Simulation of DPF Media, Soot Deposition and Pressure Drop Evolution

Kilian Schmidt, Stefan Rief, Andreas Wiegmann
Fraunhofer ITWM, Fraunhofer-Platz 1, 67663 Kaiserslautern
Siegfried Ripperger
TU Kaiserslautern, Fachbereich Maschinenbau und Verfahrenstechnik,
Gottlieb-Daimler-Straße 44, 67663 Kaiserslautern

ABSTRACT

A technique of computing the pressure drop and deposition rate evolution during soot loading and the 3D distribution of deposited soot particles for micro-structured ceramic filter media is presented. Methods developed at Fraunhofer ITWM for generating 3D computer models representing the microstructure of the filter material and for computing soot particle deposition in the microstructure models are described.

KEYWORDS

CFD-Simulation, Micro Structure, Nano particles, Ceramic Filter Media, Diesel Soot

1. Introduction

For employment in diesel particulate filters, mainly in automotive applications, various materials are investigated as potential substrates. At Fraunhofer ITWM, the software package GeoDict is developed for characterizing materials and in particular filter media by 3D models of their microstructure. The properties of filter media, which can be computed based on microstructure models, are deposition rate and pressure drop evolution and the 3D soot distribution in the microstructure. By such simulations, process engineers get a better understanding of the filtration process on the micro scale. Also, expensive and time-consuming experiments can be shortened or even substituted by simulations.

In a joint 3-year research project involving Industry and Fraunhofer ITWM, diverse cordierite ceramic variants have been investigated and diesel soot filtration simulations have been performed and validated by experiments. Throughout the project, the microstructure analysis and modeling as well as the soot particle filtration simulation methods integrated in GeoDict have been refined. In a recently started 2-year Fraunhofer-internal research project, the developments are continued.

GeoDict is not only applicable to simulation of soot particle deposition in ceramic microstructures, but also to simulation of micro- or nano particle deposition in micro-structured filter media in general.

2. Method

The microstructure of a ceramic filter medium is investigated by polished micrograph sections or microtomography and measurements of porosity and permeability. Then a 3D computer model is generated with the GeoDict structure generation module SinterGeo. The microstructure modeling approach implemented in SinterGeo is quite user-interactive up to now. The user performs a sequence of structure generation methods and morphological operations in order to match the visual appearance of the microstructure of the real material. The sequence of operations performed by the user is recorded by GeoDict as macro. By varying the parameters in the GeoDict macro, the fine adjustment for matching porosity, chord length distribution and permeability of the real material and the generated model is performed. By this technique, the microstructure of 6 distinct cordierite ceramic variants has been modeled and validated by measurements.

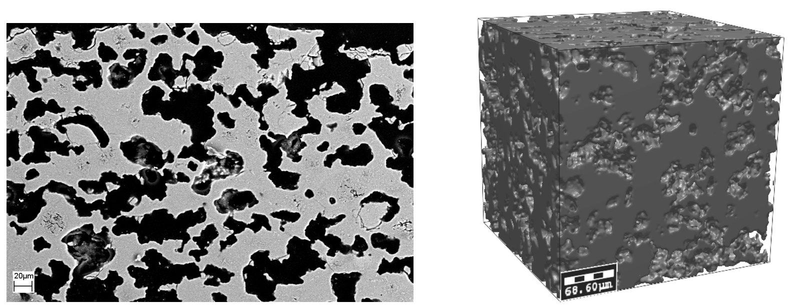

Figure 1: polished micrograph section (left) and 3D computer model generated with GeoDict / SinterGeo (right).

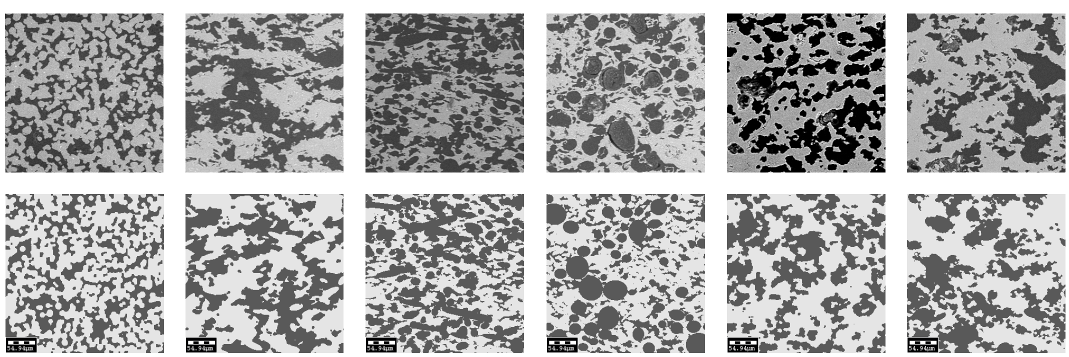

Figure 2: polished micrograph sections (upper row) of 6 distinct cordierite ceramic variants and 2D sections of 3D models generated with GeoDict / SinterGeo (lower row).

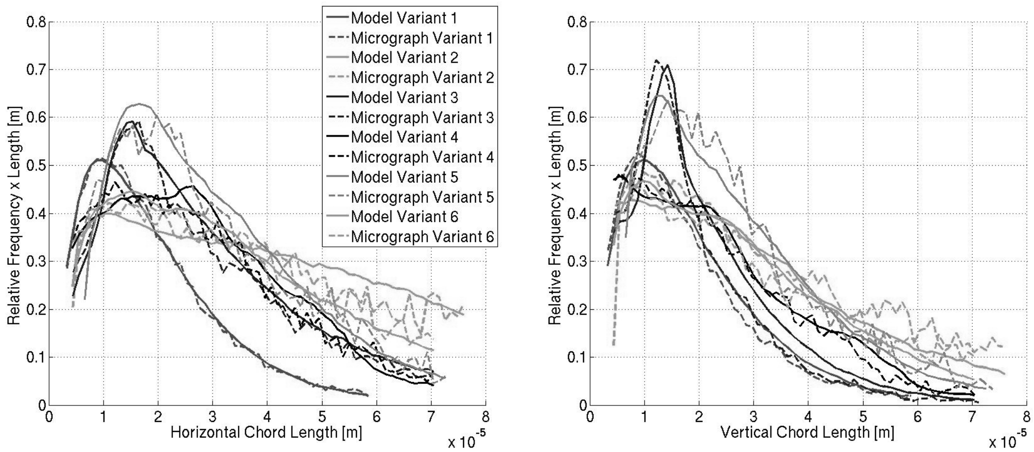

Figure 3: horizontal (left) and vertical (right) chord length distributions of polished micrograph sections and models from Figure 2.

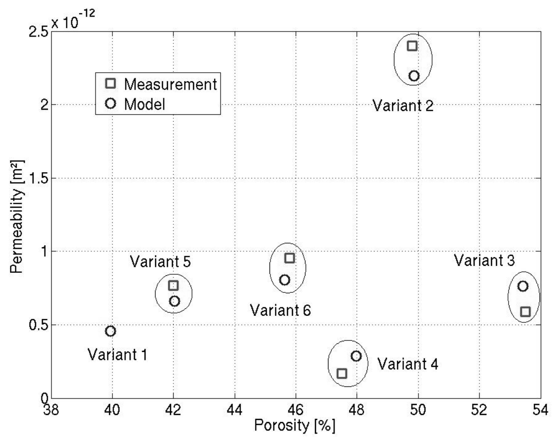

Figure 4: measured and computed porosities and permeabilities for real materials and models shown in Figure 2.

Once the microstructure of the real material has been reconstructed as 3D computer model, porosity, pore size distribution and pore shapes of the model can be varied by varying the parameters in the GeoDict structure generation macro. The variations of the microstructure model can then be investigated by simulation in order to identify an optimized microstructure variant.

GeoDict / SinterGeo is also applicable for reconstruction of a wide spectrum of microstructures unlike ceramics, such as fibers, packings, dense sinter materials or foams.

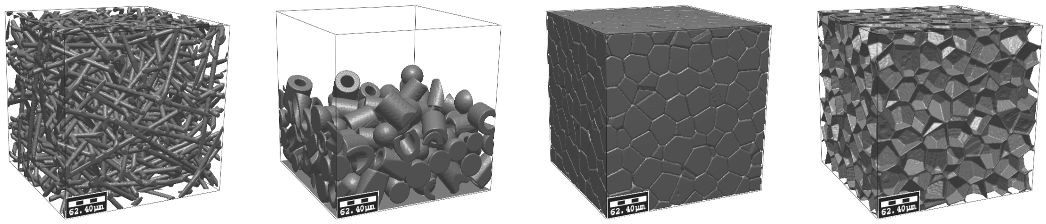

Figure 5: miscellaneous microstructure models generated with GeoDict / SinterGeo.

The soot particle filtration simulation is carried out with the GeoDict module FilterDict. The air flow through the microstructure model and the trajectories of particles, driven by flow and diffusion, are computed alternately and iteratively. The flow is recomputed each time a significant number of particles has deposited in the microstructure and effects a change of the flow. High performance codes developed at Fraunhofer ITWM for flow computation on Cartesian grids and particle trajectory computation by the Lagrangian approach with adaptive time steps are utilized. The effect on the air flow of permeable soot layers deposited locally in the microstructure is modeled by introducing the Brinkman-term into the Stokes-equations.

$$\begin{aligned} \mu\Delta V - \frac{\mu}{K}V &= \nabla P \quad \text{in } \Omega \\ \mathrm{div} V &= 0 \quad \text{in } \Omega \\ V &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

$$\begin{aligned} V &= \text{fluid velocity} \\ P &= \text{pressure} \\ K &= \text{local permeability} \\ \mu &= \text{fluid viscosity} \\ \Omega &= \text{void region in the microstructure model} \\ \partial\Omega &= \text{boundary of } \Omega = \text{microstructure surface} \end{aligned}$$

Figure 6: Stokes-Brinkman equations describing the fluid flow through the microstructure.

$$\begin{aligned} \frac{dx}{dt}(t) &= v(t) && \forall\, t \geq 0 \\ \frac{dv}{dt}(t) &= \gamma\Big(V(x(t)) - v(t)\Big) + \sigma\frac{dW}{dt}(t) && \forall\, t \geq 0 \\ x(0) &= x_0 \\ v(0) &= v_0 \end{aligned}$$

$$\begin{aligned} t &= \text{time} \\ x &= \text{particle position} \\ x_0 &= \text{initial particle position} \\ v &= \text{particle velocity} \\ v_0 &= \text{initial particle velocity} \\ \gamma &= \frac{6\pi\mu R}{m} = \text{particle-fluid friction coefficient} \\ m &= \text{particle mass} \\ \rho &= \text{fluid density} \\ R &= \text{particle radius} \\ W &= \text{continuous Wiener process describing diffusion} \\ \sigma &= \sqrt{\frac{2\kappa T\gamma}{m}} = \text{magnitude of diffusion} \\ \kappa &= \text{Boltzmann constant} \\ T &= \text{fluid temperature} \end{aligned}$$

Figure 7: Equations describing the particle movement within the fluid flow.

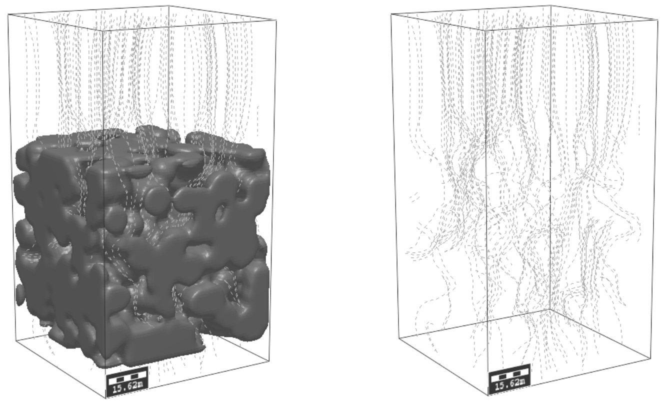

Figure 8: Filtration simulation with a 3D silicon carbide ceramic microstructure model and computation of particle trajectories (periodic microstructure model with particle trajectories left, only trajectories right).

The special shape of the soot particles, which are strictly speaking agglomerates of primary particles, and the mechanism of the soot particle deposition on the microstructure surface are modeled in detail.

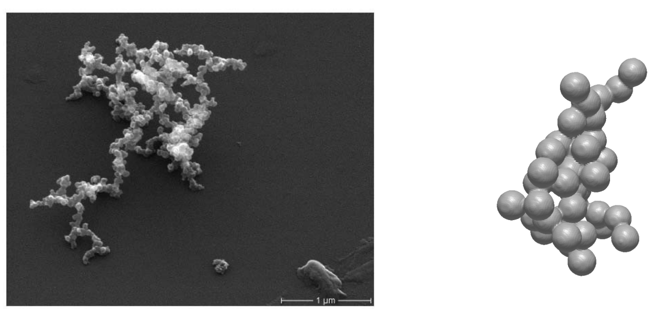

Figure 7: Micrograph of a soot particle agglomerate (left, origin: http://img.pte.at) and soot particle model used by GeoDict / FilterDict (right).

From the computed particle trajectories, the deposition rate and the 3D soot distribution in the microstructure is obtained, from the computed flow the pressure drop is derived.

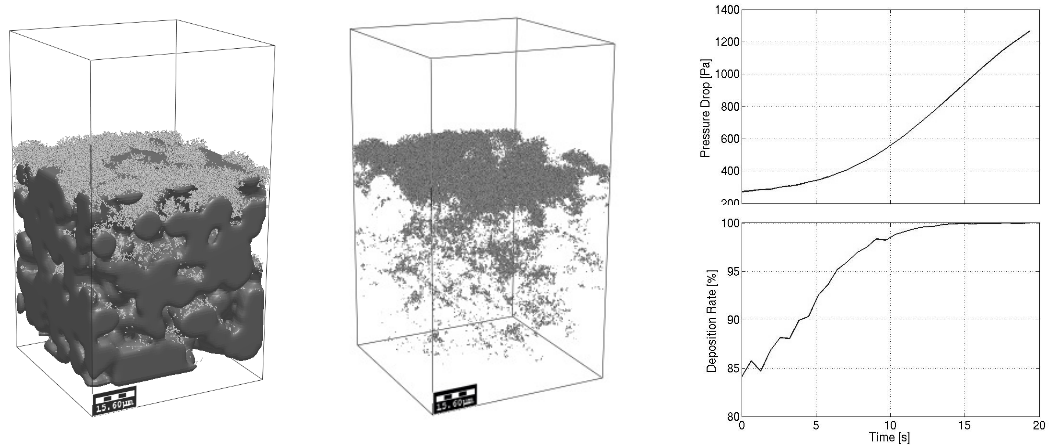

Figure 8: microstructure model with deposited soot (left), deposited soot without microstructure (center) and computed pressure drop and deposition rate evolution (right)

When the simulations are run with adequate resolution and precision, the results agree very well with measurements of pressure drop, deposition rate and 3D soot distribution in the microstructure, which have been performed by project partners in the industry. But still an enormous computing power is needed to obtain realistic simulation results. By applying sophisticated numerical methods for these computations, the required computing power can be reduced to an appropriate level.

3. Ongoing Developments

In the reconstruction process of the microstructure of a real material with GeoDict / SinterGeo, the exact matching of the chord length distributions of polished micrograph sections and the microstructure model is performed by the user, guessing and testing parameter combinations for the microstructure generation macro. This process can be automated in order to get even better agreement of real materials and models and to save time.

In order to get realistic soot filtration simulation results, the flow must be computed very accurately at the surface of the microstructure. Test simulations show that for realistic simulation of soot particle filtration, the computational grid must be resolved with about one tenth of a micron at the microstructure surface. Simulations of experiments with accordingly high resolution show very good agreement of the results of simulations and experiments, but take a long time and too much computational resources. In order to save computing resources, the grid for the flow computation can be coarsened away from the surface of the microstructure. The development of a high performance flow solver for locally coarsened Cartesian grids is continued at ITWM at the time.

The geometric soot particle diameter distribution, the soot particle flow resistivity and the permeability of deposited soot layers are still uncertain. Simulations with variations of these parameters are performed in order to determine appropriate values and to match experiments.

4. Summary and Outlook

Up to now, the approaches for ceramic microstructure generation implemented in GeoDict / SinterGeo and for diesel soot filtration simulation implemented in GeoDict / FilterDict have been proven to lead to the right results. In order to make the simulations better applicable for filter development in the industry, structure generation with GeoDict / SinterGeo is automated onward and filtration simulation with GeoDict / FilterDict is accelerated by making use of local coarsening for the flow computation.

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