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

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Outline

- Introduction
- Simulation of Filtration Processes for ceramic Diesel Particulate Filter 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
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

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

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*


Funding in BMBF project: CorTRePa
Real vs generated ceramic

SEM and vSEM
Air flow simulation

Navier-Stokes-Brinkman equations (Eulerian)

\[-\mu \Delta \vec{u} + \nabla \times \vec{u} + \kappa \nabla \cdot \vec{u} + \nabla p = \vec{f}, \quad \text{(momentum balance)}\]
\[\nabla \cdot \vec{u} = 0, \quad \text{(continuity)}\]

+ boundary conditions,

\(\vec{u}\) : velocity
\(p\) : pressure
\(\vec{f}\) : force (density)
\(\mu\) : fluid viscosity
\(\kappa\) : 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

\[
\begin{align*}
\frac{d\vec{x}}{dt} &= \vec{v} \\
\frac{d\vec{v}}{dt} &= -\gamma (\vec{v}(\vec{x}) - \vec{u}(\vec{x})) + \frac{Q E_0(\vec{x})}{m} + \sigma \frac{d\vec{W}(t)}{dt} \\
\gamma &= 6\pi \rho \mu \frac{R}{m} \\
\sigma^2 &= \frac{2k_B T \gamma}{m} \\
\langle dW_i(t), dW_j(t) \rangle &= \delta_{ij} dt
\end{align*}
\]

\[t:\] time  \\
\[\vec{x}:\] particle position  \\
\[\vec{v}:\] particle velocity  \\
\[R:\] particle radius  \\
\[m:\] particle mass  \\
\[Q:\] particle charge  \\
\[T:\] temperature  \\
\[k_B:\] Boltzmann constant  \\
\[dW(t):\] 3d probability measure  \\
\[E_0:\] electric field  \\
\[\vec{u}_0:\] fluid velocity  \\
\[\rho:\] fluid density  \\
\[\mu:\] 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 $\rho_{\text{max}}$ & corresponding flow resistivity $\sigma_{\text{max}}$
Multivariate permeability of porous voxels

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

\[
\kappa = \frac{\mu}{\sigma}, \quad \sigma = \begin{cases} 
\frac{\rho}{\rho_{\text{max}}} \sigma_{\text{max}}, & 0 < \rho < \rho_{\text{max}} \\
\sigma_{\text{max}}, & \rho \geq \rho_{\text{max}} 
\end{cases}
\]

where \(\sigma\) is resistivity, \(\rho\) is volume fractioned density.

Multivariate resistivity model:
\(\sigma_{\text{max}}\) and \(\rho_{\text{max}}\) different for *depth* filtration and *cake* filtration.
Influence of $\sigma_{\text{max}}$ and $\rho_{\text{max}}$

- $\rho^1_{\text{max}}$: max soot concentration per depth voxel determines $x$
- $\sigma^1_{\text{max}}$: max flow resistivity for (full) depth voxel determines $s1$
- $\rho^2_{\text{max}}$: max soot concentration per cake voxel determines cake height
- $\sigma^2_{\text{max}}$: max flow resistivity for (full) cake voxel determines $s2$
Determining $\sigma_{\text{max}}$ and $\rho_{\text{max}}$, Variant 1

1. By resolved scale simulations*

Resolution: 20 nm
Smallest particles: 80 nm
fiber: 4 µm
$\mu = 1.834e-5 \text{ kg/m/s}$

Structure analysis:
(solid volume fraction)
$f_{\text{max}} = 0.15$, $\rho_{\text{max}} = 270 \text{ kg/m}^3$

Flow computation:
$\kappa = 1e-15 \text{ m}^2$

$\sigma_{\text{max}} = 1.834e10 \text{ kg/m}^3/\text{s}$

Determining $\sigma_{\text{max}}$ and $\rho_{\text{max}}$, 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.

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

$$\sigma_{\text{max}} = 2.64091\times10^8 \text{kg/m}^3/\text{s}$$

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

![Image of experiment setup](image-url)
Determining $\sigma_{\text{max}}$ and $\rho_{\text{max}}$, 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
Determination of $\sigma_{\text{max}}$ and $\rho_{\text{max}}$

Experimental and simulated pressure drop evolution with error bars induced by 5 measurements and 5 different realizations of the virtual structure.
Effect of $\sigma_{\text{max}}$ and $\rho_{\text{max}}$

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. $\rho_{\text{max}}$ relates to density of primary particles, $0.45 \times 150/1800 = 0.0375$, simulation values even lower than estimates from cake height.

Micro simulation [1]
- $\rho_d = 1800 \text{ kg/m}^3$
- $\rho_{\text{max}} = 270 \text{ kg/m}^3$
- $\sigma_{\text{max}} = 1.834 \times 10^9 \text{ kg/m}^3/\text{s}$

Cake height measurement [2]
- $\rho_d = 1800 \text{ kg/m}^3$
- $\rho_{\text{max}} = 180 \text{ kg/m}^3$
- $\sigma_{\text{max}} = 2.64091 \times 10^9 \text{ kg/m}^3/\text{s}$

Fit [3]
- $\rho_d = 150 \text{ kg/m}^3$, $f_{\text{max}} = 0.45$
- $\rho_{\text{max}} = 67.5 \text{ kg/m}^3$
- $\sigma_{1,\text{max}} = 3.5 \times 10^8 \text{ kg/m}^3/\text{s}$
- $\sigma_{2,\text{max}} = 8.8 \times 10^7 \text{ kg/m}^3/\text{s}$
Predicting power of the model

Measurement vs. Simulation: pressure drop scaled by flow rates with soot
(For Prediction)

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 structures

Next issue: Thicker cake constricts the channels!
Conclusions

Multivariate resistivity model simple yet matches well against measurements

Parameters $\sigma_{\text{max}}$ and $\rho_{\text{max}}$ 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.*
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• Media, flow, filtration and honeycomb simulations performed with GeoDict

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Thank you for your kind attention