

Nano Filtration Media - Challenges of Modelling and Computer Simulation

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ABSTRACT

Nano filtration media become increasingly interesting for filtration applications as the production of nano fibers becomes cheaper. The benefit of adding nano fibers to micro fibers is the enormous improvement with respect to filter efficiency and the relatively low pressure drop add-on due to nano slip.

At the Fraunhofer ITWM, the simulation of filter media and filtration processes is traditionally performed resolving the smallest scale of the media. This approach has the advantage of keeping the model hierarchy low and the number of model parameters small. However, when entering the nano regime, two problems arise: The structures under consideration become huge. Hence, special algorithmic approaches have to be followed to overcome this hurdle. Moreover, the models for fluid flow and particle movement have to be extended by new physical effects like slip flow phenomena.

The paper gives an overview on the latest developments concerning nano filtration in the Fraunhofer software suite GeoDict / FilterDict.

KEYWORDS

Nano Filtration, Multiscale Simulation, Microstructure Simulation, CFD

1. Introduction

Filtration processes and hence, corresponding computer models and simulations are typically quite complex. This is due to several facts: Filtration media possess a porous microstructure, or even nanostructure, which has to be modelled since it heavily influences the overall filtration properties. Moreover, multiple physical phenomena occur and interact, like fluid flow, particle adhesion effects, friction, and Brownian motion, just to name a few.

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After the introductory section, a description of the modelling Ansatz is given. In Section 3, we present simulation results related to nano fiber media. Finally, we draw conclusions and give an outlook on future developments.

2. Method

The whole thickness of the filter media needs to be discretized in order to retrieve filter efficiencies that are directly comparable with measurements. An inflow region helps avoiding artifacts in the fluid flow and allows particles to develop their own

motion before entering the filter media. The computational domain is usually box-shaped, with the long side of the box taken across the filter media. The length of the other two sides is restricted by the computer memory. This box is composed of $n_x \times n_y \times n_z$ cubic grid cells. Each of these cells can be solid or empty, meaning it is part of a fiber or part of the flow domain, respectively. Fibers are discretized by setting all the cells within the fiber radius from the fiber axis to solid. The desired solid volume fraction of the filter media is achieved by randomly placing fibers and adding up their contribution. This is done by counting the number of cells that are set to solid when placing the fibers. In typical media the fibers are oriented randomly yet preferably perpendicular to the flow. Stationary slow gas flows in the no-slip regime may be described by the Stokes equations with periodic boundary conditions:

$$\begin{aligned} -\mu\Delta\vec{u} + \nabla p &= 0 \text{ (momentum balance)} \\ \nabla \cdot \vec{u} &= 0 \text{ (mass conservation)} \\ \vec{u} &= 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)} \\ P_{in} &= P_{out} + c \text{ (pressure drop is given)} \end{aligned}$$

Here μ is the fluid viscosity, \vec{u} is the (periodic) velocity and p is the pressure (periodic up to the pressure drop in the flow direction). We use the finite difference approach on staggered grids [2, 3] and interpolate the computed velocities from the cell faces in order to have a continuous velocity field that is needed for particle tracking. Note that the above linear formulation allows a simple rescaling of the flow field to adjust it to a desired mean velocity. This rescaling is only possible in the considered regime of slow flows, or low Reynolds number flows. For smaller fiber diameters, no-slip boundary conditions are not appropriate, and instead slip boundary conditions are applied [4].

$$\begin{aligned} -\mu\Delta\vec{u} + \nabla p &= 0 \text{ (momentum balance)} \\ \nabla \cdot \vec{u} &= 0 \text{ (mass conservation)} \\ \vec{n} \cdot \vec{u} &= 0 \text{ on } \Gamma \text{ (no flow into fibers)} \\ \vec{t} \cdot \vec{u} &= -\lambda \nabla (\vec{u} \cdot \vec{t}) \cdot \vec{t} \text{ on } \Gamma \text{ (slip flow along fibers)} \\ P_{in} &= P_{out} + c \text{ (pressure drop is given)} \end{aligned}$$

Here \vec{n} is the normal direction to the fiber surface, λ is the slip length and \vec{t} is any tangential direction with $\vec{t} \cdot \vec{n} = 0$. For the same pressure drop, the computed velocities for slip boundary conditions are higher than for no-slip boundary conditions. Conversely, for a given velocity or equivalently, a given mass flux, the pressure drop is lower when computed with slip boundary conditions. The challenge and restriction to our method lies in the computation of the tangential directions to the fiber surface: On cubic cells, only axis-parallel tangents can be resolved. This limits our ability to compute cases with larger slip length λ correctly.

To compute the filtration efficiency, particles are placed at random positions at the beginning of the inflow region. These particles are then tracked according to their complex equations of motion that are based on the air flow. Assuming that the particle concentration is low enough, this air flow is not altered by the presence of the particles. If during this tracking procedure a particle touches a fiber surface, then, in the *caught on first touch* model, it is captured and accounted for as filtered. The percentage of captured particles is called the filtration efficiency. All results presented in this article are based on this caught on first touch model. Three distinct effects that

contribute to the filtration efficiency are commonly described in the literature [4]. First, simply by following a stream line of the flow, a particle may get so close to a fiber that it touches. This effect is called *interception*. Secondly, a particle may leave a curving stream line and travel straight due to its inertia. This effect is called *inertial impaction*. Finally, very small particles may be influenced by random hits of air molecules. This effect is called *Brownian diffusion*. To account for interception, the particle should travel with flow velocity \bar{u} ,

$$d\bar{x} = \bar{u}(\bar{x}(t))dt.$$

Here $\bar{x}(t) = (x_1(t), x_2(t), x_3(t))$ is the position of the particle at time t . Recall from above that \bar{u} was computed using the Stokes equations with slip or no-slip boundary conditions. The introduction of friction with the friction coefficient γ adds the effect of inertial impaction, neglecting the feedback of the particles motion on the fluid flow. The friction model is based on Stokian friction of spherical particles [5], supplemented by the Cunningham Slip Correction Factor $C_c(Kn)$ as introduced in [6] for solid particles at NTP conditions. $Kn = \lambda / R$ is the Knudson number defined as the ratio between the mean free path λ and the radius R of the particle. We explicitly introduce the particle velocity as a separate variable \bar{v} and write

$$d\bar{v} = -\gamma \times (\bar{v}(\bar{x}(t)) - \bar{u}(\bar{x}(t))) dt,$$

$$d\bar{x} = \bar{v}(\bar{x}(t))dt,$$

$$\gamma = 6\pi\rho\mu \frac{R}{C_c m},$$

$$C_c = 1 + Kn \left[1.142 + 0.558e^{-0.999/Kn} \right].$$

For fixed fluid density ρ and particle radius R the friction coefficient tends to infinity as the particle mass m tends to zero. In the limiting case $m = 0$ the previous equation is recovered, i.e. for $m = 0$ the particle velocity is simply the fluid velocity. Finally, interception, inertial impaction and Brownian motion of particles altogether are described in [5] by a stochastic ordinary differential equation

$$d\bar{v} = -\gamma \times (\bar{v}(\bar{x}(t)) - \bar{u}(\bar{x}(t))) dt + \sigma \times d\vec{W}(t),$$

$$d\bar{x} = \bar{v}(\bar{x}(t))dt,$$

$$\sigma^2 = \frac{2k_B T \gamma}{m},$$

$$\langle dW_i(t), dW_j(t) \rangle = \delta_{ij} dt.$$

Here T is the ambient temperature, k_B is the Boltzmann constant and $d\vec{W}(t)$ is a 3d probability (Wiener) measure.

3. Simulation Results

We consider five different filtration media. Media 1 is a microfiber media with 1, 2 and 4 μm fibers volumetrically equally distributed. Its fiber content is 5 %. Media 2 is like Media 1 with additional nanofibers with the diameters 100, 200 and 400 nm. The nanofiber content is only 0.5 % and all nanofiber types are volumetrically equally distributed. Media 3 is again a microfiber media with similar properties as Media 1, but different initialization of the random number generator. Media 4 and 5 are based on Media 3 and possess on top a nanofiber layer of thickness 2,5 μm and 10 μm , respectively. The voxel length is chosen to be 100 nm in all cases and the simulated geometric extensions are 512 x 512 x 512 voxels corresponding to 51.2 x 51.2 x 51.2 μm^3 . The five different media are illustrated in Figure 1 – 3.

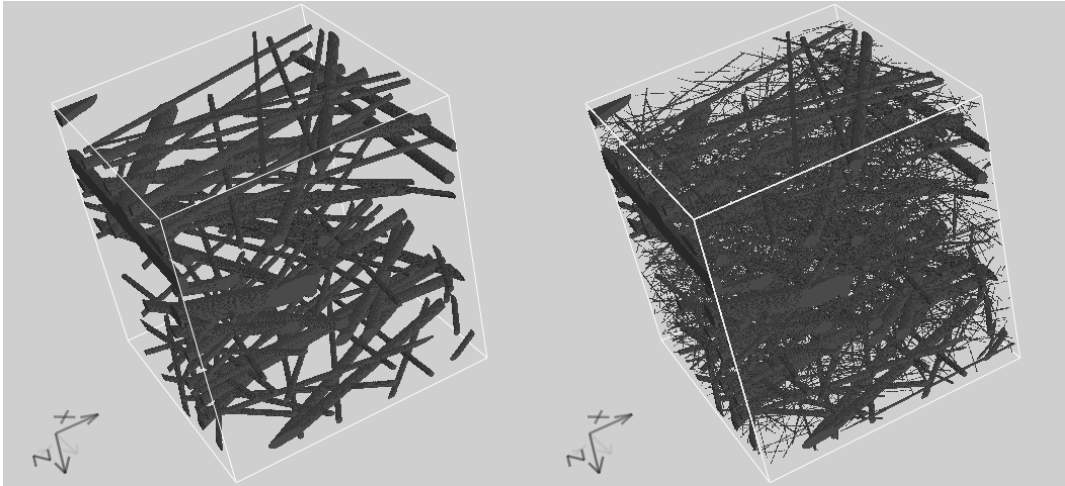


Figure 1: Media 1 (left) and Media 2 (right).

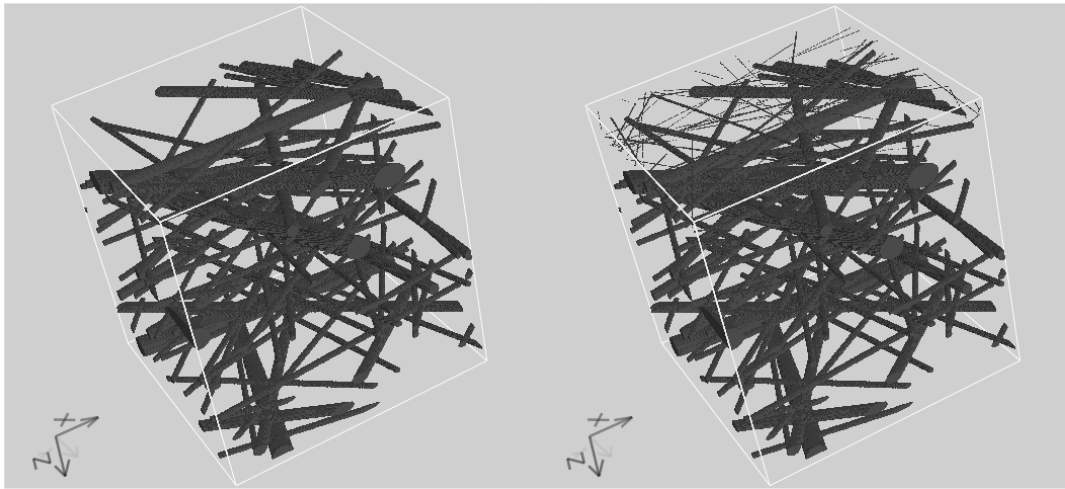


Figure 2: Media 3 (left) and Media 4 (right).

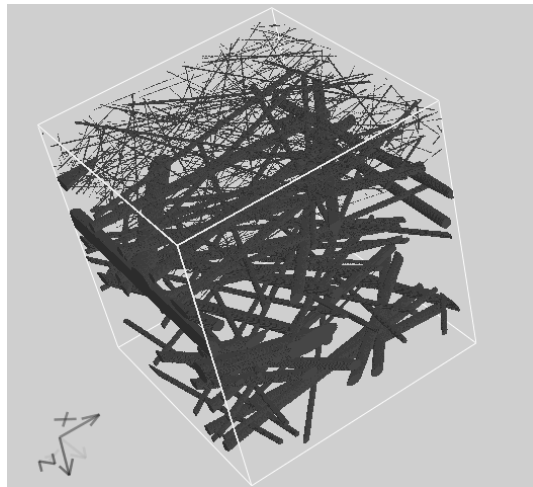


Figure 3: Media 5

We computed the permeability of each of the five media using air at 20 °C and a slip length of 118 nm [6]. The permeability values are given in Table 1.

Media	1	2	3	4	5
Permeability [m^2]	3,89e-12	6,44e-13	4,35e-12	3,71e-12	2.48e-12

Table 1: Simulated permeabilities of Media 1 – 5.

Comparing Media 1 with Media 2, we observe a permeability decrease by a factor of 6, which is quite surprising by looking at the low additional volume of nanofibers. The changes from Media 3 to Media 5 are quite moderate from a geometrical point of view, since the additional nanofiber layer is thin and the additional material content is low. Nevertheless, the permeability decrease is clearly visible.

In Figure 4 and 5, flow velocities that correspond to the permeability simulations are shown.

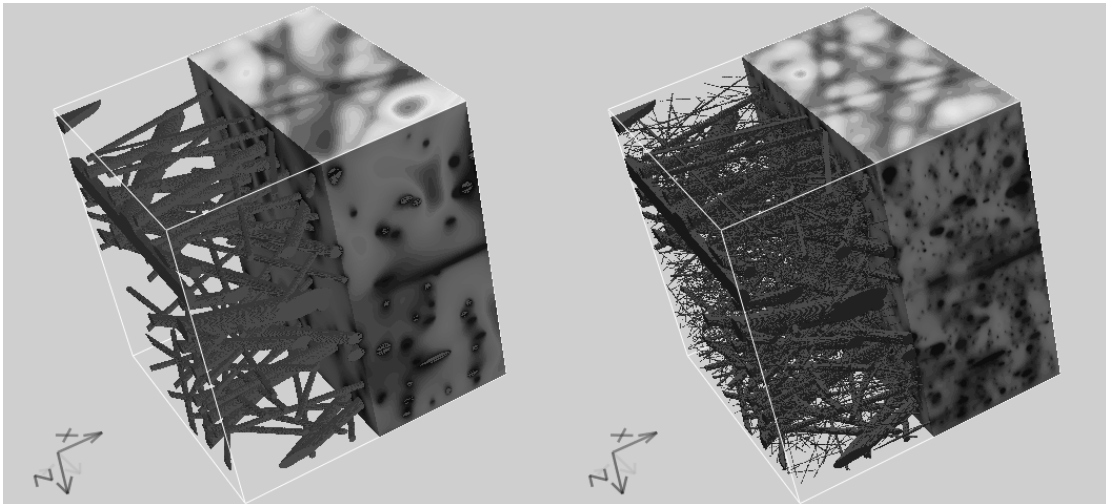


Figure 4: Visualization of the flow velocities in Media 1 (left) and Media 2 (right).

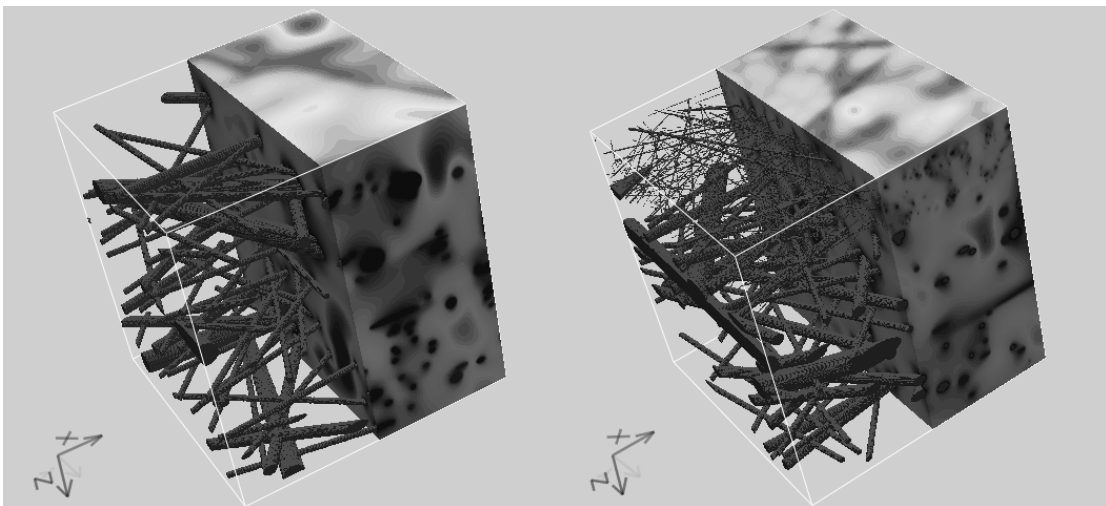


Figure 5: Visualization of the flow velocities in Media 3 (left) and Media 5 (right).

Now, we want to get an idea of the filtration properties of the different media. Therefore, NaCl particles in the range of 50 to 500 nm are considered. The fluid is again air at 20 °C. The mean flow velocity is chosen to be 5 cm/s. The computed filtration efficiencies are scaled to a media thickness of 1 mm. In the cases of Media

4 and 5, only the coarse substrate is scaled. Figure 6 and 7 show the results for the five media.

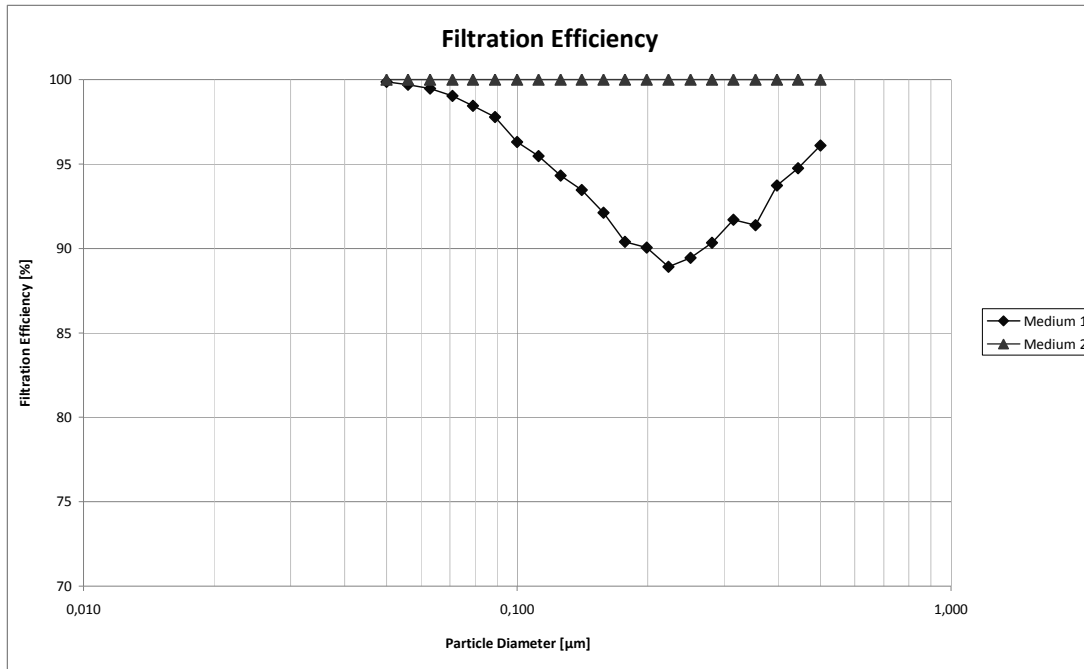


Figure 6: Initial filtration efficiencies of Media 1 and Media 2.

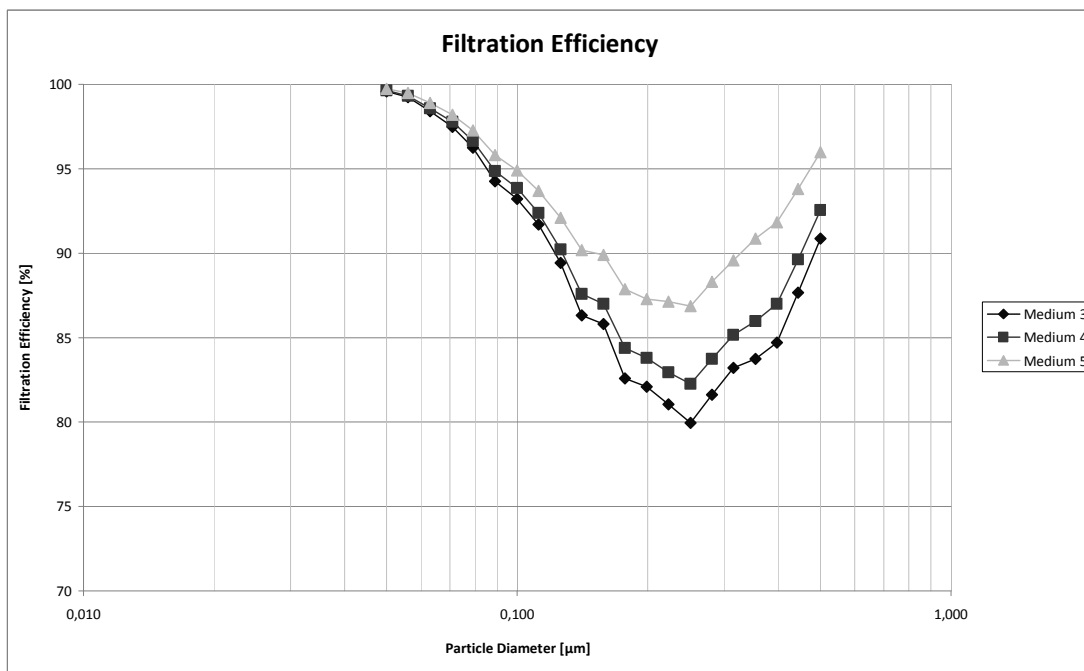


Figure 7: Initial filtration efficiencies of Media 3 – 5.

The changes from Media 1 to Media 2 are tremendous as in the case of the permeability values. Keeping in mind, that we only scaled the coarse substrate in the cases of Media 3 – 5, and that we effectively simulate additional nanofiber layers of thickness 2.5 μm and 10 μm , a pronounced increase in the filtration efficiencies can be observed.

4. Conclusions and Outlook

In the present work it is demonstrated how filter media with nanofibers can be handled numerically. The comparison of microfiber media and media with additional nanofibers shows reasonable results. One finds that the additional nanofibers lead to a big improvement of the filter efficiency.

Resolving the smallest scale of a filter media with nanofibers one has to solve very large problems. Therefore, in this work, the spatial extend of the geometries under consideration is rather small. To simulate the filter lifetime one has to resolve the whole thickness of the media, which leads to much larger geometries. One way to overcome this problem is to use adaptive grid solvers, which are currently under development for the GeoDict / FilterDict software suite.

Acknowledgments

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