



Computer simulation of air filtration including electric surface charges in three-dimensional fibrous microstructures

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Abstract

The dependence of filter properties such as pressure drop, filter efficiency, and filter lifetime on the geometric structure of fibrous filter media is of great practical importance. In particular electrostatic forces are highly dependent on this structure. Many textiles have an irregular structure, which cannot be represented by functions of say porosity. Thus, it is necessary to model the three-dimensional structure of the textiles and electrostatic charges on their surfaces. To study the filtration properties, we use a Lagrangian formulation of particle transport in the calculated complex flow field and solve a Poisson equation with jumps in the electric conductivity and singular source terms on the fiber surfaces. The electric field is obtained as the negative gradient of the potential. Depending on the size of the particles, the micro structure of the filter, the electric field and the shape of the fibers, we simulate pressure drops, filter efficiencies and filter lifetimes. Since controlled variations of structural parameters like fiber orientation, fiber shape, spatially varying pore size distribution or gradients in the fiber density and the distribution of electrostatic charges on the fiber surfaces are easily achieved within the simulation, our results constitute a systematic and quantitative approach for the simulation of air filtration in fibrous filter media.

Keywords: Simulation, Nonwoven, Particle Separation, Electrofiltration, Clogging

Introduction

The mathematics of stochastic geometry [1] allows the creation of realistic computer models of filter media. A simple model for nonwoven based on the three parameters porosity, fiber diameters and one-parameter fiber directions is derived in [2]. The model also applies for the layers of typical filter media. Layers are modeled as a nonwoven, and then stacked. In [3], the steady state fluid dynamics simulations and the study of air filtration by a Lagrangian formulation of the particle transport were reported. In the virtual filter media large particles get caught by inertia effects or sieving effects, while very small particles are trapped mostly due to diffusive effects [4]. When deposited particles are allowed to affect the steady fluid flow, also the dynamic changes in pressure drop and the clogging of the filter can be predicted. Here we report improvements in the treatment of electrostatic charges compared to [5], where also the effects of electrostatic charges on the fiber surfaces on electrically charged particles are included in the model.

Layered media model

The first ingredient in the simulation of air filtration is a three-dimensional representation of the filter media in the computer. We use a voxel model, where a large enough cutout of the media is discretized by a uniform Cartesian grid with edge-length h . This h has to be chosen in such a way that the grid resolves the smallest occurring fiber diameter. For example, for smallest fiber radius in the nonwoven $5\mu\text{m}$, $h = 2.5\mu\text{m}$ will resolve this fiber with 4 voxels per diameter. This introduces the next parameter in the model: the side lengths of the cutout. The cutout must be large enough to model a representative portion of the media. On the other hand, available computer memory limits the size of the cutout. A third consideration is that the thickness of the filter media should be resolved completely. Thus, if the media is 2 mm thick and a voxel is $2.5\mu\text{m}$, then about 840 voxels are needed in the flow direction including a little empty space before and after the media. Then the capability to compute the air flow and particle motion through the geometry limits the extent of the lateral directions.

The producers of nonwoven usually use up to 4 types of fibers. They may have a certain specific weight (polyester, polyamide, etc.), a specific cross sectional shape, a certain length, a certain crimp and a certain distribution of fiber types. From this information, a probability for each fiber type can be derived. For example, if all fibers are made of polyester at 1.37g/cm^3 , have a round cross section, are 7cm long and spiral shaped at 0.5 revolutions per centimeter with the only difference in thicknesses of $10\mu\text{m}$ and $15\mu\text{m}$, and the same amount of both types of fibers is used, then the probability of $10\mu\text{m}$ fibers is $0.69 = 15^2 / (15^2 + 10^2)$ and that of $15\mu\text{m}$ fibers is $0.31 = 10^2 / (15^2 + 10^2)$.

Under the restrictions on the computationally feasible cutout, the fibers may often be modeled as straight and infinitely long; for example when the fiber is say 7cm long with two revolutions per 10 cm but the longest edge of the cutout is 2mm. The model is then complete after choosing the porosity of the media and the anisotropy of the fibers. Usually, the air flows perpendicularly to the machine direction, which is also the main anisotropy. We usually think of it as the z-direction of the model. Last but not least, the porosity is prescribed. For filter media layers it ranges between 80% to 98% porosity. To build a virtual nonwoven, we create random fiber positions, fiber types and fiber directions. The position is uniformly distributed in the cutout; the fiber type is drawn according to its probability, and the fiber direction according to the choice of anisotropy. This fiber is discretized into voxels and entered into the domain, with the option to overlap or not to overlap with previously entered fibers. This procedure is repeated until the percentage of voxels not covered by fibers is lower than the desired porosity. If the achieved porosity is too far from the desired one, the procedure is repeated in the hope to find by chance a configuration that satisfies the porosity requirement. However, for large enough domain it is usually not a problem to achieve less than 1% deviation from the desired porosity. Finally, two or more of these layers can be stacked to achieve a realistic representation of layered filter media. Figure 1 shows a simple example of such a layered structure. Two highly porous layers are chosen not to represent a real air filter media (where at least one layer of lower porosity should be present) but for the sake of clear differentiation and three-dimensional view of the media.

Flow simulation

We consider low Reynolds numbers typical for some air filtration processes and solve the Stokes equations with periodic boundary conditions:

$$\begin{aligned}
\mu \Delta \vec{v}_0 + \vec{f} &= \nabla p && : \text{momentum balance} \\
\text{div } \vec{v}_0 &= 0 && : \text{conservation of mass} \\
\vec{v}_0 &= 0 \text{ on } \Gamma && : \text{no-slip on fiber surfaces}
\end{aligned}$$

To drive the flow, a constant body force in the z-direction is applied. Through periodicity, artificial fiber ends are felt by the flow on the cutout surfaces in the x- and y-directions where a fiber ends on the opposite cutout surface. This influence is another reason why a large enough cutout must be used in the computations. The three components of the velocity \vec{v}_0 as well as the fluid pressure p are all available at voxel centers after the calculations, with zero-values assigned inside the fiber voxels.

Model of surface charges and computation of electric field

The charges are assumed as constant given forces on the fiber surfaces, the fiber voxel walls that neighbor fluid voxels. For the moment, a single constant amount of charge ρ is assigned on all such voxel walls. The following boundary value problem is solved for the potential:

$$\begin{aligned}
\Delta u &= \rho \chi(\partial\Omega) && : \text{singular force Poisson equation} \\
\vec{E} &= \nabla u && : \text{the electric field}
\end{aligned}$$

Here u is periodic in the x- and y-directions, and satisfies zero Dirichlet boundary conditions on the boundaries at $-z_0$ and $nz + z_0$ in the z-direction. By construction, these boundaries lie away from the fibers and there is no conflict between singular forces on fiber surfaces and these Dirichlet conditions. Due to the periodic boundary conditions, the potential feels a non-integrable amount of charges, and tends to infinity in the nonwoven as the Dirichlet boundary is moved away from the nonwoven. That is, the potential u depends on the position where the Dirichlet condition is located. However, the electrical field \vec{E} remains almost unchanged from the location of the Dirichlet boundary as soon as this boundary is sufficiently far away from the nonwoven. This electric field enters in the equation of motion for the particles together with the charges on the particles as described in the next section.

Filter efficiency simulation

The two most important aspects to filter efficiency simulations are the motion of the particles in the fluid and the treatment of the interaction of the particles with the fibers. The first aspect is dealt with by a simple decoupling into the solution of two steady state partial differential equations (the Stokes flow and the electric field) and the solution of a stochastic ordinary differential equation (for the particle motion). This means that particles do not influence the air flow and particles do not collide with other particles. This is of course only valid under the assumption that there is a very low concentration of particles in the flow and that the particles are small enough. In the Lagrangian formulation, the variables are the position and velocity of the spherical particle. The influences are given by the friction with the fluid, the electrostatic attraction and Brownian motion.

$$\frac{d\vec{x}}{dt} = \vec{v}$$

$$d\vec{v} = -\gamma \times (\vec{v} - \vec{v}_0(\vec{x}(t)))dt + \frac{Q\vec{E}}{m}dt + \sigma \times d\vec{W}(t) \quad (*)$$

$\gamma = 6\pi\rho_F \nu \frac{R_p}{m}$:	friction coefficient
\vec{x} :	particle position
R_p :	particle radius
m :	particle mass
Q :	particle charge
\vec{E} :	electric field
\vec{v} :	particle velocity
\vec{v}_0 :	fluid velocity
$d\vec{W}(t)$:	three-dimensional Wiener process
$\langle dW_i(t), dW_j(t) \rangle = \delta_{ij}dt$	
$\sigma^2 = \frac{2k_B T \gamma}{m_p}$:	fluctuation-dissipation theorem
ρ_F :	fluid density
ν :	fluid viscosity

In the simplest setup, particles touch a fiber and stick to it at first collision, more advanced models of inelastic collision and adhesion forces between fibers and particles were described in [3]. To simulate the filter efficiency, for any given particle size a fixed number of particles of this size are placed at random locations in the inflow region of the filter media. Then, the transport through the media due to the fluid flow, electrostatic charges and Brownian motion is computed. The efficiency is computed for each particle size as the percentage of filtrated particles that got stuck on a fiber compared to all the particles that entered the flow.

Filter lifetime simulation

For filter lifetime simulations, the same simulation as for the filter efficiency calculations is used, with a few additions. Particles are placed at random positions in the inlet as before, but now they are drawn according to the distribution of particle sizes in the test dust, e.g. discretized to 23 different particle sizes for SAE fine Arizona dust. The deposition locations of these particles are tracked, and after a certain amount of dust is either deposited or moved through the media, the deposition locations are used to modify the nonwoven geometry. All the independently computed (deposited) particles are now entered into the nonwoven geometry, switching flow voxels to solid voxels or porous voxels. This is possible for particles much smaller than a voxel by keeping track of the mass deposited in a voxel from many small particles. For the new geometry, the static Stokes flow and electrostatic fields are recomputed, and a current estimate of the pressure drop becomes available. Fig. 2 and 3 show the same nonwoven filter media under the same flow regime and with the same amount of dust entered into the flow. In Figure 2, no electrical charges are present while in Figure 3 electrical charges have led to additional particle deposition.

The rules for the determination of the surface charges and for the conversion of deposited particles into solid or porous voxels are still subject of investigation. Very high resolution calculations where dust particles are well resolved by voxels are under way to determine these rules. Ultimately, only correct prediction of measurements will justify these choices.

Conclusion

We have described a layered nonwoven model, fluid flow computations, electrostatic computations, filter efficiency and filter lifetime simulation techniques. All known relevant effects for air filtration are incorporated in the models, that start with a simple voxel based geometry model on which the flow, electric fields and collisions are evaluated. Particles can be advected and deposited in the media, leading to filter efficiency and pressure drop curves that are qualitatively similar to measurements on real media. This simple model setup relies heavily on large scale scientific computing, but will also benefit from future work in determining simulation parameters both by experimental work and specifically designed simulations, for example to determine rules of distribution of electrostatic charges.

References

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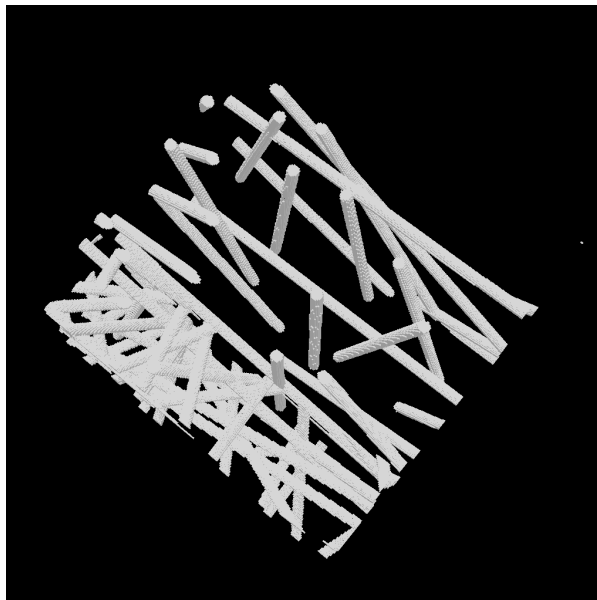
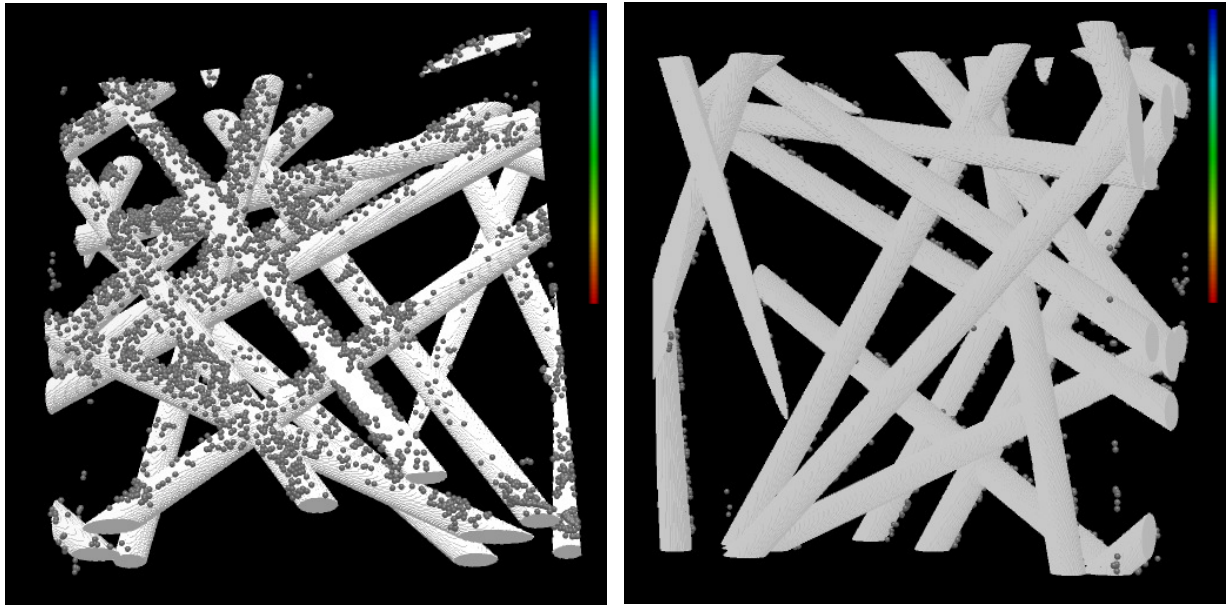


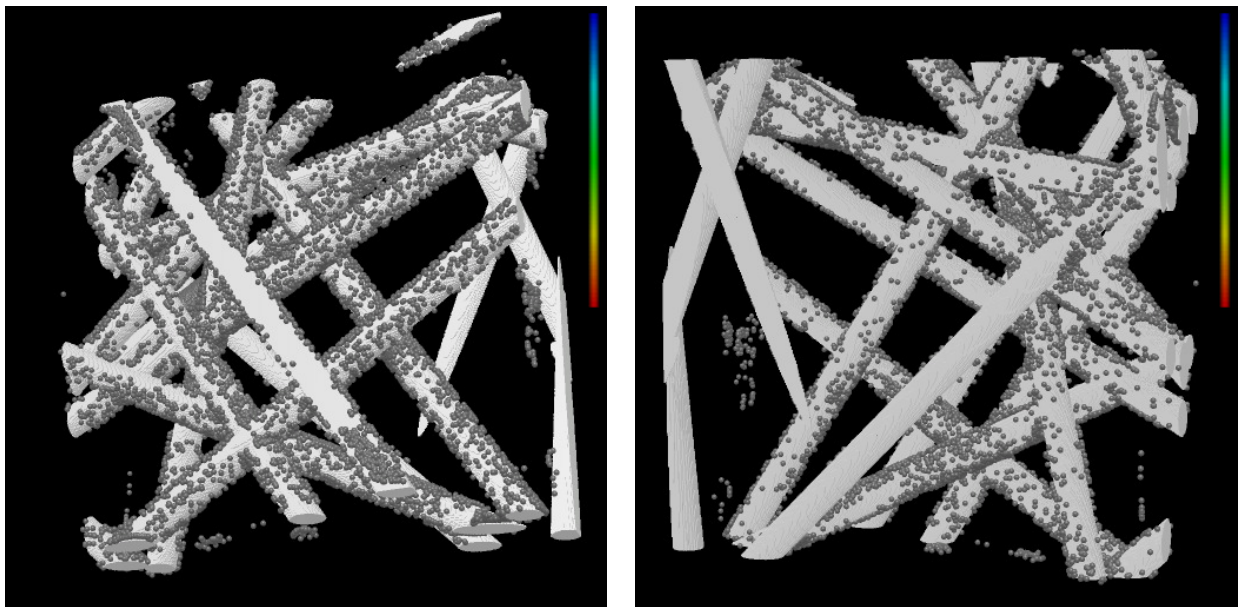
Fig. 1: Layered media of $716^3 \mu\text{m}^3$ volume. The same fibers are used, but the first $179\mu\text{m}$ are filled with isotropic fibers covering 5% of the volume, and the last $537\mu\text{m}$ of the volume are filled with fibers strongly oriented in the machine direction and covering only 2% of the volume.



a)

b)

Fig. 2: Particle deposition on fibers in a porous layer. Particles sizes are distributed according to the SAE fine test dust. They are deposited at random positions in a plane perpendicular to the flow direction and then to their deposition locations by the stochastic ordinary differential equation (*), without electrostatic charges on the fiber surfaces. a) front view, b) rear view.



a)

b)

Fig. 3: Particle deposition on fibers in a porous layer. Particles sizes are distributed according to the SAE fine test dust. They are deposited at random positions in a plane perpendicular to the flow direction and then advected to their deposition locations by the stochastic ordinary differential equation (*). The parameters are the same as in Figure 2. Here the influence of electrostatic charges on the fiber surfaces is taken into account. a) front view b) rear view.