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GeoDict and FilterDict: Software for the Virtual Material Design of New Filter Media

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Abstract

The demands on filter media grow rapidly. Yet, the time to develop new media becomes shorter and shorter as development cycles across most industries speed up under the pressure of globalization. Based on this need, and much helped by great improvements in computing machinery, our group strives to implement computer models and algorithms for filter media, gas and fluid flow therein, solid particles, particle transport, particle deposition and all the way to the clogging of the media.

Keywords: virtual material design, particle filtration simulation, microstructure simulation

Introduction

Filtration is everywhere, and the filter media is everything in filtration. These statements refer to the fact that filtration processes occur everywhere from within biological systems to automobiles and chemical engineering to medicine, and the fact that it is mostly the filter media that governs the filtration properties of a filter. The demands on the filter media grow rapidly. Yet, the time to develop new media becomes shorter and shorter as development cycles across most industries speed up under the pressure of globalization. Based on this need, and much helped by great improvements in computing machinery, our group sets out to implement computer models and algorithms for filter media [1], gas and fluid flow therein, solid particles, particle transport, particle deposition and all the way to the clogging of the media. Coming more from a mathematical and computer science rather than a process engineering background, one looks for similarities rather than differences in the many different filtration regimes. In this paper, we first describe what we mean by virtual material design in general, and what our software **GeoDict** does for it, and then narrow this general concept down to filter materials, where we apply our **FilterDict** module.

1. Virtual Material Design with GeoDict: Media Models and Property Simulation

The two classical approaches in filtration simulation are system simulation and single fiber simulation. As an example of the first case, the filter in its interaction with the exhaust system of an automobile is simulated. The scale is of the order of 2 to 200 centimeters, and the filter material is modeled as a porous media, as very few computational cells with “averaged” properties such as porosity, permeability, etc. In the second case, the deposition of particles on a single fiber, and detailed effects such as influence of electrostatic charges, local flow velocity, previously deposited particles, adhesion between materials etc. are considered. The scale here is of the order of 200 nanometers to 20 microns, and the goal is to predict "averaged" properties of the filter media.

The simulation gap lies on the scale between these two. The microscopic three-dimensional effects such as complex pore structure, variations in fiber diameters or fiber orientation, variations of grain sizes in sintered materials, etc., can not be accounted for with either type of simulation.

Requirements on the Media Model

This is where media models come into play. They have to fulfill several requirements.

Media models must be based on "real" input quantities that media developers think in. Examples are porosity, fiber diameters and fiber anisotropy for nonwoven, or pore size distributions, media thickness, specific surface area, etc., to name but a few.

Media models must be generated completely automatically from these desired parameters. A big issue with many simulation tools is that it takes even simulation experts a lot of time to *set up* the calculations. This must be avoided because it invariably shifts the focus from the media design to computer science issues.

Media models must be generic. This means that at a certain stage of the simulation chain, it must not matter whether the filter media is a textile, sintered, or foam. The model must allow assigning the different surface behavior and other specifics, but for reusability of the Software, a standard representation of the media is extremely desirable.

Media models must be combinable. For example in felts, layers of woven and nonwoven alternate in a design made both for strength and filtration properties. To reduce the complexity of the media model generation, it is highly desirable to be able to compose such felt models from woven and nonwoven models.

Media models must be compatible with 3d images of real materials. Natural scepticism of our audience invariably leads to the desire to skip the step of modelling the media, and work directly on otherwise obtained computer representations of existing media in order to validate the next step, the property simulation. The best such representations come from computer tomography, which yields three-dimensional greyscale images of the media. A lot of effort may be spent on extracting the data needed to perform simulations on these data sets, if the representation is chosen as tetrahedral or other volume meshes. More importantly, this effort is often not automated, and requires again a simulation expert to be performed.

These requirements have led to a very simple choice of format for the media model [2]. It is simply a three-dimensional indexed image. This means that a certain brick-shaped, rectangular portion of the media is cut up into many little cubes called voxels, with a fixed side length h, which we call the resolution of the geometry. To give an example, a typical resolution might be 1 micron, and a media model might consist of 400 by 400 by 1000 voxels, yielding a portion of the media of length 400 microns in two of the directions, and 1000 microns in the third. Such aspect ratios are typical of models used in filtration, because the thickness of the media should be resolved by the simulations. Figure 3 shows a two-dimensional cross section view of a sintered media model and a three-dimensional view of a nonwoven media model.

Media Model Validation

There are four stages in establishing the validity of a media model.

1. The first plausibility check is simply by inspection. Two-dimensional and three-dimensional visualizations of the media model can be compared with microscopic or tomographic images of real media. Scanning electron microscopy, Laser Scan microscopy, Synchrotron tomography, and several other techniques have been used by our partners to acquire such data sets, and inspection can often reveal faults in the model, that may or may not be relevant after all. To give an example, our nonwoven model consists only of straight fibers, while real fibers are often crimped. The human eye can thus immediately tell the difference, while in permeability calculations we found this simplification not to resulting significant deviations from measurements.
2. The second plausibility check lies in geometric analysis. Many features of the media can be measured, but are not obvious from the microscopic or tomographic image. The most important one for filtration applications are pore sizes and pore size distributions that are often used to characterize media. Since the pores are not the subject of the media model, but rather the solid portions (fibers, grains, foam, etc.), the control over the pore size distribution of the models is only indirect: The model is generated, and then the three-dimensional pore space is analyzed. Since no single definition of pore size applies for complex geometries, different algorithms are being developed that follow the physical methodology and attempt to reproduce the same quantities (pore throat diameter vs. pore volume, etc.) as these real measurements. Figure 4 shows pore size measurements by the mercury intrusion method vs. the computed pore size distribution of a media model of the same material.
3. Next, the agreement of computed and measured properties of existing media should be achieved. This will usually only be attempted after stages 1 and 2 are passed, because it is conceivable that simulation results such as filter efficiency will agree with measurements even though the underlying media model is completely wrong. In this case, the model will never be able to predict the effect of modifications of material parameters, and would not be useful for its original purpose, which can not be achieved with three-dimensional images of existing media: the last stage, namely the computer-aided virtual material design of the media.
4. For the property prediction to work, the media model must agree with reality, but several other aspects must be taken care of equally well. Usually, in stage three some unknown parameters (e.g. particle-surface adhesion, particle shape factor, etc) were fit to achieve the agreement between measurement and simulation. Now, in the final stage, no more parameter fitting is allowed. Instead, the assumption is that at least in a certain regime, for a certain type of material, the parameters are all known, and the effect of material modifications can be predicted. In practice this simply requires a set of measurements that were not used for the calibration of the parameters, but taken in the same regime as other measurements (e.g., a filter media with 10 µm fibers instead of 8 µm fibers, or similar). This type of controlled setup is hard to find in industry, and the goal is to establish settings with known parameters through extended use of the simulation software in a variety of projects, ranging from publicly funded basic research to trend studies with individual companies.

Property Simulation

Properties of the media are generally estimated by the following procedure: A physical process is modeled by a partial differential equation with boundary conditions and values of the coefficients. As an example, the Stokes equations describe the motion of a fluid for very slow regimes that occur in many filtration applications, and the pressure difference, together with the media model, provides the needed boundary conditions. The media is viewed to consist of a collection of empty and solid voxels, and the flow can only occur in the empty space. On the surfaces of the solid voxels, the velocity is prescribed to be zero, while the pressure difference is converted into a driving force for the flow equations. Figure 1 shows the Navier-Stokes-Brinkmann equations, the most complete formulation of steady fluid flow used in our computations: they include the nonlinear inertia term and a Darcy-type permeability κ that is capable of modeling effects that are not resolved by the voxels.

$$\begin{aligned} -\mu\Delta\vec{u} + \nabla\vec{u}\cdot\vec{u} + \kappa^{-1}\vec{u} + \nabla p &= \vec{\mathrm{f}} \text{ (momentum balance)} \\ \nabla\cdot\vec{u} &= 0 \text{ (mass conservation)} \\ \vec{u} &= 0 \text{ on } \Gamma \text{ (no-slip on fiber surfaces)} \end{aligned}$$

$$\begin{aligned} \vec{\mathrm{f}} = (0,0,f) &: \text{ force in flow(z)-direction,} \\ \kappa &: \text{ porous voxel permeability,} \\ \vec{u} &: \text{ velocity,} \\ \mu &: \text{ fluid viscosity,} \\ p &: \text{ pressure and} \\ \Gamma &: \text{ surfaces of fibers or deposited particles.} \end{aligned}$$

Figure 1. Navier-Stokes-Brinkmann equations and notation.

From each of the three computed mean velocities for a given pressure difference in the three coordinate directions, a column of the effective permeability tensor can be determined from Darcy's equation:

$$\begin{aligned} \vec{u} &= -\begin{pmatrix} \kappa_{11} & \kappa_{12} & \kappa_{13} \\ \kappa_{21} & \kappa_{22} & \kappa_{23} \\ \kappa_{31} & \kappa_{32} & \kappa_{33} \end{pmatrix} \nabla p \\ \kappa_{ij} &= u_{ij}\frac{L}{\Delta P} \end{aligned}$$

where u_{ij} is the component of the mean velocity in direction i under applied pressure difference ΔP in direction j across the width of the media L. Such a permeability, mean flow velocity or equivalently, flow resistivity can be compared with measurements on the real media once the media model has been established.

Other properties than can be computed in a similar fashion include effective elastic tensors, effective diffusivity or effective thermal conductivity of media. Important for filtration applications is the ability to compute electric force fields from surface charges. In each case the validity of the mathematical model must be carefully checked. In the example above, the existence of a stationary solution to the Navier-Stokes-Brinkmann equations is assumed, which means that pressures and velocities may not be very large, because this would result in a turbulent, in particular not stationary, solution.

2. Virtual Filter Media Design with FilterDict: Interaction of Particles with the Media

The Virtual Filter Media Design via **FilterDict** was developed based on the media model and the detailed solution of the flow equations by adding the transport and deposition of particles on surfaces on top of and inside the media model. The approach is again a compromise between accuracy and computational feasibility, based on the insight that useful simulations should not take longer than one night to produce results. The compromise places the following restrictions on the applicability of the method:

We alternate an Eulerian approach for a partial differential equation with a Lagrangian approach for many stochastic ordinary differential equations by decoupling the solution of the flow problem from the motion of the particles. The particles do not influence the flow while they are traveling through the media, and do not collide with each other. For these assumptions to be reasonable, particles should be rather small and rather scarce. In this fashion, many particles can be transported through the media based on the same flow field. When too many have deposited, the assumption of a fixed flow field becomes questionable, and the media model must be modified to now also include previously deposited particles. Based on this updated media model, a new flow field is computed, and the process is started again. In this fashion, even the clogging of the media can be simulated.

The Flow Model

The Navier-Stokes-Brinkmann equations [6] are used in all our filtration simulation applications: only the parameters decide whether the fluid is a liquid or gas by choice of viscosity μ, e.g. as 1.84e-5 Pas, for air at 20°C, as 2e-2 Pas for diluted blood at 22°C or 1e-5 Pas for oil at -25°C. The surface locations, the different forces and the time-dependent localized modification of the permeability κ distinguish the media, flow regimes and particles in the different applications.

The Particle Model

In **FilterDict**, particles are spherical for computational efficiency and for lack of better knowledge of their shapes. They have a known density, and by using non-physical densities, shape factors for different types of particles (soot, sand, droplets, etc) can be introduced implicitly. The particles also carry additional information such as electric charges, adhesion forces against other materials that can govern bounce off with energy loss, and a history of previous collisions with fibers.

Particle Transport

The particle information is important for all three terms that contribute to the particle velocity. The radius and density (as mass) enter into the friction of the particle against the flow, charges and mass enter into the electrostatic attraction, and also into the diffusive part of the motion. Figure 2 gives the precise formulation for the particle transport without collisions. Particles can be positioned anywhere in space, while the fluid velocity is only available at a discrete set of points in space, for example on cell walls in case of one particular finite difference solver [7]. To approximate fluid velocities at the particle location, these discrete velocity values are linearly interpolated.

$$
\begin{aligned}
\frac{d\vec{v}}{dt} &= -\gamma \times (\vec{v}(\vec{x}) - \vec{v}_\circ(\vec{x})) + \frac{Q\vec{E}_\circ(\vec{x})}{m} + \sigma \times \frac{d\vec{W}(t)}{dt} \\
\frac{d\vec{x}}{dt} &= \vec{v} \\
\gamma &= 6\pi\rho\mu\frac{R}{m} \\
\sigma^2 &= \frac{2k_B T\gamma}{m} \\
\left\langle dW_i(t), dW_j(t) \right\rangle &= \delta_{ij}dt
\end{aligned}
$$

t:	time
$\vec{x}$:	particle position
$\vec{v}$:	particle velocity
R:	particle radius
m:	particle mass
Q:	particle charge
T:	ambient temperature
k_B:	Boltzmann constant
$d\vec{W}(t)$:	3d probability (Wiener) measure
$\vec{E}_\circ$:	electric field
$\vec{v}_\circ$:	fluid velocity
ρ:	fluid density
μ:	fluid viscosity

Figure 2. Lagrangian description of particle motion.

The Collision Model and Particle Deposition

Because the particles are spherical, only the distance of the particle center from the nearest obstacle needs to be computed in order to detect collisions. To further accelerate this computation, the media model is equipped with a so-called distance function, which provides information about the distance to the nearest obstacle voxel for all empty voxels. If the particle radius is smaller than the distance function value at its position, then no collision can occur. The distance map must be updated periodically by the deposited voxels, at the same time that the flow field is updated. For each material combination of particle – fiber interaction, adhesion and restitution parameters are set. Adhesion means the attraction force that a particle must overcome in order to bounce off the fiber. Restitution governs the energy loss of the particle in case it bounces off. It is partially due to the adhesion between the particle and the fiber, and additionally also models an inelastic response of the fiber, i.e. a small irreversible motion or plastic deformation of the fiber. One of the great challenges to the simulation is to find the appropriate values for these parameters in each new filtration setting, for each new material combination.

The flow and collision models account for most mechanisms of filtration: except for the influence of their mass and electric charges, particles follow the streamlines and can be caught by **direct interception**. Due to their mass, they can leave stream lines and can be caught by **inertial impact**. Due to electrostatic charges, they may be attracted to fibers or repelled from fibers and get caught via **electric forces**. For small particles, the effect of Brownian motion is significant, and they can be caught by **diffusive deposition**. Particles may be caught between typically three or more fibers under **sieving**, and in the course of the simulation also by previously deposited particles, via **clogging effects**. Effects of gravity or other extension may be easily added to the models as needed.

Model of Media Clogging

The recalculation of the flow field after a certain amount of particles has been deposited allows the simulation of filter lifetime and filter clogging. When enough particles were deposited to invalidate the assumption of a constant flow field, these deposited particles are converted into additional obstacles to the flow. We distinguish two modes.

In the easier case, the particles are resolved by the computational grid for the flow calculations, and we simply set previously empty voxels to solid voxels wherever particles have deposited [3, 5]. The flow field is recomputed, and a new pressure drop is available that corresponds to a certain amount of filtered particles. Based on this new flow field, particles are again deposited, now with the possibility to also get caught by the new obstacles, the previously deposited particles.

The more difficult case is the one where the particles are not resolved by the computational grid [6]. An example of this is soot filtration, where soot agglomerate particles may be a factor 100 smaller than the filtering structures. They are known not to form a solid, but rather a highly porous sort of filter cake. Many thousand soot particles may fit into a single flow voxel, which is neither empty nor full when this happens. The voxel will only sustain a certain amount of soot, before it acts like a solid voxel for collision purposes, i.e. deposition occurs in neighboring voxels, while it is still permeable for the fluid. The parameters for this behavior can be set in the simulation, but are very hard to establish. Currently, we establish them by simulations on a smaller scale, with resolved particles depositing on a single fiber. The computed parameters such as porosity and permeability depend on issues like particle sizes, mean flow velocities etc., which illustrates the tremendous difficulties the simulation faces. Once a porosity, and depending on that, a permeability is established for a voxel, this permeability value enters in the Brinkmann term ($\kappa^{-1}\vec{u}$) extension of the Navier-Stokes equations. Figure 5 shows results of a computation where soot was deposited in a sintered structure. It can be seen that the growth of deposited particles extends also into the empty space in front of the media. This illustrates that by the same methodology also cake or surface filtration simulation is feasible. What is still missing for that regime is the additional simulation of the cleaning process. We expect this cleaning process to be one of several near future topics to work on. Figure 5 also illustrates another major aspect of the filtration simulation work: to provide the visualization techniques for the complex results of the simulation.

Conclusions

We have presented the thoughts, models and equations behind our software for virtual material design. The individual aspects are mostly not new, but the scale of the computations and the complexity of the simulated behavior are greater than in most other works. By parameter studies and dedicated material modifications, already the simulation alone provides many insights into the interplay of particle filtration mechanisms. Some comparisons of simulation results with experiments can unfortunately not be shown due to secrecy agreements, but they are quite promising. On the other hand, much collaboration with experimenters and simulators from industry and academia must still happen in order to fully realize the potential of the proposed technology.

References

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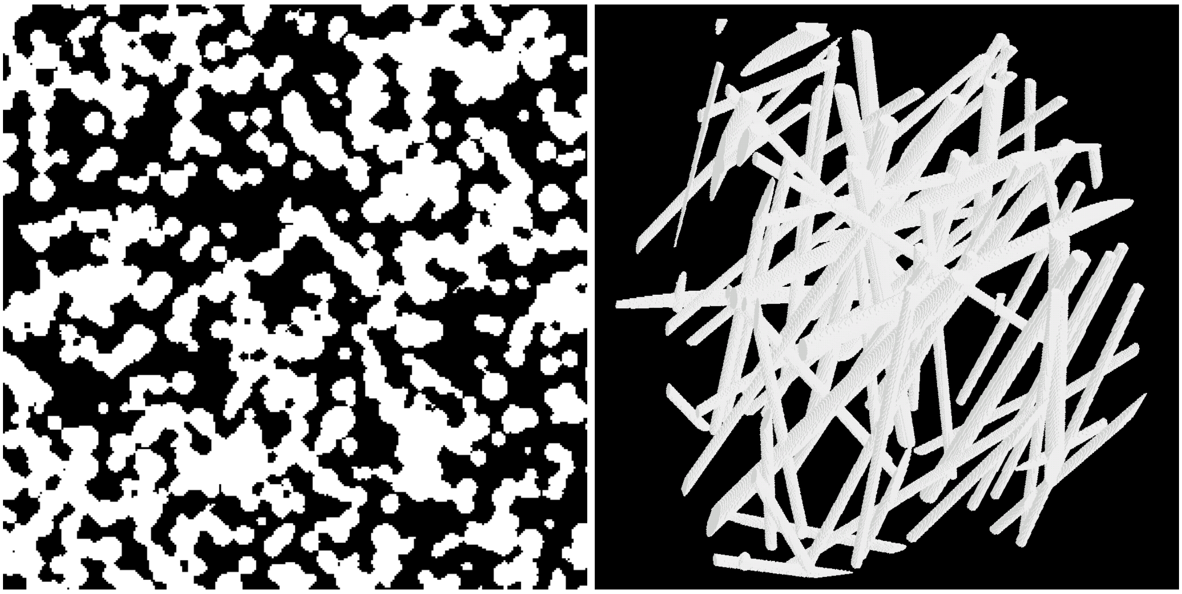

Figure 3. a) Two-dimensional cross section view of a sintered media model with about 50% porosity and b) a three-dimensional view of a nonwoven media model with about 95% porosity.

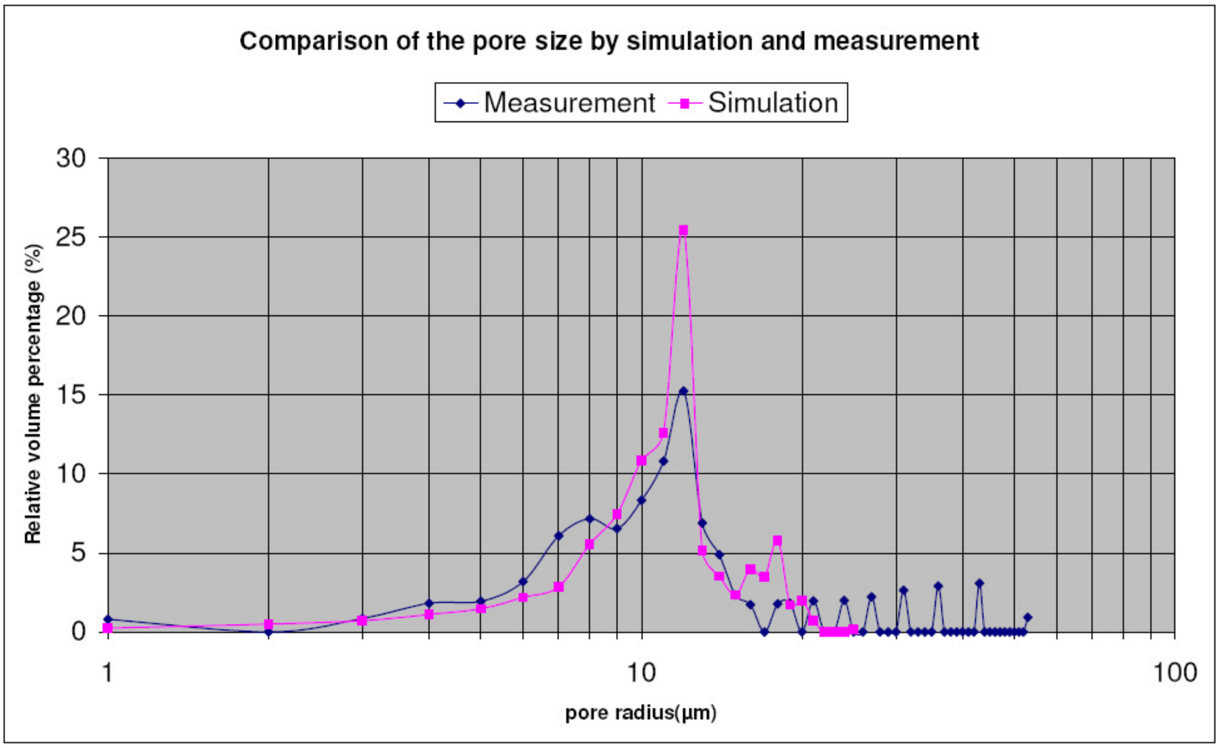

Figure 4 shows pore size measurements by the mercury intrusion method in dark blue vs. the computed pore size distribution of a media model of the same material in pink. The media was described by a frequency distribution of 20 fiber types. The discrepancy for large pore sizes bigger than 30 microns is still under investigation, and is currently considered an artefact of the experimental method.

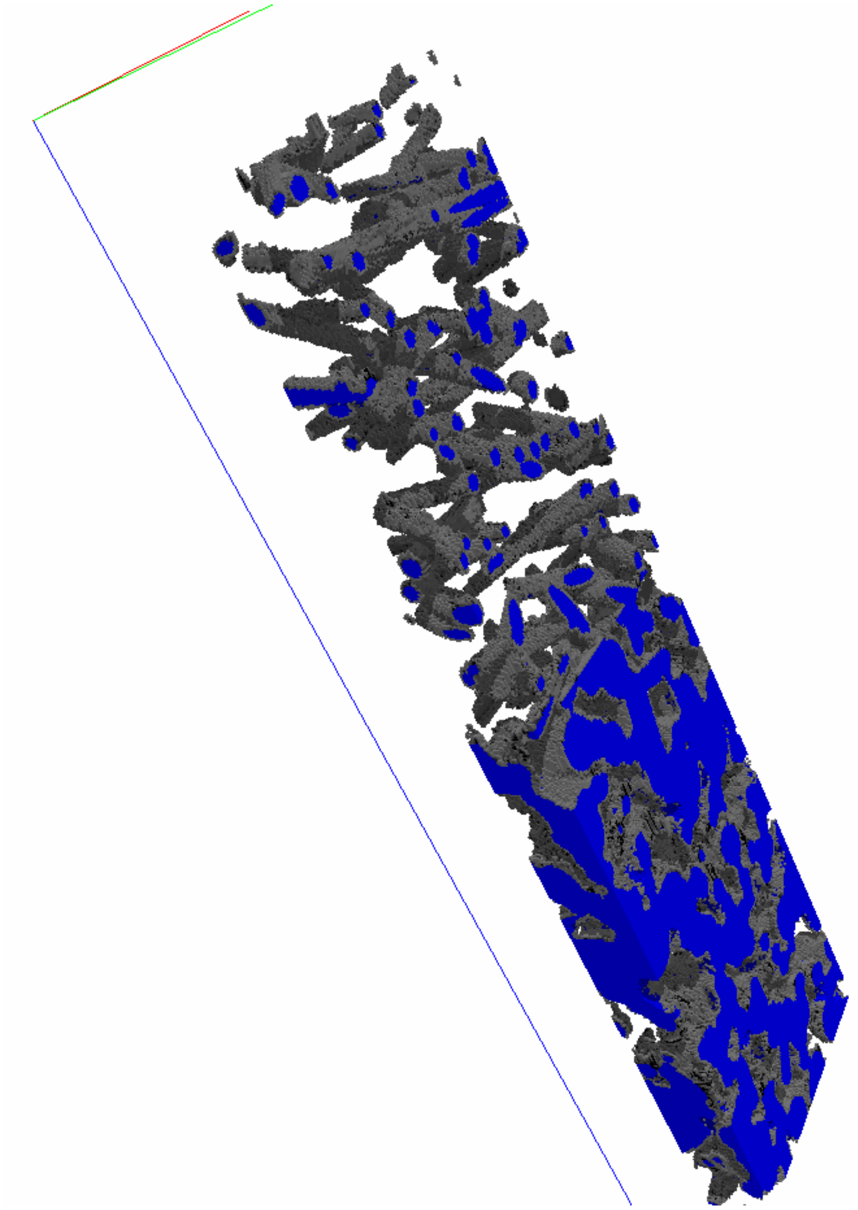

Figure 5 shows a generated sintered structure in blue with soot deposits in grey. Darker grey means denser soot deposits; empty space indicates pores (not yet) filled with soot. The cutout represents the full length of the filter media, but only a portion of the computational domain, for better inspection of the deposition patterns.