Fraunhofer Institut
Techno- und
Wirtschaftsmathematik

Virtual Material Design and Air Filtration Simulation Techniques inside GeoDict and FilterDict

Andreas Wiegmann, PhD, Stefan Rief and PD Dr. Arnulf Latz
Fraunhofer Institut für Techno- und Wirtschaftsmathematik,
Kaiserslautern, Germany

Abstract

In case of depth filtration in fibrous filter media, pressure drop, permeability, filter efficiency, and filter lifetime depend strongly on the micro structure. In addition to the filter mechanisms which are present already for a single fiber we also simulate sieving effects and electrostatic forces that are highly dependent on the geometry of the material. The procedure decouples into several steps: First individual layers of the fibrous filter media are modeled and then stacked into a random three-dimensional representation with given mean properties such as porosity, fiber types and fiber directions. Next, the air flow through the media is computed by solving the steady Stokes equations, and the electric field given by surface charges on the fibers is computed by solving a Poisson problem with singular source terms and appropriate boundary conditions. Then, a stochastic ordinary differential equation models Brownian motion, friction with the air, inertia of particles due to mass, as well as attraction or repulsion due to electric forces. Particles may collide with fibers and stick due to adhesion or bounce off if they have enough energy. They may also be sieved by being stuck between three or more fibers. By iterating this procedure, and computing new flow fields after significant amounts of particles were filtered, even filtration by previously filtered particles is simulated and the clogging and pressure drop of filters can be estimated.

Introduction

Mathematical methodologies from stochastic geometry [1] allow creating very realistic computer models of nonwoven. These models also apply for the layered structures of typical filter media. Each individual layer can be modeled as a nonwoven, and the layers can then be stacked. A simple model for nonwoven based on the three parameters porosity, fiber diameters and one-parameter fiber directions is derived in [2]. In [3], the methodology for steady state fluid dynamics simulations with a parallel Lattice Boltzmann code and the study of air filtration by a Lagrangian formulation of the particle transport was reported. In these generated random nonwoven geometries 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. Now, also the effects of electrostatic charges on the fiber surfaces on electrically charged particles are included in the model, and can give vastly increased filter efficiencies compared to the uncharged case.

Nonwoven model

The first item in the simulation of air filtration in a nonwoven is a three-dimensional representation of the nonwoven in the computer. Here, a so-called voxel model is used. In such a model, 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 fiber diameter that occurs. For example, for smallest fiber radius in the nonwoven 5µm, $h = 2.5\mu m$ will resolve this fiber with 4 voxels of edge-lengths h per diameter. This already introduces the next parameter in the model: the side lengths of the cutout. They must be long enough to model a representative portion of the media. On the other hand, available computer memory puts a limit to the size of the cutout. The thickness of the filter media should be resolved completely. Thus, if the media is 2 mm thick and a voxel is 2.5µm, then about 840 voxels are needed in the flow direction to allow also for a little empty space before and after the media. Then the capability to compute the air flow and particle motion through the geometry puts some restraints in the lateral directions, limiting us to 200 to 400 voxels in calculations.

The producers of nonwoven usually use up to 4 or 5 types of fibers. They may have a certain specific weight depending on the raw material (polyester, polyamide, etc.), a specific cross section shape, a certain length, a certain crimp and a cewrtain 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 $1.37 g/cm^3$, have a round cross section, are 7cm long and spiral shaped at 0.5 revolutions per centimeter with thickness 10µm and 15µm, and the same amount of both types of fibers is used, then the probability of 10µm fibers is $0.69 = 15\,\hat{}\,2/(15\,\hat{}\,2+10\,\hat{}\,2)$ and that of 15µm fibers is $0.31 = 10\,\hat{}\,2/(15\,\hat{}\,2+10\,\hat{}\,2)$.

Under the restrictions on the computable cutout, the fibers may often be modeled as straight and infinitely long; compare 7cm with 2mm. The model is then complete when one allows choosing the porosity and anisotropy of the fibers. Usually, the air flows perpendicularly to the machine direction. For concreteness we assume this is the z-direction of the model. Using polar coordinates, the directional distribution of the fibers in the nonwoven is given by its density, a function $p(\vartheta,\varphi)$ of altitude $\vartheta \in [0,\pi)$ and longitude $\varphi \in [0,2\pi)$. Due to the isotropy of the xy-plane, $p(\vartheta,\varphi)$ is independent of φ. The density of the directional distribution is

$$p(\vartheta,\varphi) = \frac{1}{4\pi}\frac{\beta \sin\vartheta}{(1+(\beta^2-1)\cos^2\vartheta)^{3/2}} \quad , \qquad \vartheta \in [0,\pi), \varphi \in [0,2\pi).$$

We call β the anisotropy parameter. The case $\beta = 1$ is the isotropic case, for increasing β the fibers tend to be more and more parallel to the xy-plane. For real nonwoven, β ranges from 3 to 10 depending on the compression applied to the nonwoven.

Last but not least, the porosity can be prescribed. For filter media layers it ranges between 80% to 98% porosity. Algorithmically, it can be realized very simply. 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 β. This fiber is discretized into voxels and entered into the domain, with the option to allow or disallow overlap with previously entered fibers. This procedure is repeated until the percentage of voxels not covered by fibers for the first time 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.

Flow simulation

We consider the rather slow flows typical for some filtration processes and solve the Stokes equations with periodic boundary conditions:

$$\mu\,\Delta\vec{v}_0 + \vec{f} = \nabla p \quad : \text{ momentum balance}$$

$$div\;\vec{v}_0 = 0 \quad : \text{ conservation of mass}$$

$$\vec{v}_0 = 0 \text{ on } \Gamma \quad : \text{ no-slip on fiber surfaces}$$

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.

Computation of the electric field

The charges are assumed as given forces on the fiber surfaces, i.e. on those 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:

$$\Delta u = \rho(\partial\Omega) \quad : \text{ singular force Poisson equation}$$

$$\vec{\mathrm{E}} = \nabla u \quad : \text{the electric field}$$

Here u is periodic in the x- and y-directions, and satisfies 0 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.

It is intuitively clear that this should be the case when considering a delta source on a single flat sheet centered in the nonwoven with periodic boundary conditions in x- and y-directions and Dirichlet conditions applied at various distances from the sheet. Due to the symmetries, the potential arising from this configuration is just a function of the z variable, and because it must satisfy the Poisson equation it is obvious that it is a piecewise linear function with a kink (angle determined by the magnitude of the charge) at the location of the delta. When the location of the Dirichlet boundary is moved away from the source, this hat function simply moves upward. That is, as $z_0 \to \infty$, $u \to \infty$ uniformly on $[0, nz]$. But the shape of the function remains unchanged, and the electric field $\vec{E}$ is independent of the choice of z_0.

Filter efficiency simulation

There are two important aspects to filter efficiency simulations. The first is the motion of the particles in the fluid. The second is 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 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 dust 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.

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

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

$\gamma = 6\pi\rho_F \nu \frac{R_P}{m}$:	friction coefficient
$\vec{x}$:	particle position
R_P:	particle radius
m:	particle mass
Q:	particle charge
$\vec{E}$:	electric field
$\vec{\mathrm{v}}$:	particle velocity
$\vec{\mathrm{v}}_0$:	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. Fig. 1 shows such filter efficiency curves that were computed for the empty media as well as partially loaded media. In Fig. 2, the effect of electrostatic charges on the deposition patterns is depicted. On the right, no electric charges are present and the deposition occurs only on the side of the fiber facing the flow (from left to right). On the left electric surface charges are present, and it is clearly seen that more particles are captured on the side of the fiber facing the flow, but even more importantly, electrostatic charges can attract particles from the slow flow region behind the fiber to the back side of the fiber, in the end more than doubling the amount of particles captured by the single fiber.

Filter lifetime simulation

For filter lifetime simulations, the same simulation is used as for the filter efficiency calculations, with a few modifications and 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 fine Arizona dust. The deposition locations of these particles are tracked, and after a predetermined amount of dust is computed, these deposition locations are used to modify the nonwoven geometry. All the previously independently computed (deposited) particles are now entered into the nonwoven geometry, switching flow voxels to solid voxels. This is possible even for particles much smaller than a voxel by keeping track of the mass deposited in a voxel from many small particles. For this modified geometry, the static problems of the steady fluid flow and electrostatic fields are recomputed, and a current estimate of the pressure drop becomes available. The next generation of particles is deposited, and their deposition rates can be used to compute again filter efficiencies for the partially clogged medium, illustrated in Fig. 1. Fig. 3 shows the pressure drop resulting for the whole media from such a procedure, as well as the pressure drop in some heavily clogging portion of the media where all the particle deposition is occurring. Fig. 4 shows a nonwoven filter media at end-of-lifetime. Many large and small particles have already deposited in an almost dendritic growth at the front of the nonwoven, which demonstrates nicely the ease with which cake filtration can be demonstrated in future modified versions of the simulations. The simulation was stopped, however, because the pressure drop had reached a certain predetermined magnitude. The exact rules for the conversion of deposited particles into solid or porous voxels are still subject of investigation. For example, very high resolution calculations where dust particles are well resolved by voxels are under way to determine these rules. Ultimately, only correct prediction of filter lifetime measurements will verify these choices.

Conclusion

We have described the nonwoven model, fluid flow computations, electrostatic computations, filter efficiency and filter lifetime simulation techniques incorporated into ITWM's GeoDict and FilterDict software. 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. Then even subvoxel-sized particles can be advected and deposited in the media, leading to filter efficiency and pressure drop curves that are very close 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 geometry changes based on deposited particles that are much smaller than a voxel.

References

[1] J. Ohser u. F. Mücklich, "Statistical Analysis of Microstructures in Materials Science", John Wiley & Sons (2000)

[2] K. Schladitz, S. Peters, D. Reinel-Bitzer, A. Wiegmann, J. Ohser, "Design of acoustic trim based on geometric modeling and flow simulation for nonwoven", ITWM Technical Report Nr. 72, January 2005.

[3] A. Latz, A. Wiegmann, "Simulation of fluid particle separation in realistic threee dimensional fiber structures", Filtech Europa, Düsseldorf, October 2003.

[4] R.C. Brown, "Air Filtration, An Integrated approach to the Theory and Application of Fibrous Filters", Pergamon Press, Oxford (1993).

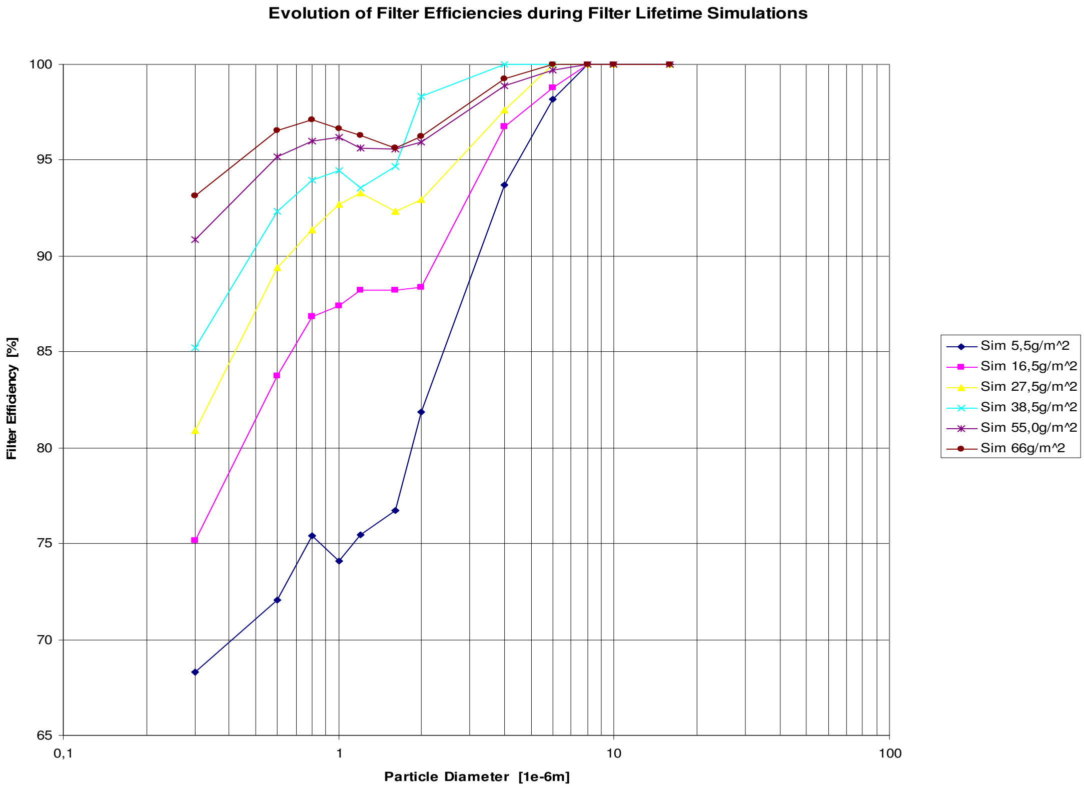

Fig. 1: Increase of filtration efficiency while the filter media clogs. At fixed intervals of dust deposition during a filter lifetime simulation, the filter efficiency is reevaluated. The pore sizes decrease and the filter efficiency particularly for small particles goes up as the filter media clogs.

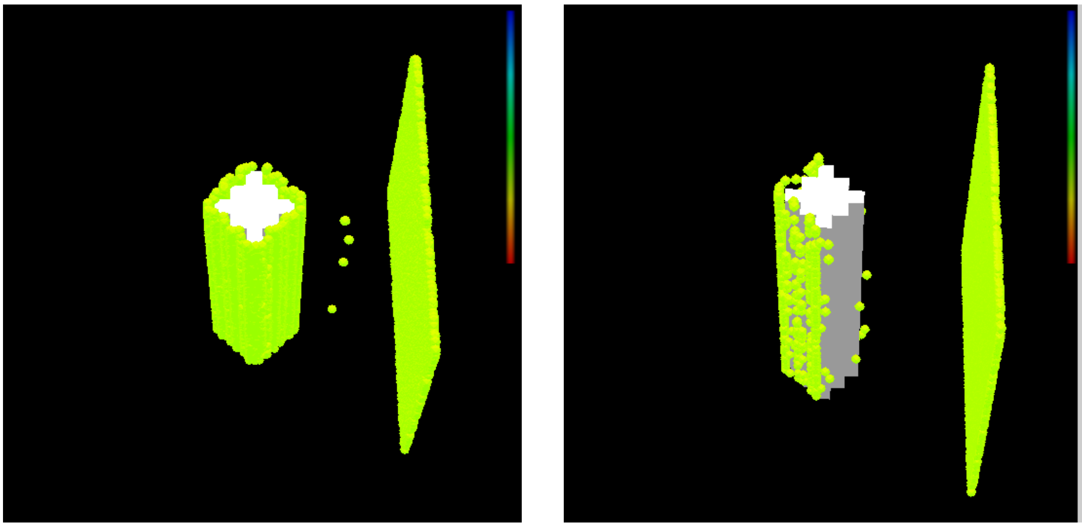

Fig. 2: Effect of an electrostatic field (left) on the particle deposition on a single fiber. Particles are started at random positions, and cover the front of fiber more densely in the presence of the electrostatic field, but most notably are also attracted to the back of the fiber in this case. The particle sheets on the right in both figures are non-filtered particles in their final position where they leave the computational domain.

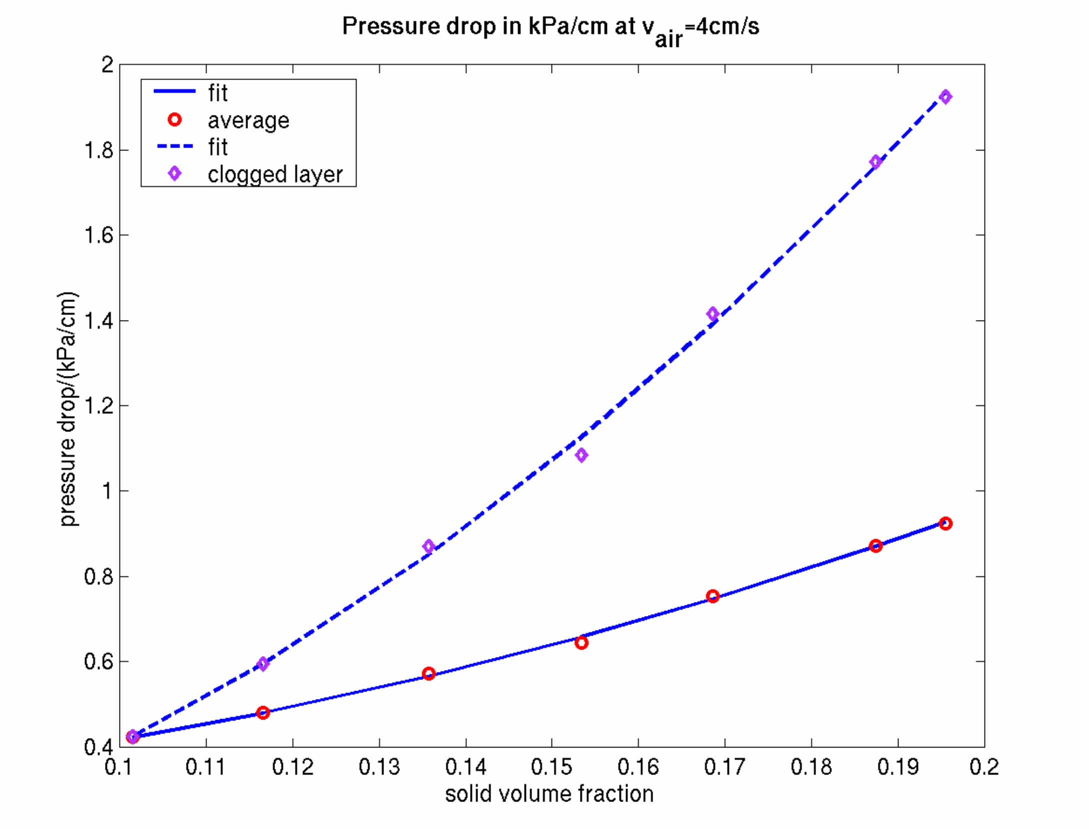

Fig. 3: Increase of the pressure drop while the filter media clogs. At fixed intervals of dust deposition during a filter lifetime simulation, the pressure drop is reevaluated. This is done for the complete media as the solid line but also for the actually clogged portion of the media in the dashed line. The information regarding pressure differences in parts of the media is easily accessed from simulation data but very hard to come by via experiments on real clogged filter media.

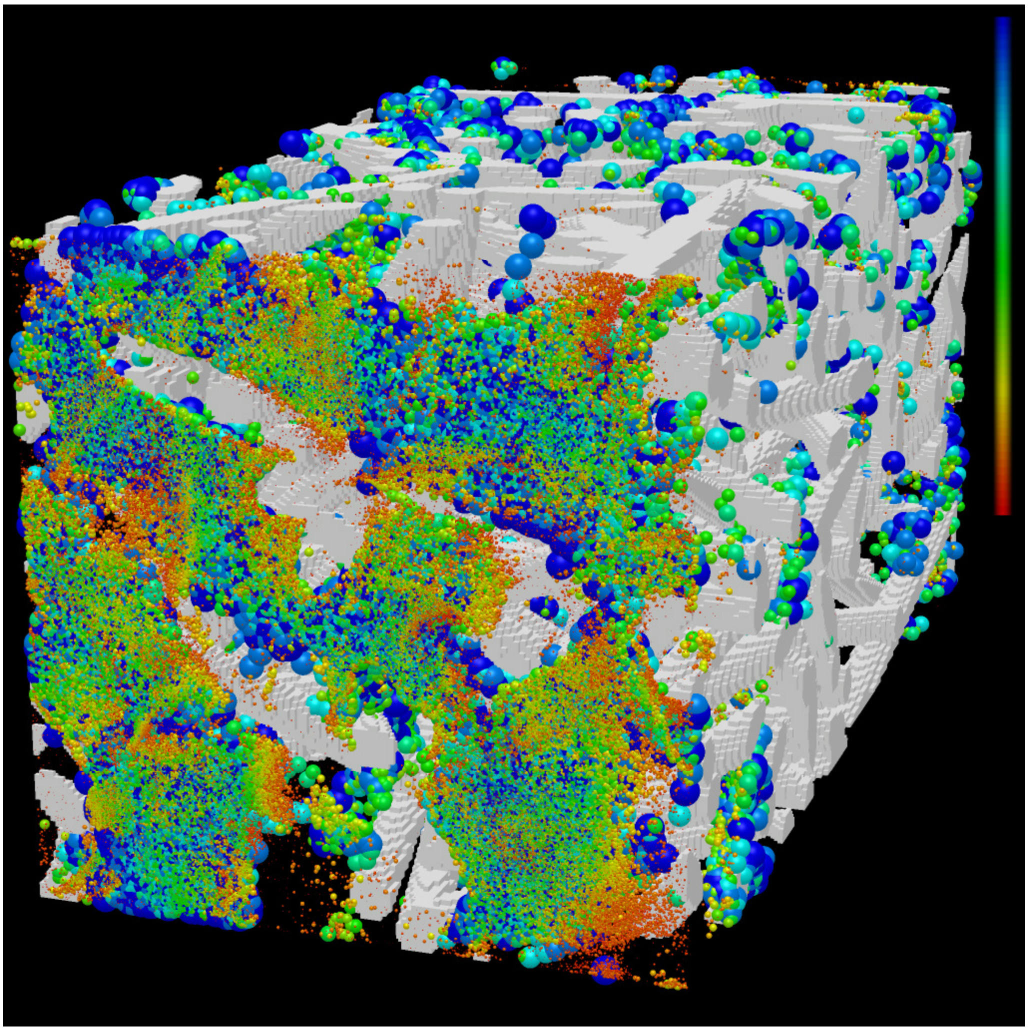

Fig. 4: Staple fiber fleece with dust particles, at end-of-lifetime. Different particle sizes in Arizona dust are illustrated by the color, with red indicated the smallest and dark blue indicating the largest of 23 occurring particle sizes. The colorful front face shows plenty of dendritic growth of particles on top of previously deposited particles.