Fraunhofer Software Tools GeoDict/FilterDict for the Simulation of Diesel Particulate Filters

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Summary:

Diesel particulate filters are gradually making their way into series production to keep emissions of fine dust to a minimum. But which filters are most efficient at extracting the noxious particles? How do the geometrical details of the filter material affect the filter properties? Until now, researchers and developers have had to conduct a series of tests to answer questions like these: They build prototypes, which then have to prove their abilities in experiments. This involves using a huge number of test filters.
A new simulation software could in future significantly reduce the number of prototypes required, cutting the time and cost of development – and offer some powerful new features, as well. For the first time, the 3-D simulation software FilterDict gives full insight into the filtration process. It allows simulating how fast and how far particles penetrate into the filter, for example – using any kind of filter material. As its input variables, FilterDict requires the filter material model from the microstructure generator GeoDict, various physical parameters, and the particle size distribution. The program calculates the path of the soot particles through the filter media. The simulation shows how much soot is deposited in which part of the filter. Therefore, the design of the filter can be optimized to achieve long regeneration intervals, low fuel consumption and a high engine rating.
The simulation program has already passed its first practical test. In an experiment conducted with fellow scientists at Bosch, the researchers examined two diesel particulate filters, and compared the results with those of the simulations. Now, Bosch and ITWM are extending their cooperation to simulate up to a hundred filters. Unsuitable designs can then be excluded from the outset – the researchers only build prototypes of filters that achieve satisfactory results in FilterDict. Only these are tested in the laboratory.

Keywords:

Virtual Material Design, Filtration Simulation, Computational Fluid Dynamics

1 Introduction

Filtration plays a key role in many technical applications, as well as in everyday life. For example, filters are used in air conditioning systems, in medical applications and in the food industry for various separation tasks. Especially in automotive applications they are of predominant importance. Fir instance, diesel particulate filters have been in the center of interest for several years now.
Filters have to fulfill certain performance criteria which are partly in contradiction to each other: Filtration efficiency and filter lifetime should be on a high level, whereas the overall pressure drop is aimed to be small. In the car industry, the size of the filter is typically strongly limited due to manufactures' specifications. On the other hand, there exist various possibilities to design a filter. Questions arise for the best fiber crossection and optimum fiber orientation, etc. Is a layered medium always better than a homogenous one? How do pleats influence the pressure drop? Quite often, the interplay of all these design parameters is not fully understood. Hence, prototyping can be very costly and time consuming. One way with a great potential to overcome these difficulties is computer simulation.
At the Fraunhofer ITWM, numerical methods and software tools ([3], [10]) have been developed for microstructure simulation and virtual material design. Structure generators exist capable to create virtual geometry models of nonwoven and woven media, sinter structures, foams and membranes. These models are resolved at the micrometer scale. Taking a representative volume of the medium, flow simulations compute effective properties like permeabilities and flow resistivities of the virtual media. Adding a computer code for particle tracking, initial filter efficiencies and filter lifetime computations become possible.
The paper is organized as follows: In Section 2, the methods of virtual structure generation are presented. The physical models and simulation methods are explained in Section 3. Both sections contain various illustrating examples. Finally, in Section 4, we give a brief summary and an outlook on future developments.

2 Virtual Filter Geometries

The starting point of any filter simulation is a realistic three-dimensional computer model of the geometry. With regard to virtual material design the possibility to rely on purely computer generated structures is essential. In Fig. 1 and 2, four virtual structures are shown which may be used in a filtration application. The geometries are generated by the Fraunhofer software **GeoDict** [15]. All geometries are generated on basis of regular cubical meshes. In general, this approach requires a huge number of cells which are called voxels. On the other hand, extremely efficient algorithms exist which exploit the highly structured mesh. Moreover, it ensures high flexibility such that the simulation chain can also be fed by tomographic data sets.
Subsequently, the methods are described how these structures are generated.

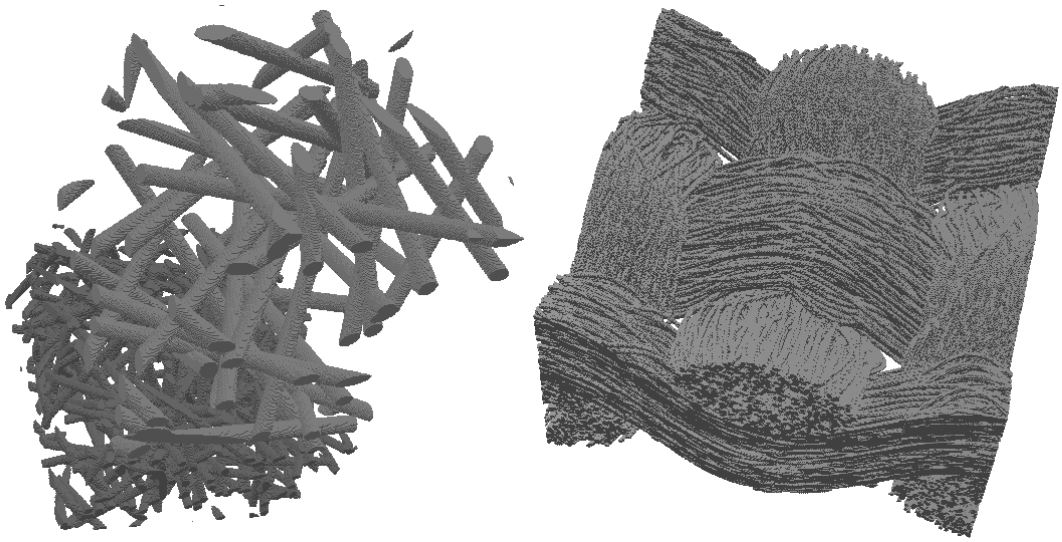

Fig. 1: Virtual structures: Two layered nonwoven (left) and woven structure (right)

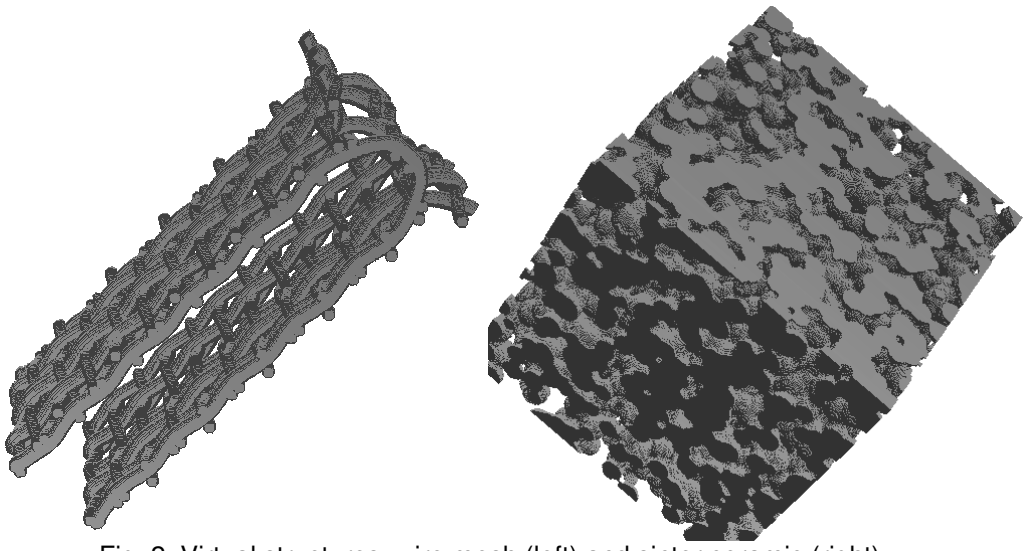

Fig. 2: Virtual structures: wire mesh (left) and sinter ceramic (right)

2.1 Virtual Nonwoven

The generation of virtual nonwoven is based on a stochastic fiber generator [11]. The generator is controlled by a set of parameters that is readily interpreted geometrically. For instance, porosity or fiber volume fraction is selectable. Additionally, several fiber properties like densities, lengths, crossections and orientations can be prescribed. Finally, the resolution of the underlying voxel mesh and the overall dimensions have to be entered. After the specification of the parameters, the fiber generation starts by randomly computing fiber axes and entering the fibers into the voxel mesh. The generation is stopped when the specified fiber volume fraction is reached. In case that the volume fraction could not be reached, GeoDict changes the initialization of its random number generators and starts again. The algorithms do not work completely randomly, but they are designed to guarantee the specified properties with selectable tolerance. Since GeoDict also allows adjusting the initialization of the random number generator, all geometries are reproducible.
In view of simulations, the dimensions should be chosen sufficiently large to give representative results. *Representative* means that the results do not change when the dimensions are further enlarged. To fix ideas, the geometries in Fig. 1 have this property with respect to flow simulations. For filter simulations representative frequently implies to resolve the medium in flow direction completely. The size of the required mesh may reach several millions of voxels: Let us consider a medium with thickness of 1.5 mm and smallest fiber diameter of 20 µm. To ensure reasonable results in a flow computation the smallest fiber diameter should be resolved by at least 4 voxels. Hence the edge length of a voxel is 5 µm, and we need 300 voxel in flow direction. Having approximately the same lateral dimension and additional inlet and outlet regions, we easily end up with millions of voxels.

2.2 Virtual Woven

Virtual woven structures require precise deterministic rules following the weaving pattern of their real counterparts. On the right hand side, Fig. 1 shows a virtual woven possessing a basket weave pattern. Moreover, the yarns consist of many thin fibers. These fibers do not follow a strict deterministic rule, but have some randomness build-in reflecting certain irregularities also present in the real woven.

2.3 Virtual Sinter Structures

The generation of sinter structures comprises two steps: First, the stochastic fiber generator (see Section 2.1.) is used to create packings of spheres and cylinders. To achieve satisfactory results, it is often a good idea to look at the shape and size distribution of the real sinter grains and try to match these distributions. During the second step, morphological operations [11] are applied to generate the sinter necks. Iteratively using the operations dilatation and erosion creates exactly the intended connectivity, i.e. virtual sinter necks.

2.4 Complex Geometries

The methods presented in the previous sections can be considered as elementary building blocks for more complex geometries. The voxel mesh approach naturally allows for combining layers of *elementary* structures. Thus, media having gradients with respect to some property are easily created (Fig. 1, left). Another interesting example is the nonwoven with binder in Fig. 3. The binder is added into the nonwoven in complete analogy to the sinter necks in Section 2.3.

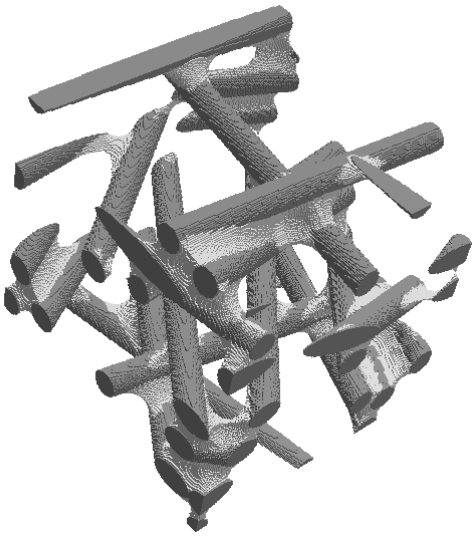

Fig. 3: Virtual nonwoven with binder

In view of virtual material design, we want to finally mention an interesting opportunity for tomographic data sets. If one is interested to redesign a certain layer of an existing medium, one can substitute this layer by a virtual structure. The effect of the replacement can then be studied by simulation.

3 Simulation of Filtration Processes

Depending on the filtration application in mind, the simulation efforts to compute certain filter properties may differ significantly. In some situations, a single flow simulation is sufficient to determine the requested effective permeabilities or flow resistivities. Computing filter efficiencies additionally requires the solution of particle transport through the medium. Certainly, the most demanding application is the simulation of an entire filter lifetime.

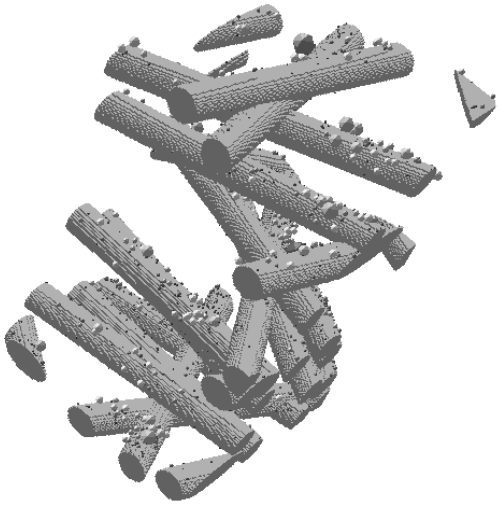

Fig. 4: Simulation of a fibrous medium with deposited dust particles

In the following sections, we describe the physical models and numerical methods currently available in the Fraunhofer GeoDict/FilterDict software [15].

3.1 Flow Simulation

Slow flow regimes are typical for most filtration processes. Hence, flow solvers for the solution of the Stokes equations are well-suited for the simulation. The Stokes equations describe incompressible viscous flow in case of small velocities, i.e. when inertia is negligible:

$$-\mu\Delta\vec{u} + \nabla p = \vec{f} \text{ , (conservation of momentum)} \quad (1)$$

$$\nabla \cdot \vec{u} = 0 \text{ , (conservation of mass)} \quad (2)$$

+ boundary conditions.

In (1) and (2), $\vec{u}$, p, $\vec{f}$ denote the velocity vector, the pressure and the external body force, respectively. To solve the system, boundary conditions have to be prescribed, e.g. velocity profiles at the inlet and outlet of the computational domain. For the numerical solution of system (1), (2), we have two codes. The first code is based on a Lattice-Boltzmann method [4]. The approach of the second code combines a finite volume discretization with the fast Fourier transform [13].
For high velocity flows, the Navier-Stokes equations should be used. This system is quite similar to (1), (2), but contains an additional convective term accounting for inertia effects:

$$-\mu\Delta\vec{u} + (\rho\vec{u}\cdot\nabla)\vec{u} + \nabla p = \vec{f}\text{, (conservation of momentum)} \tag{3}$$

$$\nabla\cdot\vec{u} = 0\text{, (conservation of mass)} \tag{4}$$
$$\text{+ boundary conditions.}$$

In (3), ρ denotes the fluid density. To solve (3), (4) numerically, the already mentioned Lattice-Boltzmann code [4] is available.
Combining free and porous flows enables us to simulate diesel particulate filters (see Section 3.3), where deposited soot particles are not resolved by voxels, but modelled as porous media. For this type of application, we employ the Navier-Stokes-Brinkmann equations [8]:

$$-\mu\Delta\vec{u} + (\rho\vec{u}\cdot\nabla)\vec{u} + \mu K^{-1}\vec{u} + \nabla p = \vec{f}\text{, (conservation of momentum)} \tag{5}$$

$$\nabla\cdot\vec{u} = 0\text{, (conservation of mass)} \tag{6}$$
$$\text{+ boundary conditions.}$$

K^{-1} is the reciprocal of the permeability of a porous medium. In the free flow domain, the permeability is zero, simplifying (5) into (3). In the porous medium, K^{-1} is typically quite large, and $\vec{u}$ is small. Therefore, we can neglect the first two terms in (5), and we obtain Darcy's law:

$$\vec{u} = -\frac{K}{\mu}(\nabla p - \vec{f})\,. \tag{7}$$

Darcy's law was found experimentally in 1856 [2]. It expresses the linear relation between velocity and pressure drop for slow flows in porous media.
(5), (6) is again solved by our Lattice-Boltzmann code.

3.2 Simulation of Initial Filter Efficiencies – Particle Transport and Deposition

The first step in computing initial filter efficiencies is the computation of the fluid flow in the virtual geometry (see Section 3.1). The second step consists in particle tracking. Here, we make certain assumptions: The particles are spherical, there is no particle-particle interaction (= low particle concentration) and the particles do not influence the flow field. After specifying the particle size distribution and a few additional parameters, particle motion is modelled by Newton's Second law:

$$\vec{F} = m\vec{a}\,, \tag{8}$$

where $\vec{F}$ denotes the force exerted on the particle, m is the particle mass, and $\vec{a}$ is the particle acceleration. The particle moves due to its inertia, due to fluid friction and due to Brownian motion. Additionally, an electrostatic force may influence the particle trajectory. For brevity, we refer to [12], [14] for further details on electrostatics. Besides inertia, which is inherent to (8), all effects are modeled as superposition of forces. We finally solve the following system of stochastic differential equations:

$$\frac{d\vec{v}}{dt} = -\gamma(\vec{v}(\vec{x}(t)) - \vec{u}(\vec{x}(t))) + \sigma\frac{d\vec{W}(t)}{dt} + \frac{q\vec{E}(\vec{x}(t))}{m}\,, \tag{9}$$

$$\frac{d\vec{x}}{dt} = \vec{v}\,. \tag{10}$$

In (9), (10), t, $\vec{x}$, and $\vec{v}$ denote time, position, and velocity of the particle, respectively. The first term on the right hand side of (9) describes the force due to friction. It is proportional to the difference of the particle and the fluid velocity. The coefficient γ is given for slow flow and spherical particles by:

$$\gamma = \frac{6\pi\mu R}{m} \text{. (Stokes friction)} \tag{11}$$

R denotes the particle radius.
The second term on the right hand side of (9) models Brownian motion by a three-dimensional Wiener-process $\overrightarrow{W}$. Let T be the temperature and k_B be the Boltzmann constant. Then, we have by the fluctuation–dissipations theorem:

$$\sigma^2 = \frac{2k_B\gamma T}{m}. \tag{12}$$

For further details of the modelling, we refer to [9], [14]. We solve system (9), (10) by an implicit Euler method.
In addition to the particle motion, we have to check for collisions of the particles with the geometry in each time step. In case a collision is detected, the particle stops and it is marked as deposited. After the simulation run, we calculate for each particle size the fraction of deposited to total number of particles (Fig. 5).

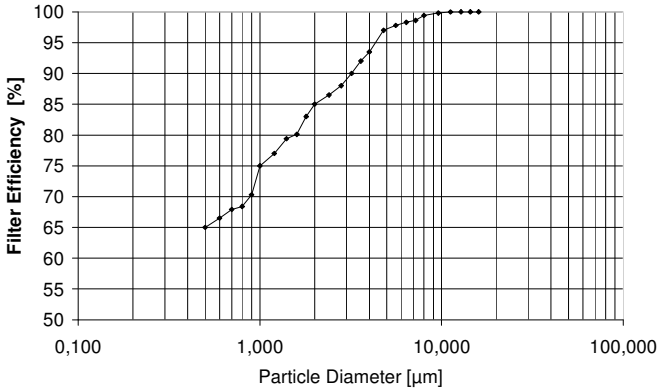

Fig. 5: Simulation of the initial filter efficiency of an air filter medium

Since the simulation provides total information on each individual particle, diagrams like Fig. 6 are possible to create. Up-to-now, this detailed analysis is experimentally not available.

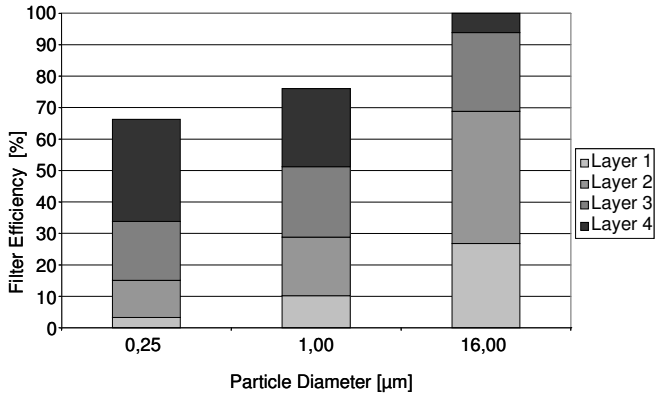

Fig. 6: Cumulative initial filter efficiencies of a four layered air filter medium

3.3 Simulation of Filter Lifetimes – Solid and Porous Deposition Mode

Filter lifetime simulations iteratively compute the flow field and particle transport as introduced in Section 3.2. An essential third simulation component comes into play, since we need to *modify* the geometry due to deposited particles. Therefore, we keep track of the volume fraction filled by deposited particles for every voxel of the geometry. Basically, there exist two modes how volume fractions influence forthcoming simulations. The first mode is called *solid deposition mode*. It is intended to be used whenever particle diameters are greater or equal than the voxel length. Hence, particles are resolvable by the voxel mesh. When the volume fraction of a voxel reaches 1, it is marked as *solid*. The flow solver considers this voxel as an obstacle, and the particle tracking considers it as a collision voxel where particle may deposit. The second mode is called *porous deposition* mode. It is used when particles are much smaller then a voxel and, hence, build up porous

substructures. Depending on its volume fraction, we assign a permeability to the voxel. Consequently, the flow computation is based on the Navier-Stokes-Brinkmann approach (5), (6). Particle deposition in a porous voxel is possible as long as a prescribed maximum volume fraction is not reached. When a voxel exceeds the maximum fill-level it is considered as a collision voxel. Obviously, filter lifetime simulations using the porous deposition model depend on the prescribed permeability and maximum volume fraction. In Section 3.4, we show how the parameters can be obtained by highly resolved single fiber simulations.

3.4 Example: Simulation of a Diesel Particulate Filter

The aim of this section is to simulate the evolution of the pressure drop of the diesel particulate filter medium in Fig. 7. The clean medium in bright grey consists of a ceramic substrate with additional fiber layer. Both geometries are purely virtual by applying the procedures from Section 2.1, 2.3 and 2.4. The resolution is 1 µm, and the dimension of the geometry is 150 x 150 x 650 voxels. With respect to porosity and cord length distribution, the virtual structure has quite similar properties as its real counterpart. The comparison is done using SEM images. Moreover, the simulated initial pressure drop is in good accordance with the measured pressure drop.

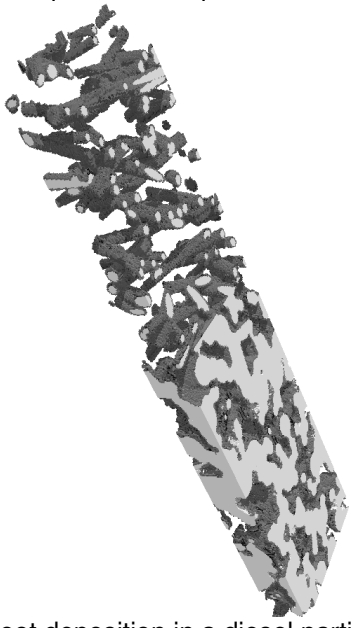

Fig. 7: Simulation of soot deposition in a diesel particulate filter medium

Since the particle diameters vary between 20 - 300 nm, the filter lifetime simulation is run in porous deposition mode. To determine the parameters of the sub grid model, i.e. maximum volume fraction and permeability of the porous medium, highly resolved single fiber simulations in solid deposition mode are performed (Fig. 8). The voxel length is set to 10 nm.

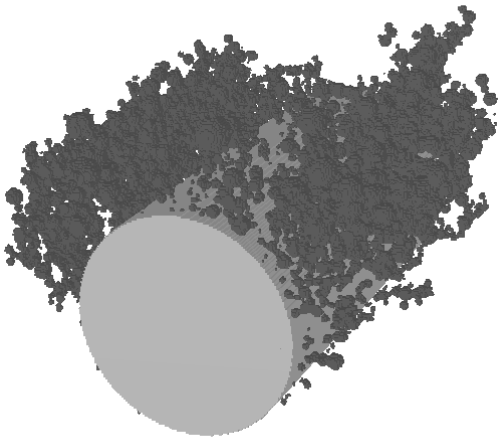

Fig. 8: Simulation of soot deposition on a single fiber

We determine the permeability and the maximum volume fraction by investigating the porous layer in upstream direction of the fiber. We obtain 15 % as maximum volume fraction and 10^{-3} Darcy for the permeability. Both parameters are then used in the filter lifetime simulation of the filter medium. Fig. 9 shows the characteristic *S – profile* when filtration switches from depth to surface filtration. The results are found in good qualitative agreement to measurements.

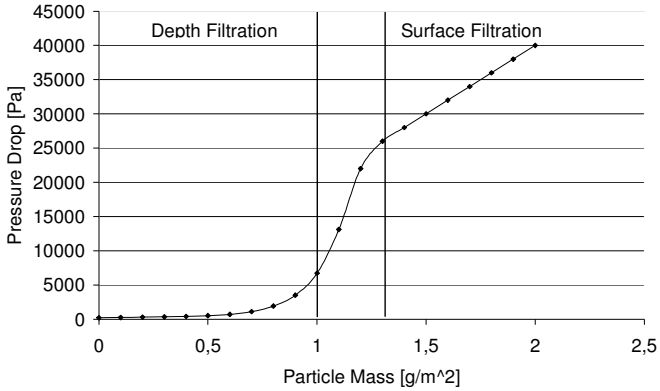

Fig. 9: Typical pressure drop evolution of a diesel particulate filter

Repeating the same simulation with the ceramic substrate only (= without fiber layer), we observe a slightly decreased initial pressure drop, but a much faster and unwanted transition to surface filtration. So, the simulation qualifies the design with fiber layer as the better medium. The same result is achieved by experiments.

4 Summary and Future Developments

In Section 2 and 3, we demonstrated the current capabilities of our software for virtual material design. Based on virtual geometry models, flow simulation software and computer codes for particle tracking and deposition, it is possible to reliably compute pressure drops, flow resistivities, initial efficiencies and entire lifetimes of filters. Hence, the simulation provides data which can immediately be compared to experiments. Moreover, it provides information which can't be obtained by any experimental setup, today. Besides the development of the basic simulation methods, great effort is spent to make the software GeoDict/FilterDict easily usable for the filter designer.

For the future, we plan to extend and improve the methods and the software in order to make it applicable in most filtration regimes and for most of the potential users. For example, simulation of standard tests, as already done for the single pass test, will be easily accessible via the graphical user interface. We want to further improve existing transport and deposition models by considering arbitrary particle shapes, particle spin, and particle-particle interaction. To allow particles to escape after deposition due to local changes in flow conditions is a necessity in certain applications. Extending the coupling of scales is also a hot topic, especially in view of the increasing usage of nano fibers. Moreover, going to smaller length scales requires appropriate fractional slip models for the flow boundary conditions. Last, but not least, the handling of elastic deformation due to fluid-structure interaction and particle impact will be a challenging task for the next years.

5 References

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