Simulation of Soot Filtration on the Nano-, Micro- and Meso-scale

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APRIL 16 – 20, 2012 · GRAZ – AUSTRIA

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GEO DICT

Outline

- Introduction
- Simulation of Filtration Processes for ceramic

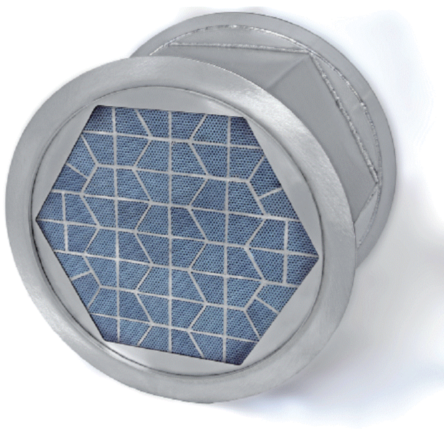
  Diesel **P**articulate **F**ilter media
  - Air flow simulation
  - Soot transport simulation
  - Soot particle deposition and conversion to porous media
  - Determining soot layer packing density and flow resistivity
- Predicting the pressure drop for a new DPF media
- Outlook towards the macro scale
- Conclusions

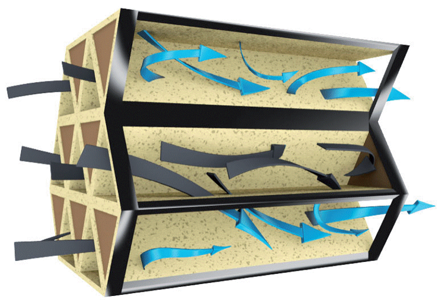
Introduction

- Goal:
  use computer simulations to design a better DPF
  - lower pressure drop
  - higher filter efficiency
  - longer life time

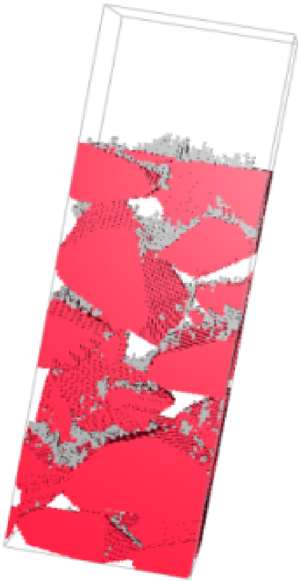
- key ingredients that govern the DPF performance: **the ceramic filter media**

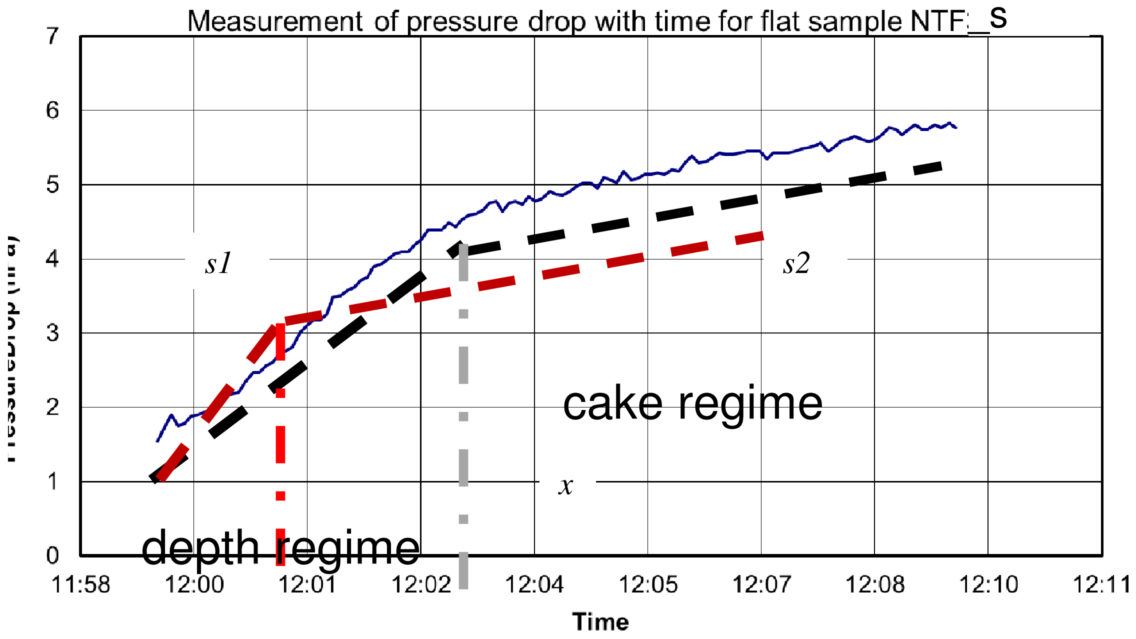
- Ceramic filter media can be simulated and predicted.
  – a multivariate resistivity model is introduced and shown to match and predict pressure drop measurements

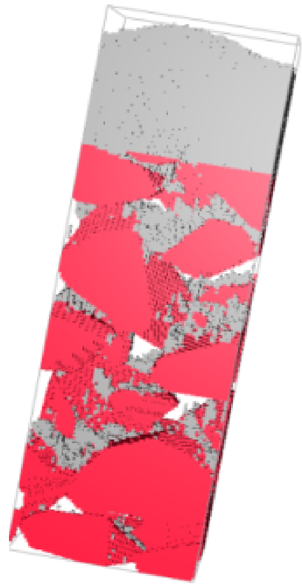




Pressure drop over time







After fast initial pressure drop increase (s1, depth filtration phase) follows long slower pressure drop increase (s2, cake filtration phase)

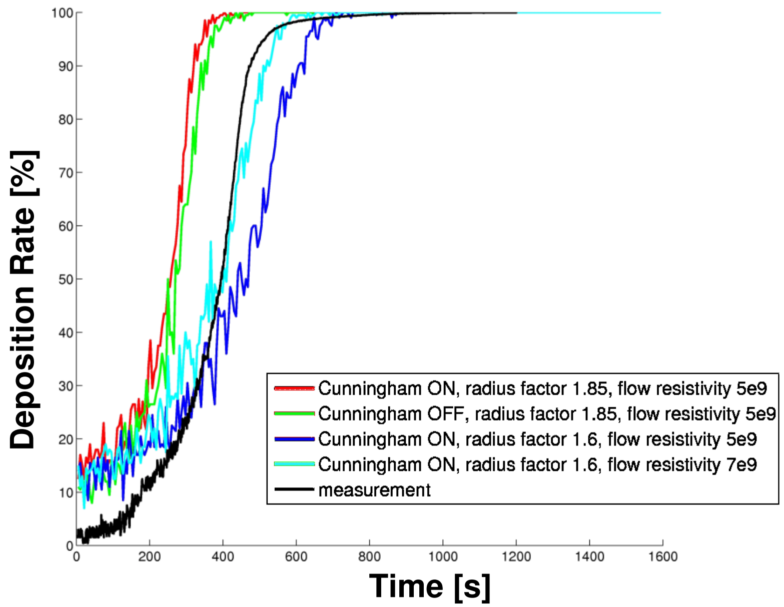
Objectives:

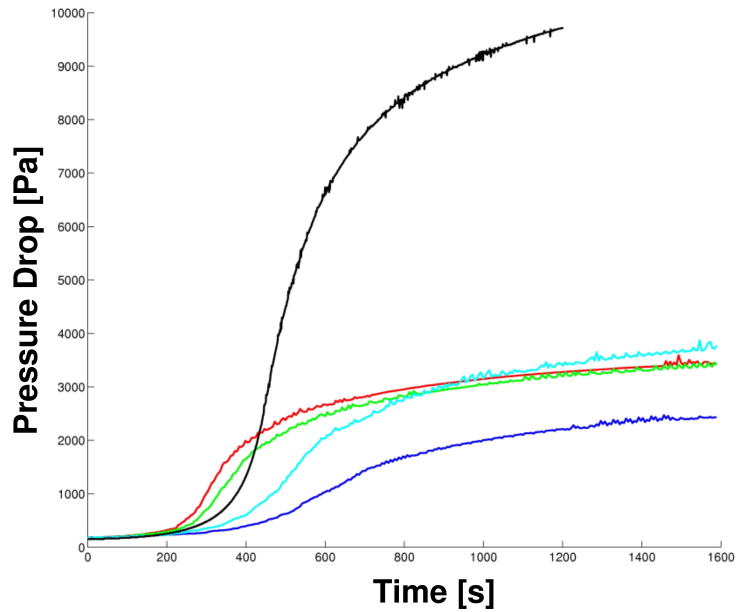
A. Match this behavior in simulations

B. Reduce depth filtration phase to lower overall pressure drop

C. Check that flat sample results are significant also for honeycombs (Fraunhofer IKTS)

Previous results





*K. Schmidt, S. Rief, A. Wiegmann, S. Ripperger. *Simulation of DPF Media, Soot Deposition and Pressure Drop Evolution.* Filtech, Wiesbaden 2009.

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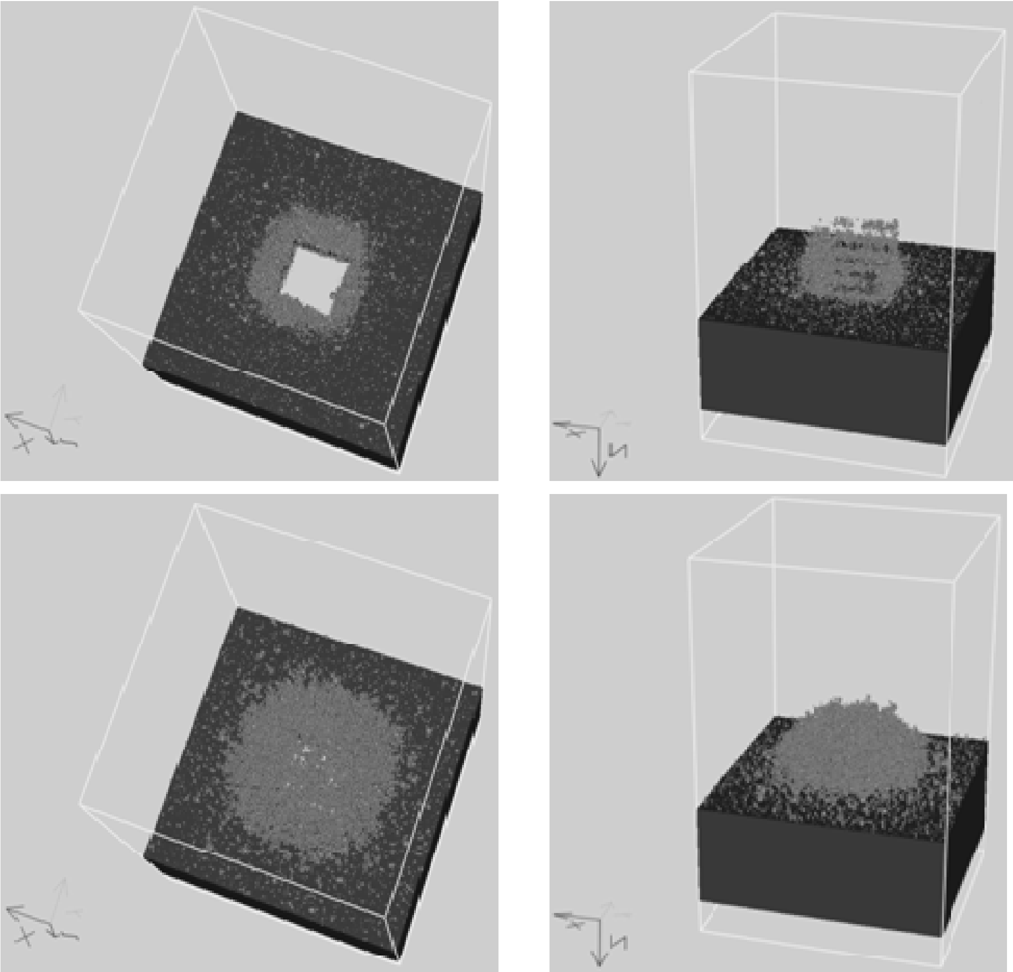
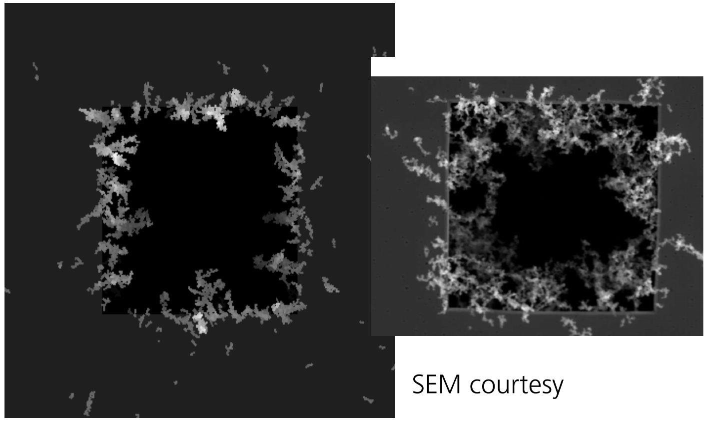
3d view, virtual SEM and real SEM (with FIB) of soot on micro sieve

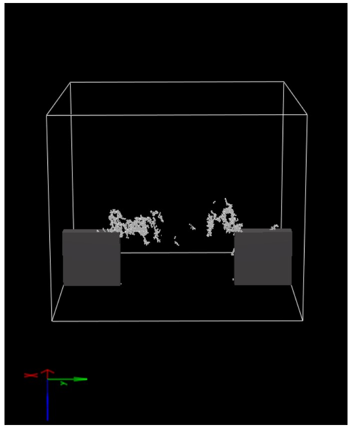


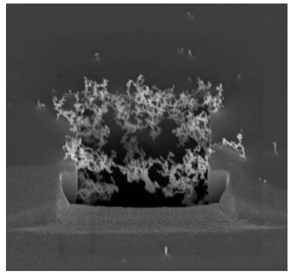


SEM courtesy

H. Schomburg,

Robert Bosch GmbH





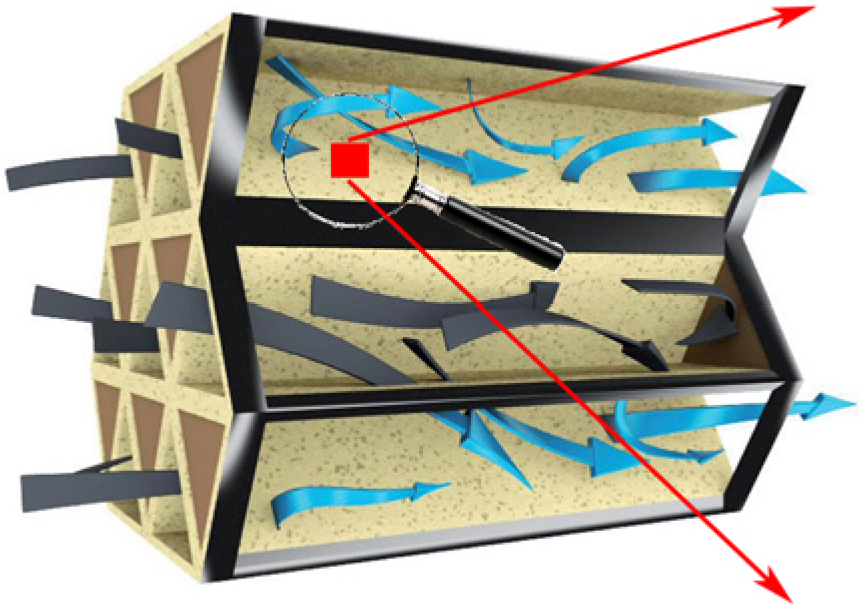
FIB & SEM courtesy

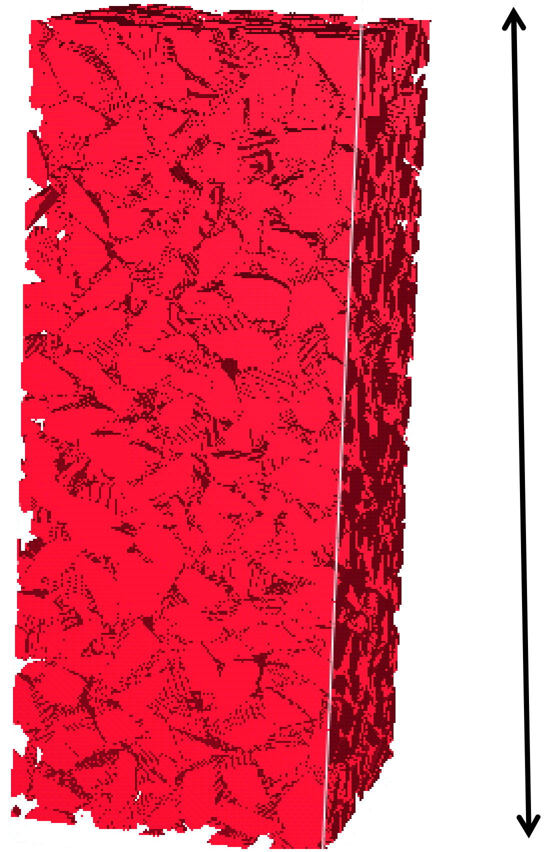
H. Schomburg,

Robert Bosch GmbH

Dissertation Kilian Schmidt, Kaiserslautern Technical University, 2011.

The scale of our simulations:



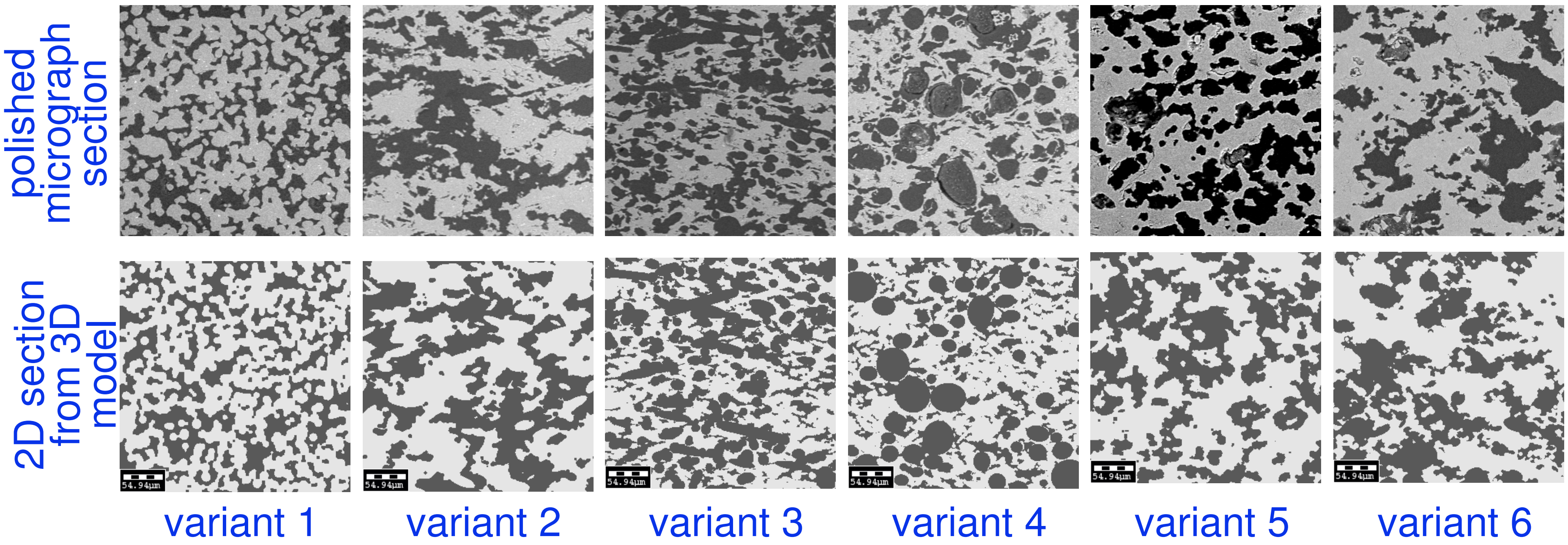


Grid cells: 1 µm x 1 µm x 1 µm
Simulations: ca. 300 x 300 x 700 cells

wall thickness: ca. 0.4 mm

DPF ceramic modeling

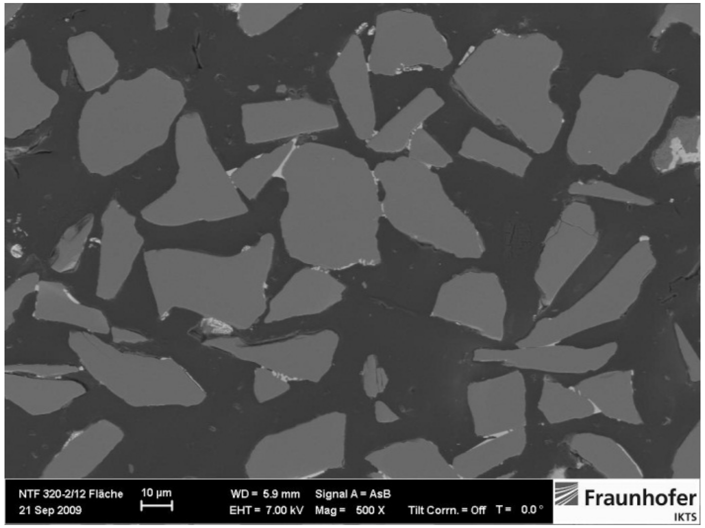
- Various ceramic variants were reconstructed and validated*



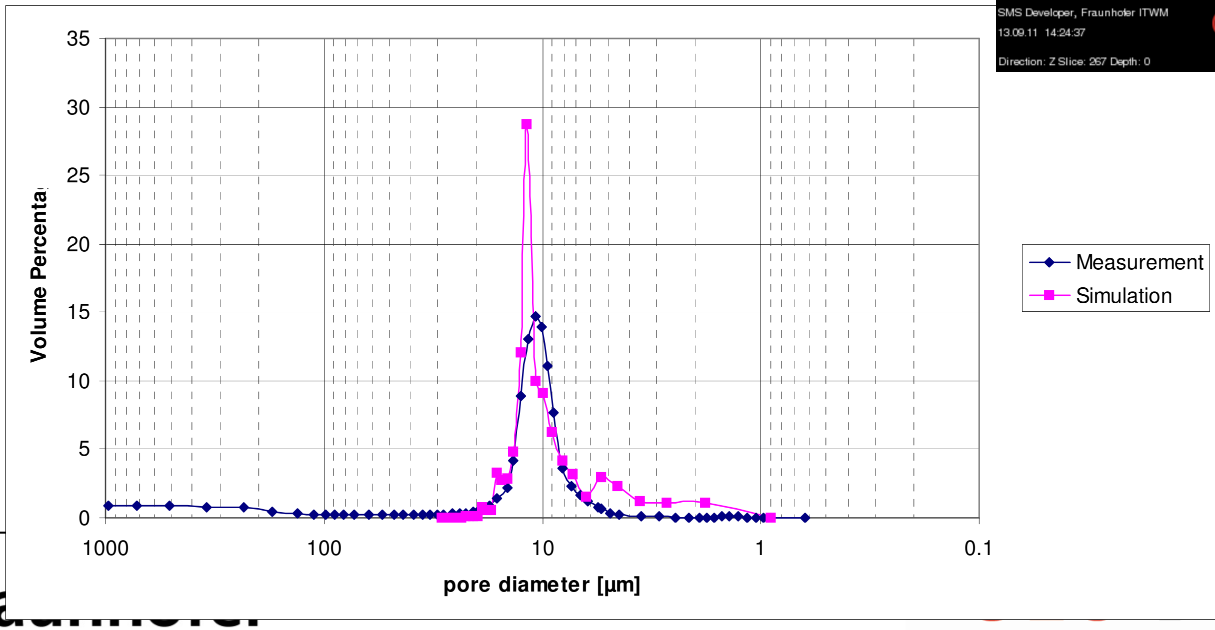
*K. Schmidt, S. Rief, A. Wiegmann, S. Ripperger. *Simulation of DPF Media, Soot Deposition and Pressure Drop Evolution.* Filtech, Wiesbaden 2009.

Funding in BMBF project: CorTRePa

Real vs generated ceramic



SEM and vSEM



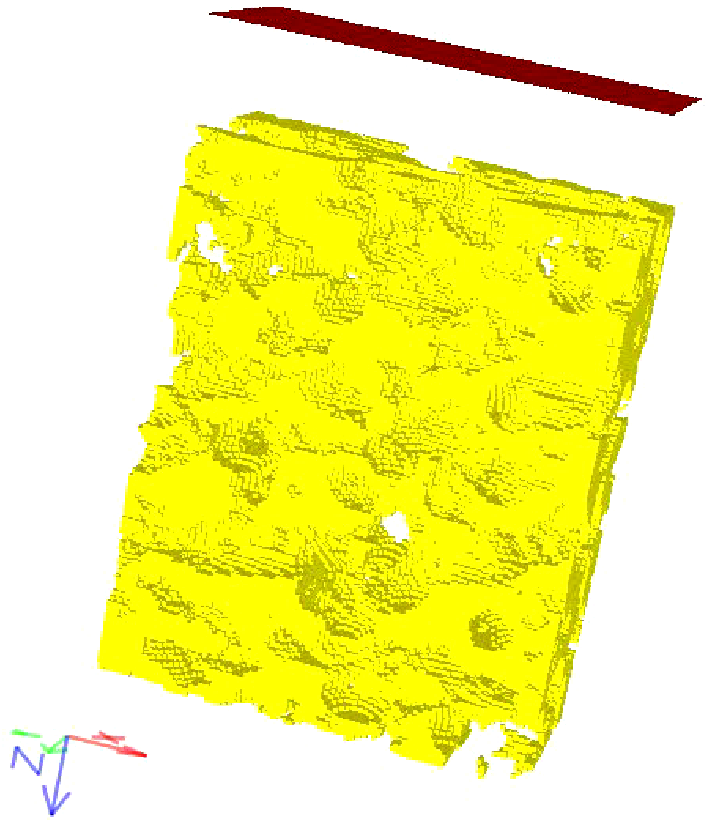
Air flow simulation

Navier-Stokes-Brinkman equations (Eulerian)

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

$+$ boundary conditions,

$\vec{u}$	:	velocity
p	:	pressure
$\vec{f}$	:	force (density)
μ	:	fluid viscosity
κ	:	permeability of porous voxel



Drop convective term: creeping flow

Brinkman term: non-zero in porous media created from subgrid scale particle deposition

Soot transport simulation

Lagrangian Particle Transport

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

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
$\vec{E}_\circ$:	electric field
$\vec{v}_\circ$:	fluid velocity
ρ:	fluid density
μ:	fluid viscosity

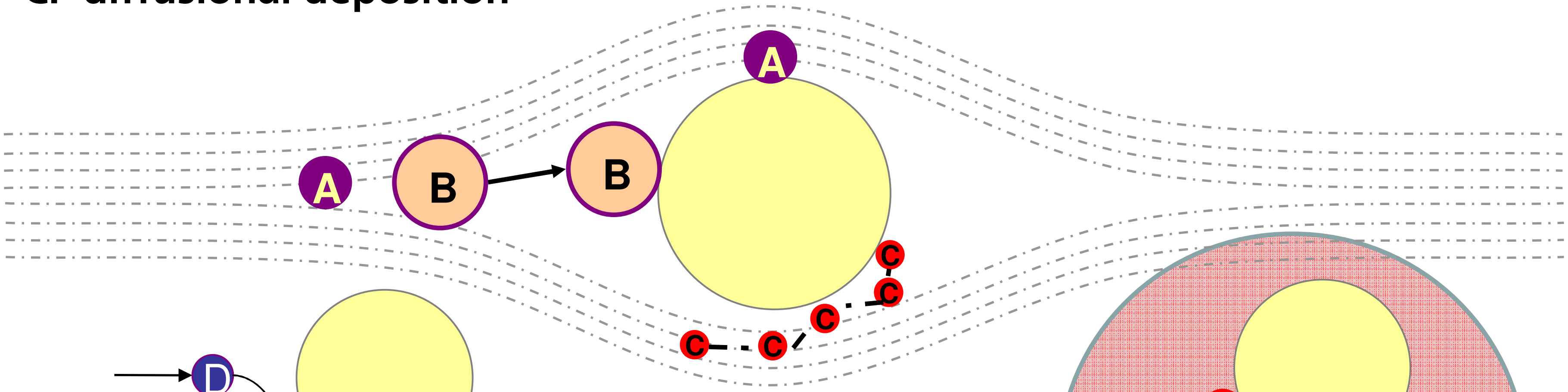
Soot collection mechanisms

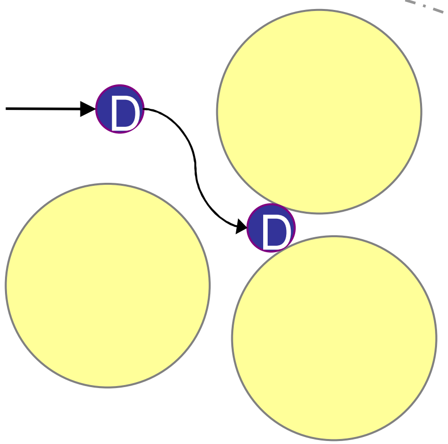
A: direct interception

B: inertial impaction

C: diffusional deposition

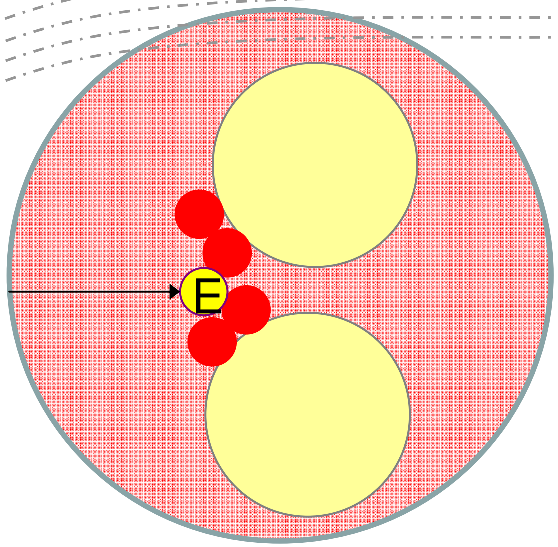
Clogging dominant effect
for soot filtration in DPF



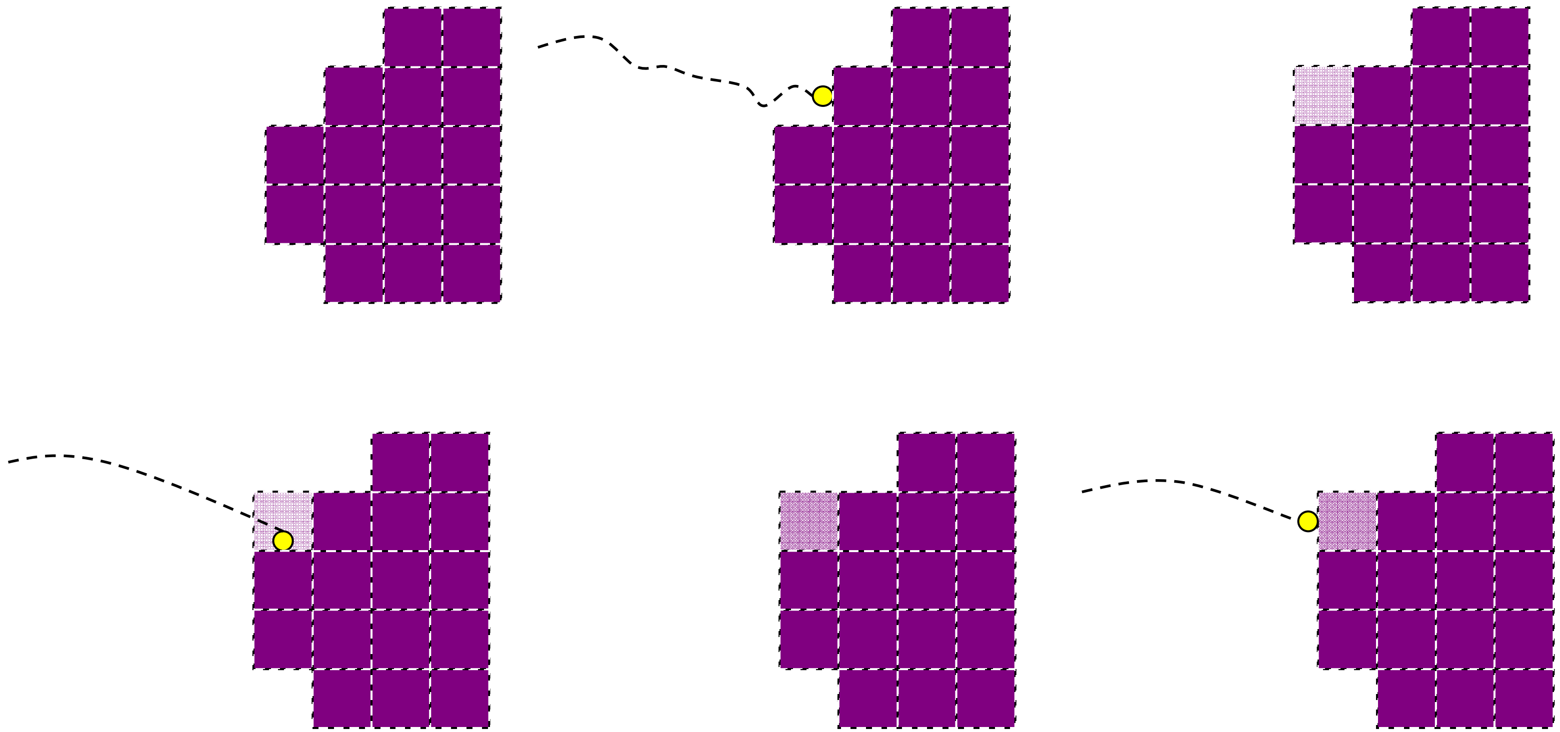


D: sieving

E: clogging

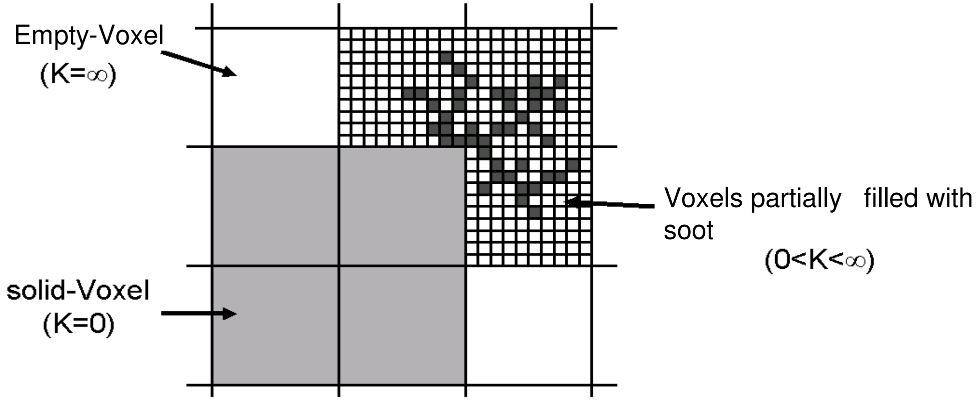


Porous media from soot



- Soot particles are smaller than flow simulation grid cells
- Key parameters: packing density ρ_{max} & corresponding flow resistivity σ_{max}

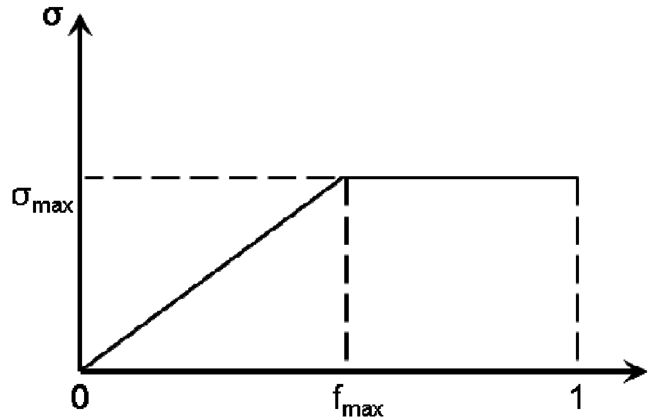
Multivariate permeability of porous voxels



- Soot particles smaller than voxels implies Soot voxels are porous.
- Brinkman term *active* in porous voxels
- permeability computed by

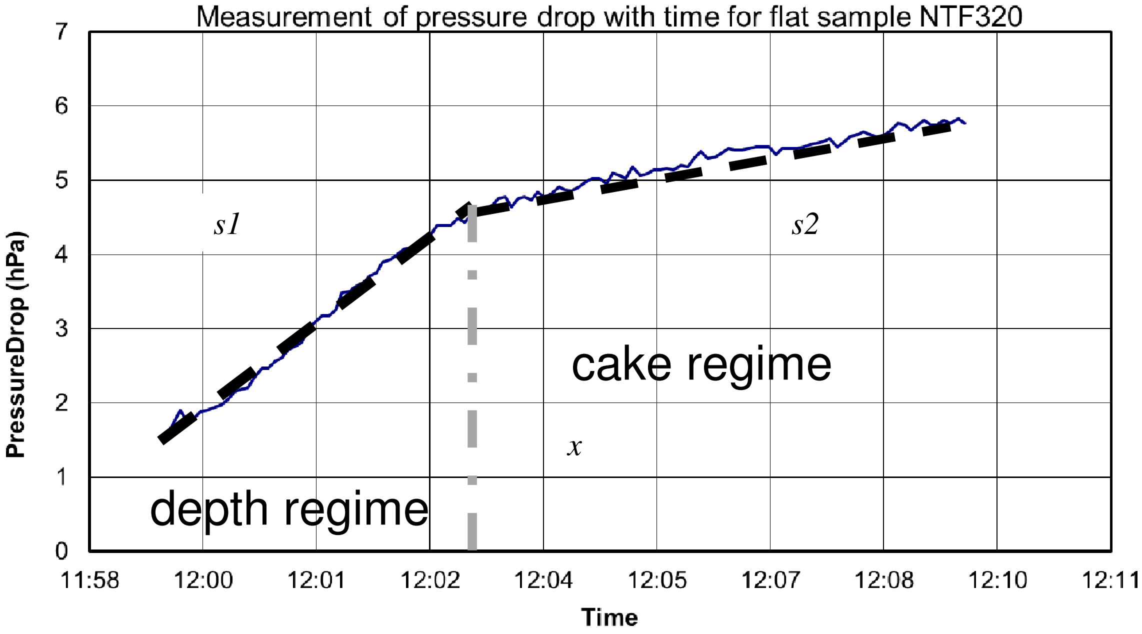
$$\kappa = \frac{\mu}{\sigma}, \qquad \sigma = \begin{cases} \dfrac{\rho}{\rho_{max}}\sigma_{\max}, & 0 < \rho < \rho_{\max} \\ \sigma_{\max}, & \rho \geq \rho_{\max} \end{cases}$$

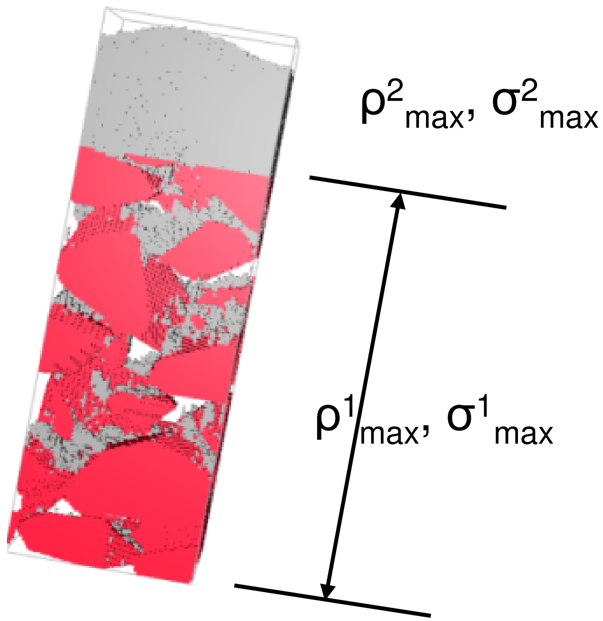
where σ is resistivity, ρ is volume fractioned density.



Multivariate resistivity model:
σ_{max} and ρ_{max} different for *depth* filtration and *cake* filtration.

Influence of σ_{max} and ρ_{max}





ρ^1_{max} : max soot concentration per *depth* voxel determines x

σ^1_{max} : max flow resistivity for (full) *depth* voxel determines s1

ρ^2_{max} : max soot concentration per *cake* voxel determines cake height

σ^2_{max} : max flow resistivity for (full) *cake* voxel determines s2

Determining σ_{max} and ρ_{max}, Variant 1

1. By resolved scale simulations*

   Resolution: 20 nm

   Smallest particles: 80 nm

   fiber: 4 µm

   μ = 1.834e-5 kg/m/s

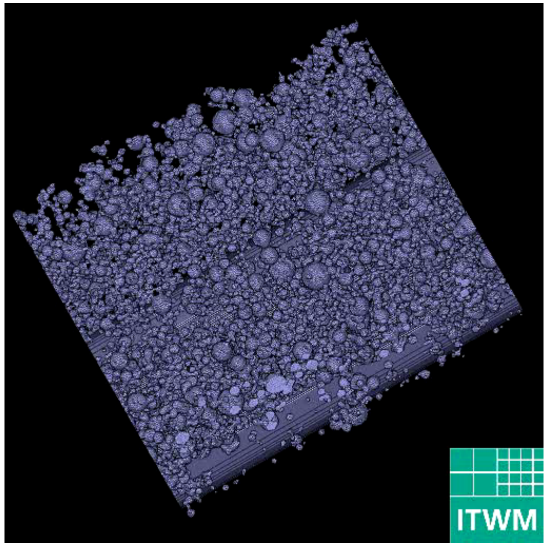
   Structure analysis:
   (solid volume fraction)

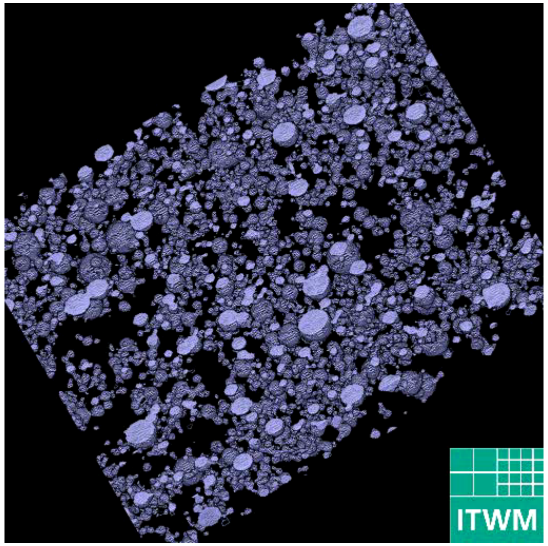
   f_{max} = 0.15, ρ_{max} = 270kg/m³

   Flow computation:

   κ = 1e-15 m²

   σ_{max} = 1.834e10 kg/m³/s





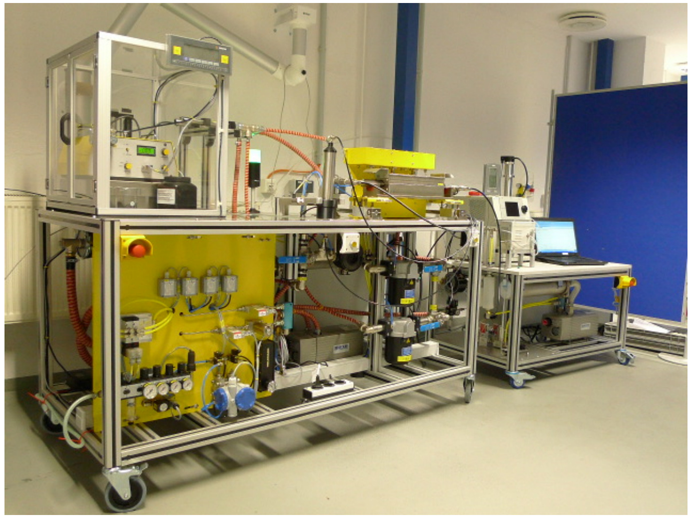
*S. Rief, D. Kehrwald, A. Latz, K. Schmidt, A. Wiegmann. *Virtual Diesel Particulate Filters: Simulation of the Structure, Exhaust Gas Flow and Particle Deposition.* Filtration, No. 4, Vol. 9, 2009, pp. 315-320.

Determining σ_{max} and ρ_{max}, Variant 2

2. By measuring cake height and pressure drop as functions of deposited soot (Fraunhofer IKTS)

   the height of the soot cake on top of flat ceramic samples was measured with time.

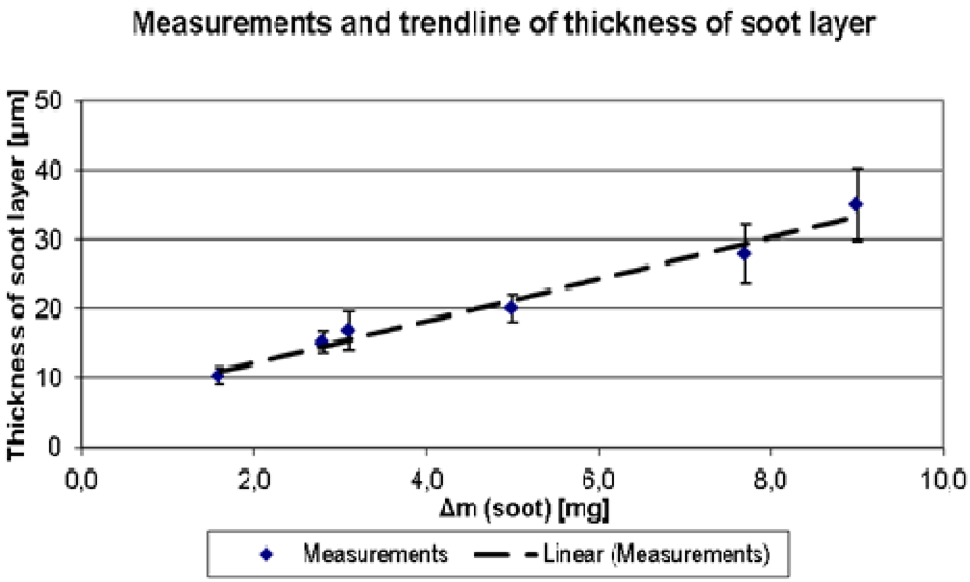
   pressure drop as a function of deposited dust was measured.



$f_{max} = 0.1$, $\rho_{max} = 180 kg/m^3$

$\sigma_{max} = 2.64091e08\ kg/m^3/s$

Lower packing density and flow resistivity than predicted by nano scale simulations!



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Determining σ_{max} and ρ_{max}, Variant 3

3. Fit simulation parameters in media scale simulation until predicted pressure drop agrees

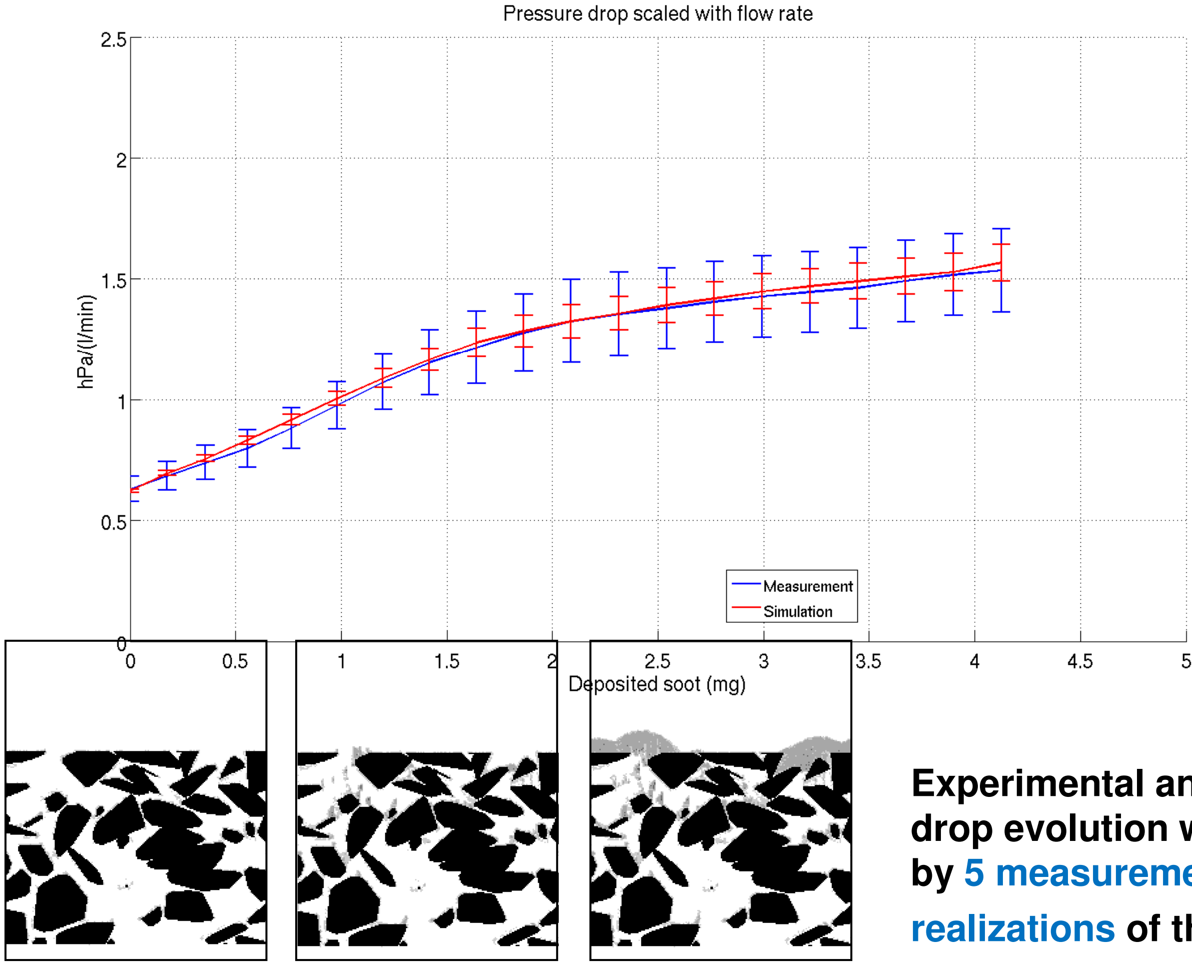
   with experimental data

   – Ceramic model

   – Filtration model

Sample NTF_S

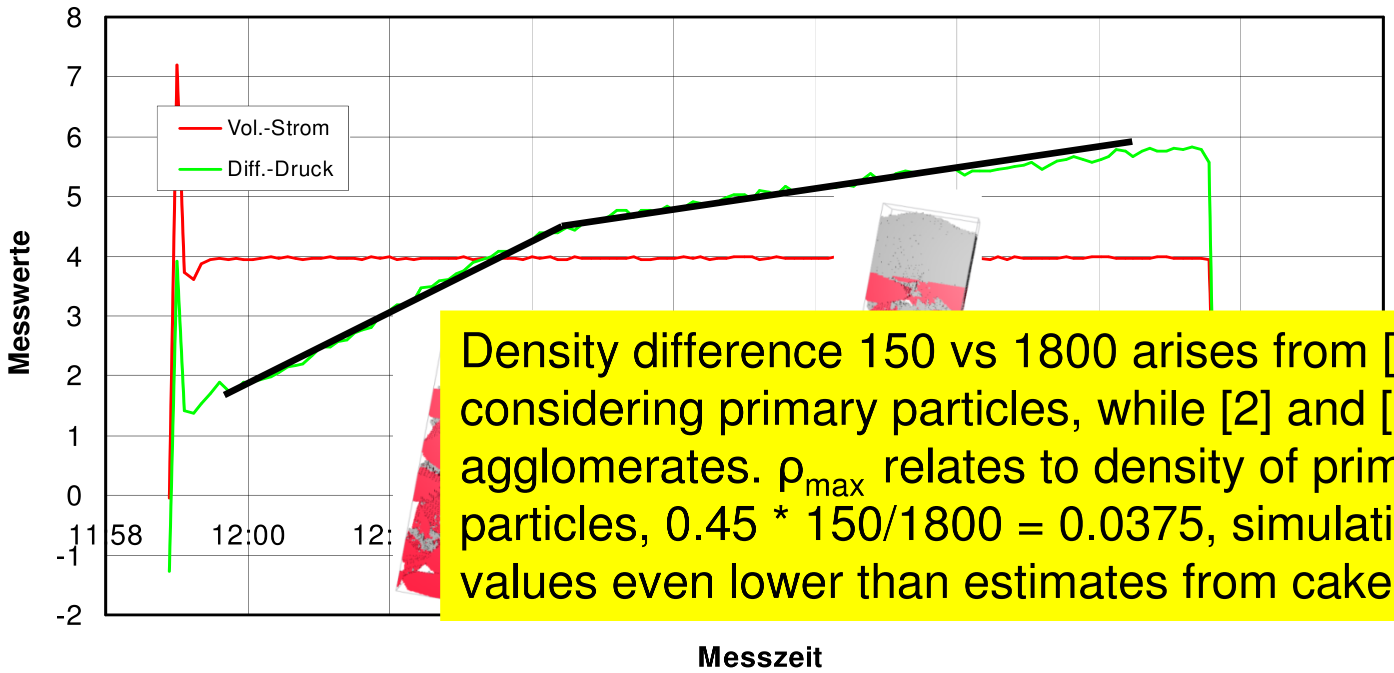
Determinationof σ_{max} and ρ_{max}



Experimental and simulated pressure drop evolution with error bars induced by 5 measurements and 5 different realizations of the virtual structure

Effect of σ_{max} and ρ_{max}

Pressure drop evolution with time for NTF_S



Density difference 150 vs 1800 arises from [1] considering primary particles, while [2] and [3] use agglomerates. ρ_{max} relates to density of primary particles, 0.45 * 150/1800 = 0.0375, simulation values even lower than estimates from cake height.

<u>Micro simulation [1]</u>

ρ_d = 1800 kg/m^3
ρ_{max} = 270 kg/m^3

σ_{max} = 1.834e10 kg/m³/s

<u>Cake height measurement [2]</u>

ρ_d = 1800 kg/m^3
ρ_{max}= 180 kg/m^3,
σ_{max} = 2.64091e08 kg/m³/s

<u>Fit [3]</u>

ρ_d=150 kg/m^3, f_{max} = 0.45,
ρ_{max} = 67.5 kg/m^3,
σ^1_{max} = 3.5e08 kg/m³/s
σ^2_{max} = 8.8e07 kg/m³/s

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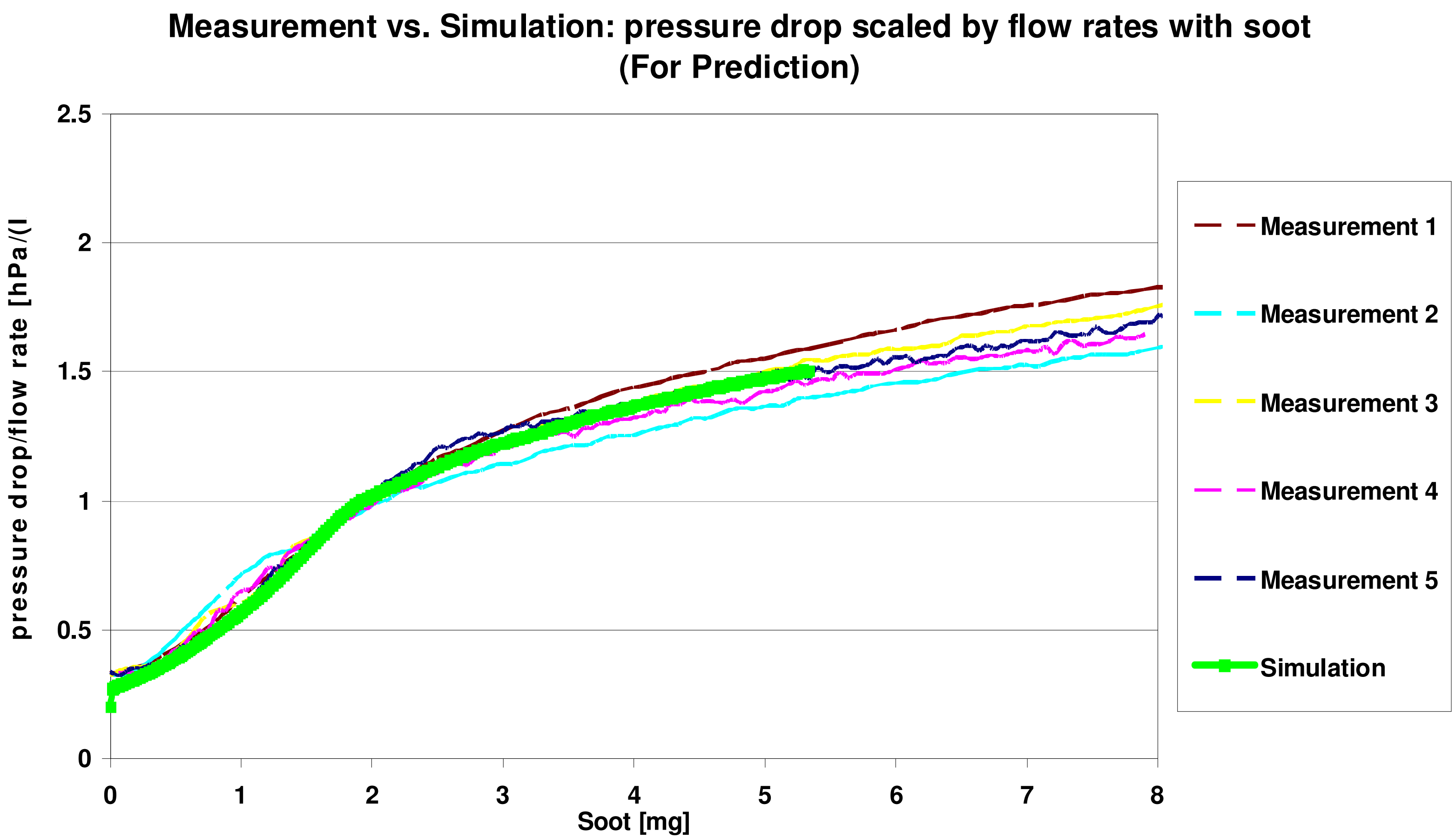
Predicting power of the model

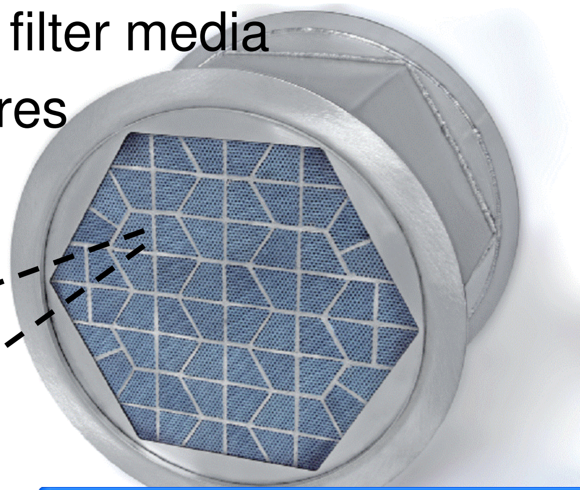


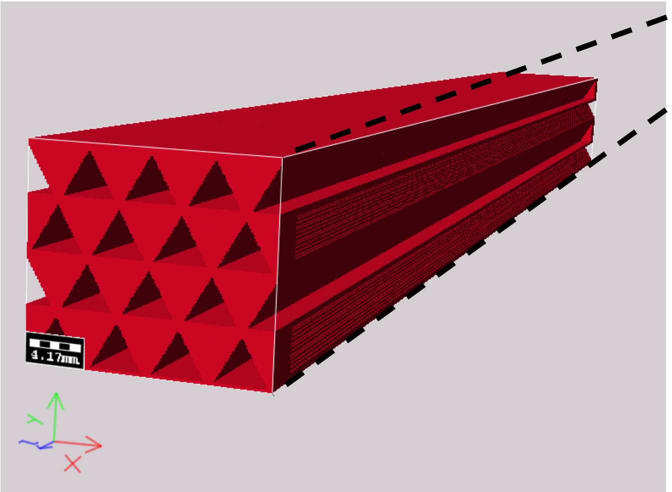
Experimental and simulated pressure drop for a different ceramic, NTF_B, with parameters found by fitting against the measurements of NTF_S.

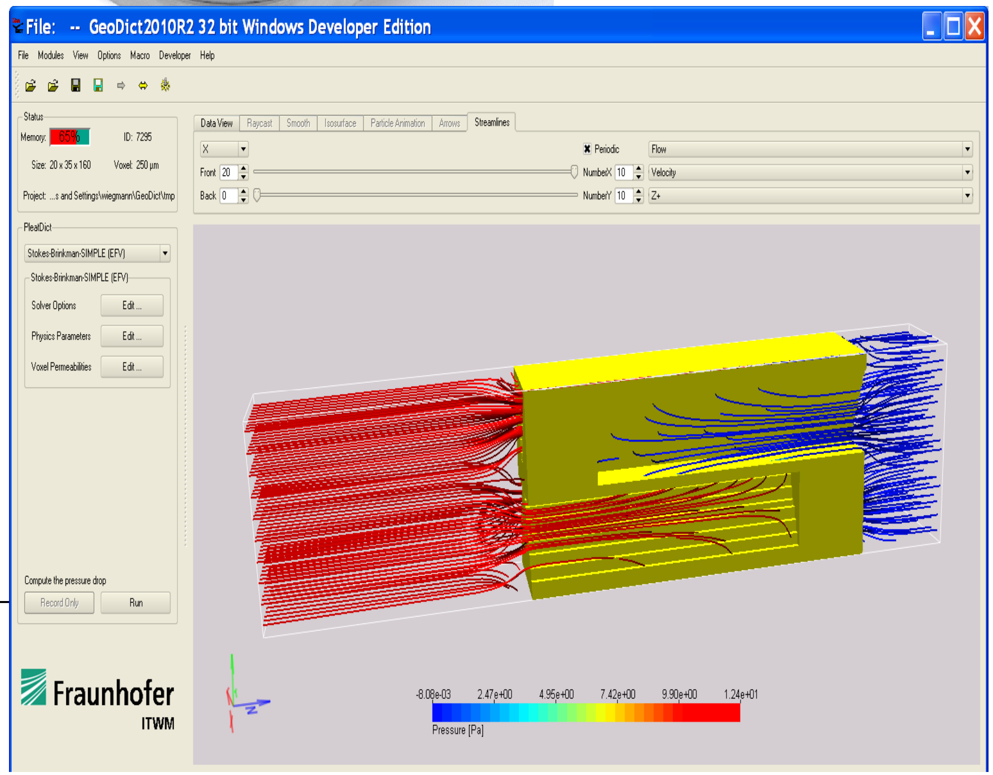
The difference between S and B lies in grain sizes and consequently pore sizes.

Outlook

- The complete filter, instead of filter media
- Next scale: honeycomb structres







Next issue: Thicker cake constricts the channels!

Conclusions

Multivariate resistivity model simple yet matches well against measurements

Parameters σ_{max} and ρ_{max} obtained by fitting against one ceramic predict correctly the pressure drop of a not too different but better DPF media.

This work confirms an important step in virtual material design:

> ***The behavior of not yet existing materials can be predicted by computer simulations, as long as the parameters were established and validated against measurements of media that are not too different from the new and virtual ones.***

Acknowledgements

- We thank Fraunhofer Society for funding the FeiFilTools MEF project

- Media, flow, filtration and honeycomb simulations performed with GeoDict

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Thank you for your kind attention

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