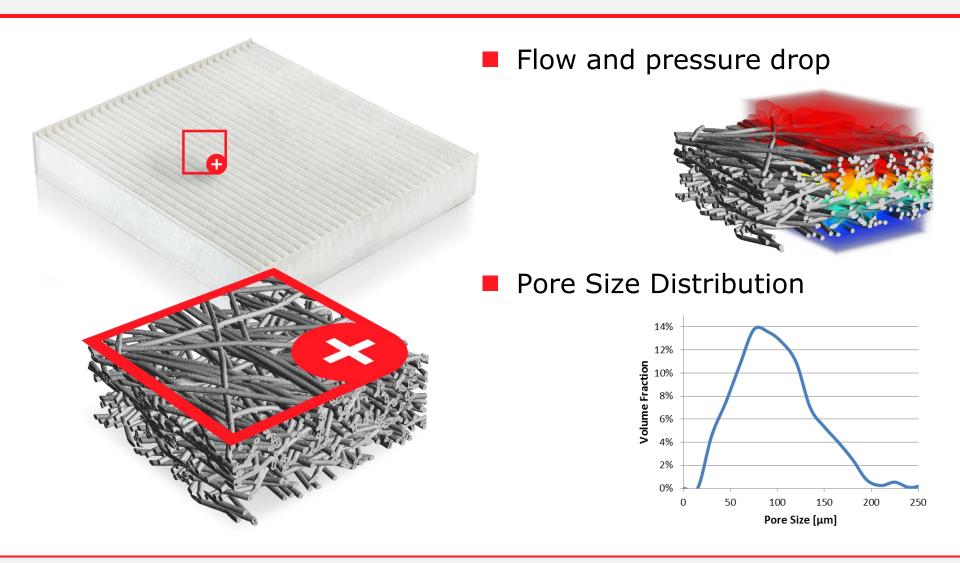


#### Case Study: Cabin Air Filter



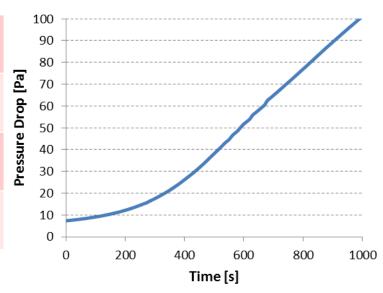


#### μCT-scan of cabin air filter sample

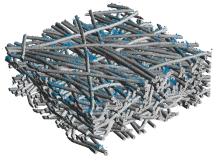


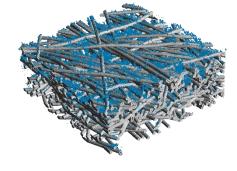
#### **Filter Life Time simulation**

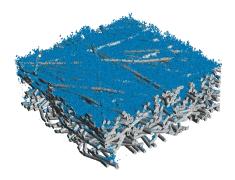
| Initial pressure drop            | 7 Pa         |
|----------------------------------|--------------|
| Pressure drop after 1000s        | 101 Pa       |
| Total deposited dust after 1000s | 93 g/m²      |
| Total filter efficiency          | 93% (weight) |













## Improved ceramic for soot filtration (patent granted to Fraunhofer IKTS and Fraunhofer ITWM)

- Liping Cheng & Andreas Wiegmann Fraunhofer ITWM, Kaiserslautern, Germany
- Jörg Adler, Uwe Petasch & Lars Mammitsch Fraunhofer IKTS, Dresden, Germany
- Originally presented at WFC 12, Graz



## Introduction Diesel Particulate Filter (DPF)

Goal: design a better DPF using simulations

- lower pressure drop
- higher filter efficiency
- longer life time



#### ceramic filter media

They can be simulated and predicted.

a multivariate resistivity model is introduced and shown to predict pressure drop measurements



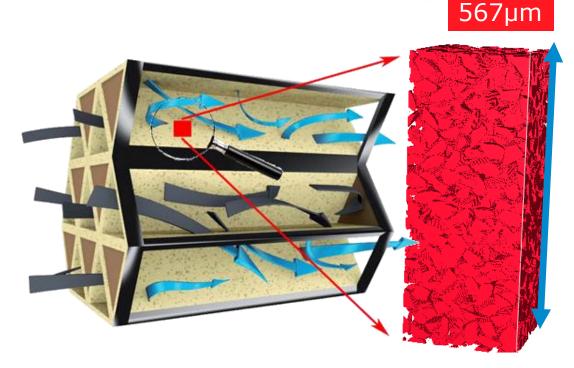




#### **Diesel Particulate Filter Simulations:**

In a Diesel Particulate Filter, soot particles are filtered in the walls of the filter, usually a 50% porosity ceramic

The energy use of the filter is due to pressure loss across the loaded ceramic, as well as along the channels of the DPF. Here, we consider the pressure loss across the wall.



Simulations:  $256 \times 256 \times 750$  cells

Grid cells:  $0.9 \mu m \times 0.9 \mu m \times 0.9 \mu m$ 

Soot particle: 25 nm - 600 nm

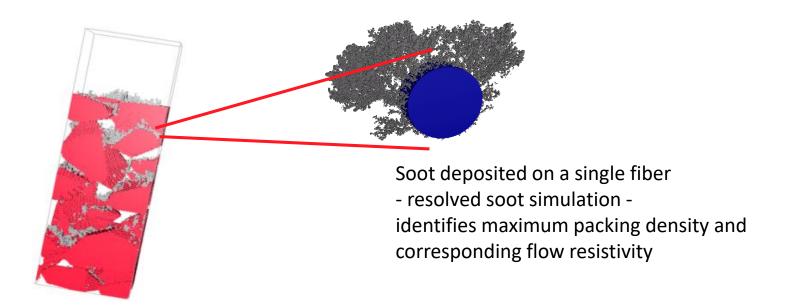
Wall thickness: 567 μm Inlet / Flow Channel: 108μm





#### **Particle Filtration Tasks:**

#### Multi-scale approach

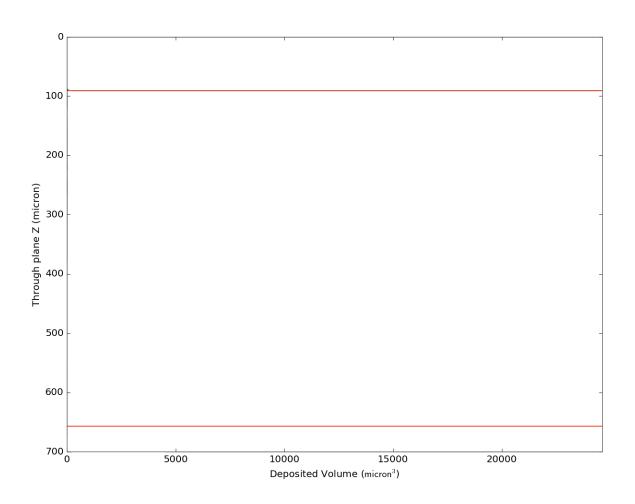


Soot deposited in ceramic DPF
- soot as porous media simulation —
requires maximum soot packing density and
corresponding flow resistivity





## **Advanced Postprocessing Video – Spatial Particle Deposition over Time**

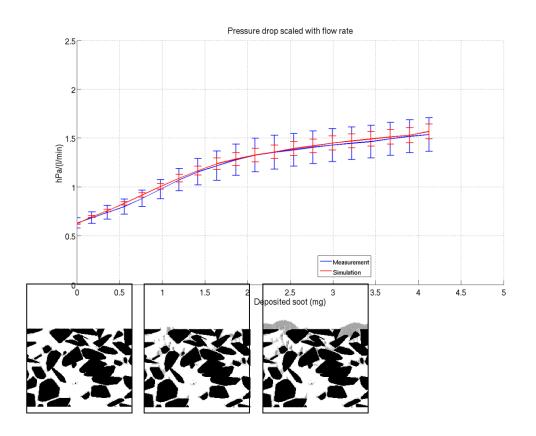








#### **Horizontal layers**



- Experimental and simulated pressure drop evolution with error bars induced by 5 measurements and 5 different realizations of the virtual structure.
- Match achieved by introducing different Brinkman parameters for depth and cake filtration.

L. Cheng et al., WFC 11, 2012.

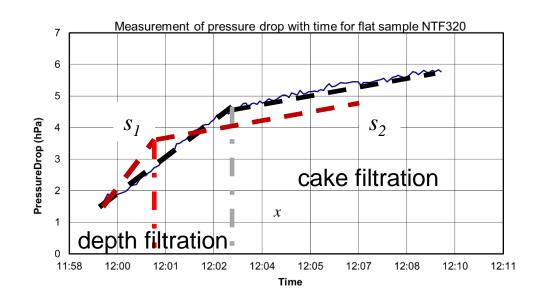


#### Reduced pressure drop over time

After fast initial pressure drop increase (slope  $s_1$ , depth filtration phase) follows long slower pressure drop increase (slope  $s_2$ , cake filtration phase)

- Matched experiment with simulations
- Shortened depth phase to lower pressure drop during cake phase
- Fraunhofer IKTS manufactured ceramic, experiment matched simulations, and patent was granted: Particulate filter, No. DE102012220181 A1 [http://www.google.com/patents/DE102012220181A1?cl=en]









#### **Honeycomb structures (DpfGeo)**

### Triangular and square honeycomb structures

Zhang, X. Numerical study of flow and pressure characteristics for Diesel particulate filters with square and triangle channels. Filtration 8 (3), 2008.

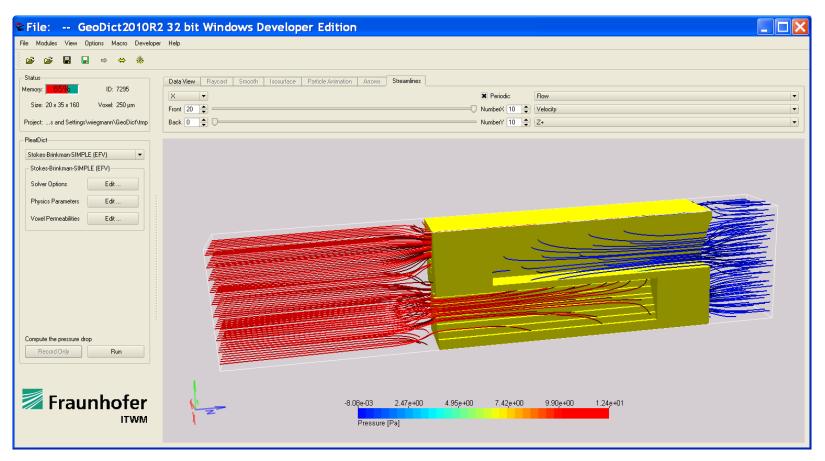


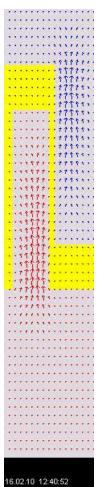






#### **Streamlines and velocity field (PleatDict)**





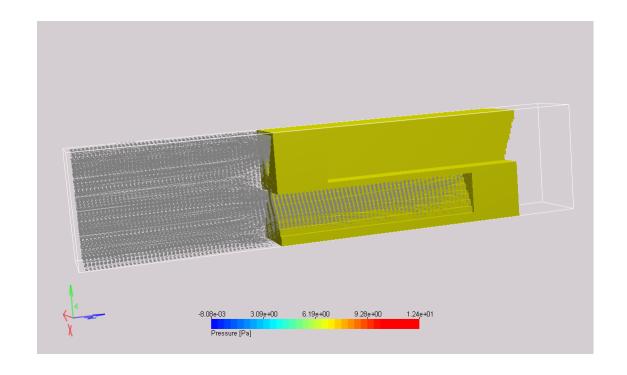








#### Paths of 0.1µm (filtered) particles







## Design of Fibrous Filter Media Based on the Simulation of Pore Size Measures

Simulation of mercury intrusion porosimetry (MIP) Simulation of liquid extrusion porosimetry (LEP) Simulation of maximum inscribed sphere (MIS)

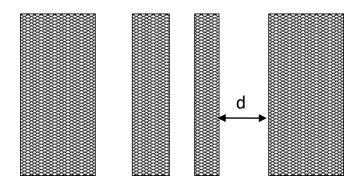
- FILTECH, Wiesbaden
- Jürgen Becker,
- Andreas Wiegmann,
- Volker Schulz



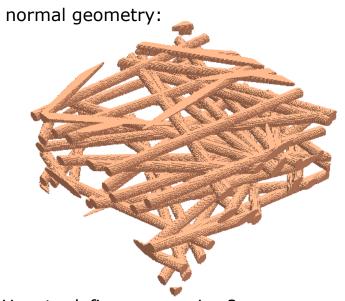


#### **Pore Size Distribution**

#### simple geometry:



Pore sizes well defined and easy to measure

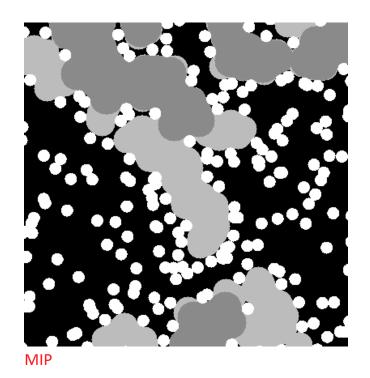


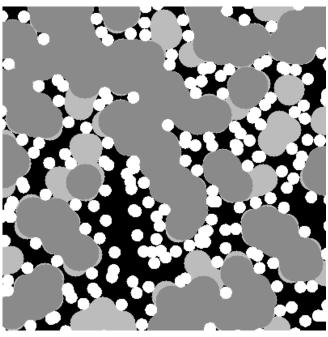
How to define a pore size ?

What is measured?



## Mercury intrusion porosimetry simulation (MIP) vs. maximum inscribed sphere (MIS) simulation





MIS



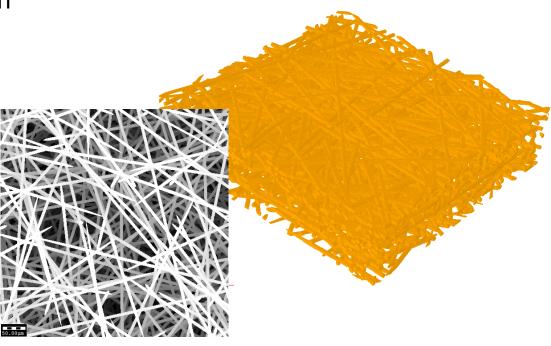
#### **3D sample structure**

digitally created 3D fibre structure

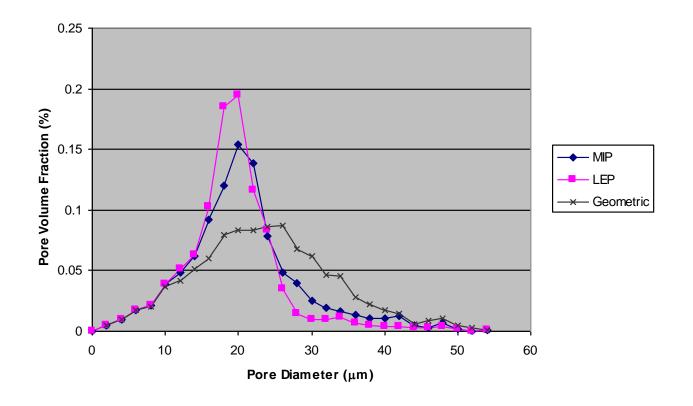
fibre diameter 7μm

porosity 82%

highly anisotropic

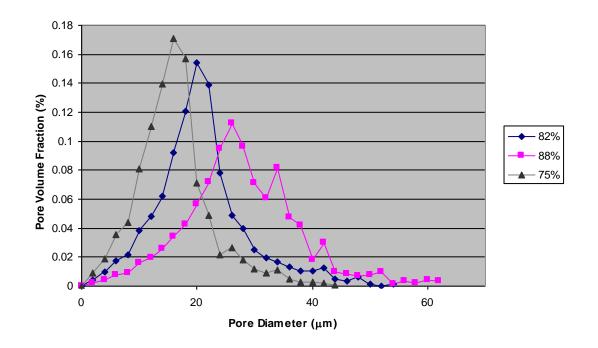


#### **Results of the simulation**



# Dependence of Pore Size Distribution on design parameters (example)

- media with porosities 75%, 82%, and 88%.
- chart shows results of simulated MIP.

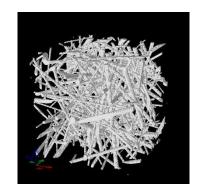


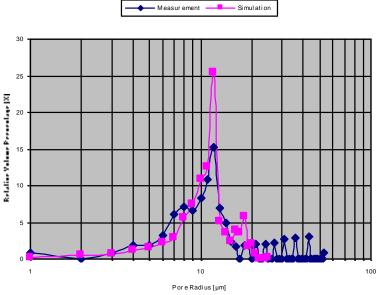
### **Comparison of measurement and simulation**

Measurement: MIP

#### Simulation:

- digitally created fibre structure using known values for porosity and fiber thickness distribution.
- simulated MIP









#### **Summary / References**

- Different measurement techniques measure different "Pore Size Distributions" (see A. Jena, K. Gupta, Fluid Particle Separation J. 4, 2002, pp. 227-241)
- Mercury intrusion porosimetry (MIP) can be simulated
- Liquid extrusion porometry (LEP) can be simulated
- Both result in fewer large pores than maximum inscribed sphere (MIS, purely geometric) approach due to requirement of connectivity with the domain boundaries
- Largest simulated through pore agrees extremely well with glass bead tests, see work by Haver & Boecker and Whitehouse Scientific



# Filtration simulation Method and Algorithm



### **Filter Efficiency simulations**

#### Basic idea:

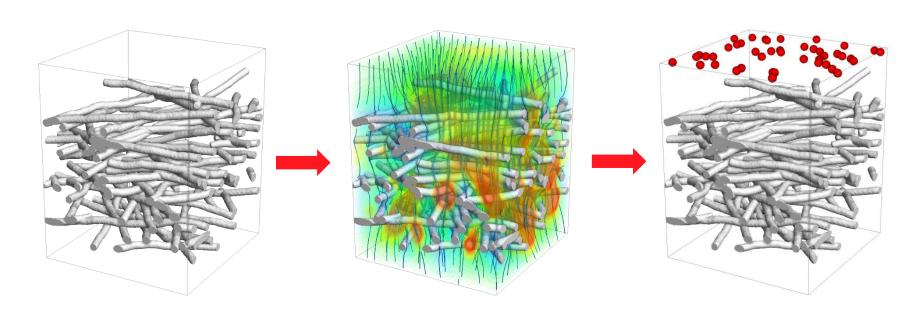
- 1. Filter media model
- 2. Determine flow field
- 3. Track particles (filtered or not?)

#### Randomness:

- Starting positions
- Brownian motion

#### Result:

Percentage of filtered particles







# Flow simulation Stationary Navier-Stokes flow

$$-\mu \Delta \vec{u} + \rho (\vec{u} \cdot \nabla) \vec{u} + \nabla p = 0$$
$$\nabla \cdot \vec{u} = 0$$

$$\vec{u} = 0$$
 on  $\Gamma$   
 $P_{in} = P_{out} + const$ 

 $\vec{u}$ : velocity

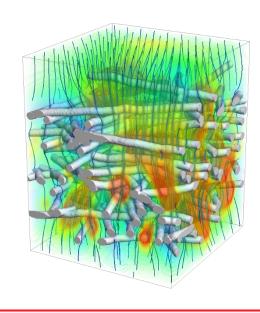
*p*: pressure

 $\mu$ : dynamic viscosity

 $\rho$ : fluid density

(momentum balance)
(mass conservation)

(no-slip on surface)
(pressure drop is given)





#### Tracking particles in a flow field

**Impulse** 

Stokes Drag

Electrostatic Force

$$m\frac{d\vec{v}}{dt} = 6\pi\mu \left(\frac{R}{C_c}\right) \left(\vec{u} - \vec{v} + \sqrt{2D}\frac{d\vec{W}(t)}{dt}\right) + Q\vec{E}$$

Cunningham Corrected Particle Radius

: particle velocity [m/s]  $\mu$  : dynamic viscosity [kg/m·s]

**Brownian Motion** 

 $\overrightarrow{u}$ : fluid velocity [m/s] Q: particle charge [C] R: particle radius [m] E: electric field [V/m]  $C_c$ : Cunningham correction D: Diffusivity [m²/s] D: particle mass [kg] D: 3D Wiener process

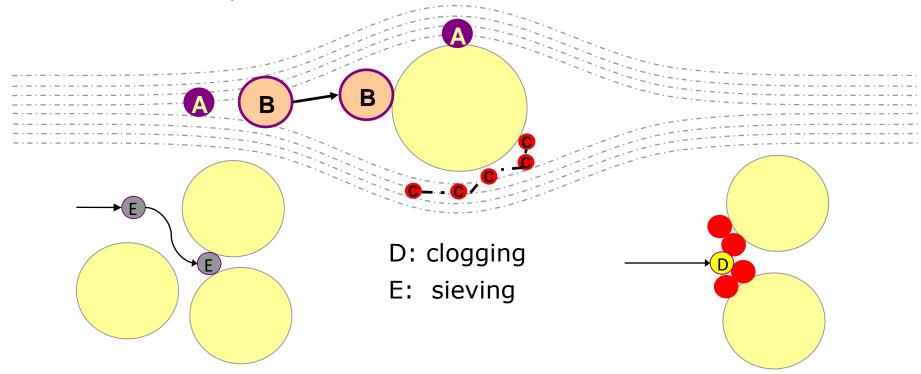


#### Filtration effects I

A: direct interception

B: inertial impaction

C: diffusional deposition



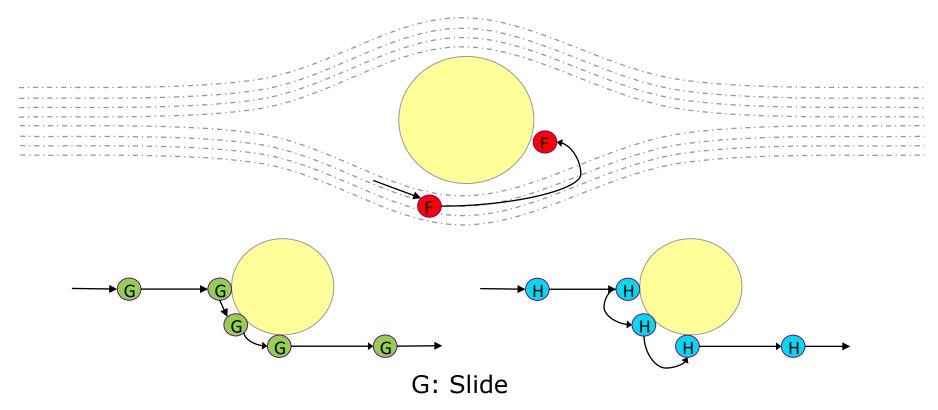






### Filtration effects II and modes of particle motion

#### F: electrostatic attraction

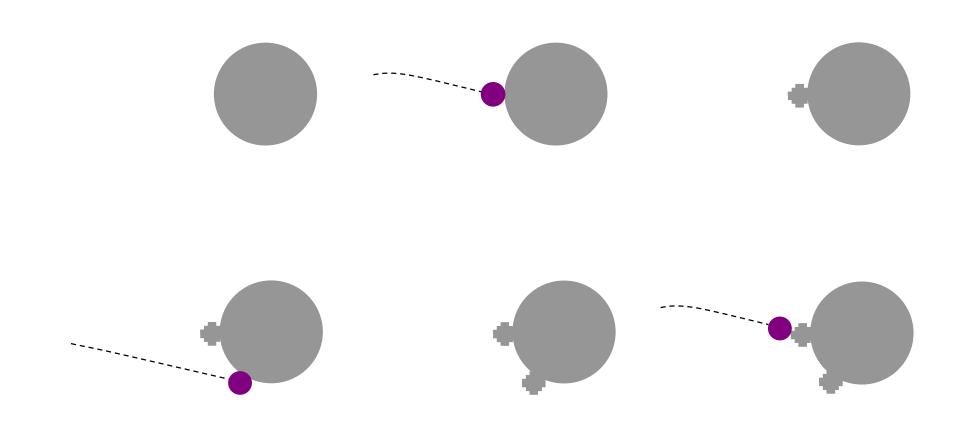


H: Bounce





# Filtration of resolved particles grid cells can be solid or empty

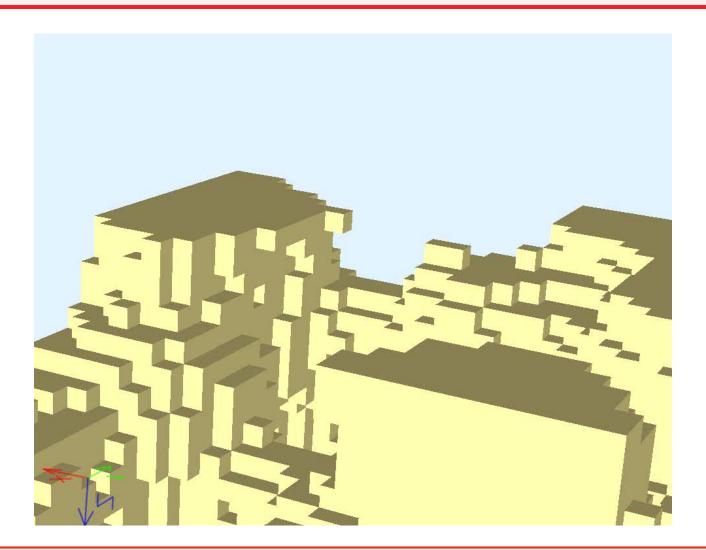






# **Soot forming cake**

# - detail of the beginning





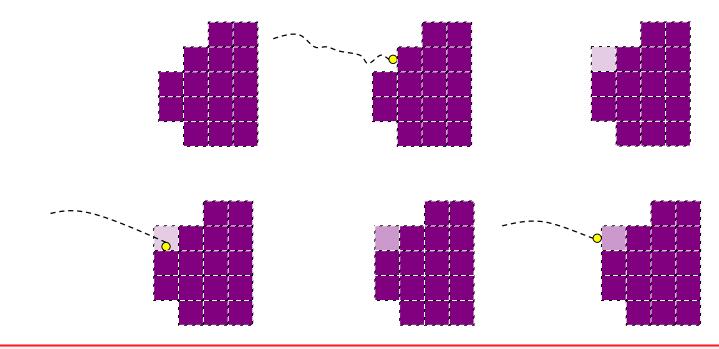


# Filtration of unresolved particles grid cells can be solid, empty or porous (& permeable)

Soot particles are much smaller than the computational grid.

When they deposit, they do not fill the computational cell, but rather form a permeable media inside and on top of the ceramic filter.

We control how much a cell can get filled, and how much resistivity to the flow the cell will have, depending on the degree of filling.

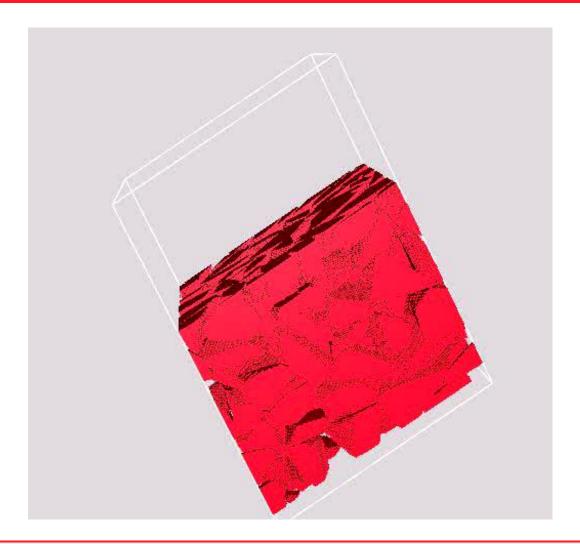






#### **Soot filtration**

# - millions of particles per time step!







# **Conclusions and Outlook**





#### **Conclusions**

- We saw 3d models for filter media, pleats and whole filters, where the media models could also result from µCT-scans of existing media
  - Cellulose, glass and synthetic fibers
  - Ceramics
  - Open-cell foams
  - Weaves
- On the models one can predict
  - Pore Size measures
  - Pressure drop, flow resistivity, permeability,
  - Filter Efficiency
  - Filter Life Time / Dust Holding Capacity
- Simulations, combined with experiments, can lead to
  - New knowledge, such as understanding of re-entrainment
  - Quantification of phenomena, such as effects of layers
  - And also patents and long-term commercial benefits





#### **Outlook**

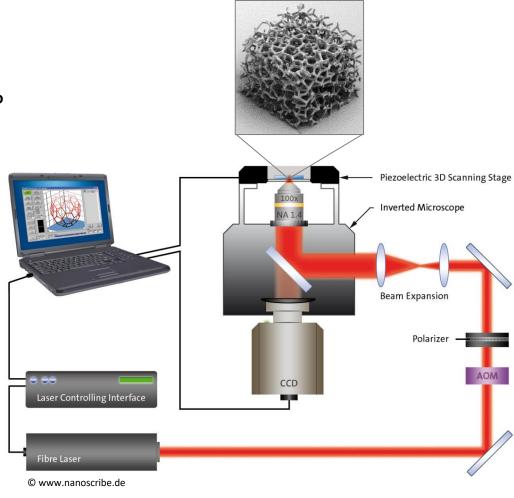
- Material-scale Simulation is here to stay more computer power and higher resolution in 3d imaging will lead to better and better material scale models than can be run in less and less time.
  - Math2Market is exploring the possibility to use cloud computing, for example.
- The material scale models will produce output that will be usable automatically in pleat-scale and filter-scale simulations.
  - For structural mechanics simulations, Fraunhofer ITWM and Math2Market are already creating UMATS from the material scale that can be used in ABAQUS simulations on the part-scale. This will be transferred to filtration phenomena as well.
- The more we work on simulation, the more we appreciate experiments, and the more we realize how much more work still lies ahead ...
  - Example: Additively manufactured filter media with fiber diameter around 1µm





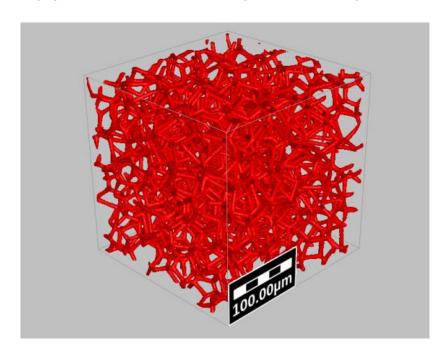
#### Center for Materials Characterization and Testing

- Printable Materials
  - Acrylate-based photoresists (IP resists)
- Local exposure via ultrashort laser pulses and two-photon absorption
- Crosslinking of liquid photoresist only in the very focus of the laser
- Wet chemical development removes unexposed photoresist
- Feature size < 150 nm</p>
- Resolution < 600 nm</p>



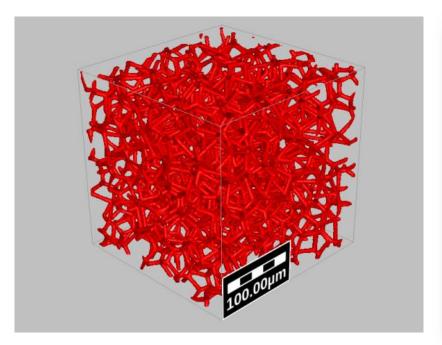


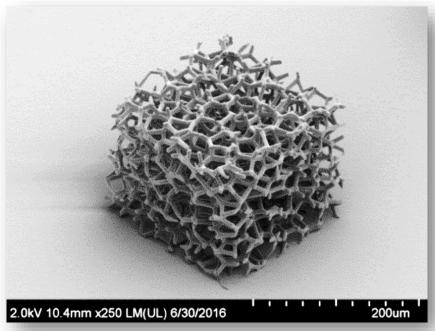
Application example: computer-optimized filtration media



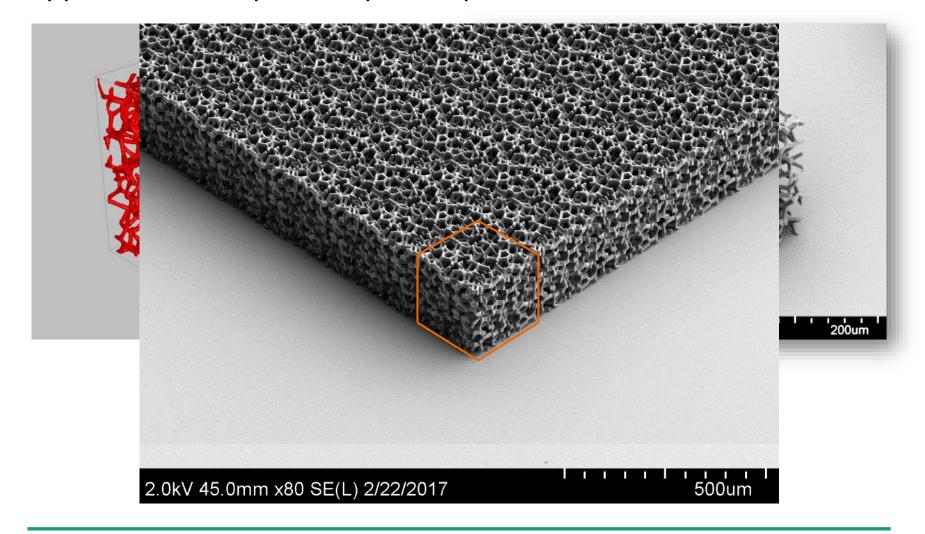


### Application example: computer-optimized filtration media



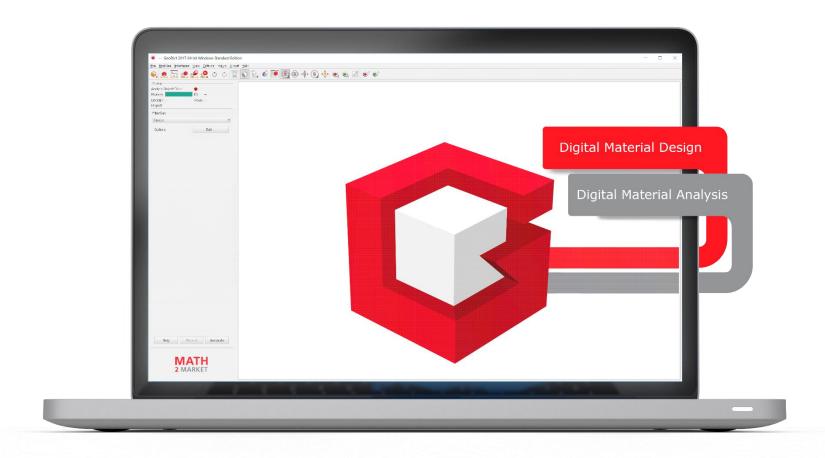


Application example: computer-optimized filtration media





# Thank you for your time and attention. Please feel free to ask questions...



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