FILTER MEDIA DESIGN BASED ON ANALYSIS OF µCT SCANS AND SIMULATION OF FILTRATION PROCESSES

Jürgen Becker, Cornelia Kronsbein, Liping Cheng(*), Rolf Westerteiger, and Andreas Wiegmann

Math2Markt GmbH, Stiftsplatz 5, 67655 Kaiserslautern - Germany

ABSTRACT

To address the growing demands on filter efficiency and life time, the industry continuously needs to improve filter materials and filters. One possibility to achieve this goal is to adjust the pore structure and fiber structure of the filter medium. Because production costs of new materials are high, it is beneficial to use computer simulations to accelerate the design cycle of new materials. In this talk, we present the necessary workflow:

At first, we take a µCT scan of a filter medium which is to be improved. On the segmented images, we can simulate filtration processes and thus understand how air flow, particle motion, particle capture and filter clogging happen in this medium.

In the next step, we want to modify the filter medium. For this, the segmented µCT images alone are not sufficient, as they could only be modified pixel by pixel. So, to enable filter media design, the µCT images must be analyzed for the geometric properties first, and then a 3D structure model must be created based on those geometric properties. This model can then be used as a starting point for the media design.

We will present how to analyze the µCT scan for porosity, fiber diameter, fiber orientation and fiber curvature and how to use those parameters to create a realistic model of the imaged sample.

KEYWORDS

Simulation, Filtration, Filter Design, FilterDict[®], GeoDict[®]

1. Introduction

To address the more and more demanding expectations of the filter markets, continuous design and development of new filter materials and products are always tasks for filter manufacturers. Traditional design involves an elaborate and expensive trial and error process in experimental laboratories. Computer Aided Design (CAD) and Computer Aided Engineering (CAE) make the process possible via modelling and simulation with computers.

For the performance of the filter, both the media and the filter design play a crucial role. The focus of this talk, however, is on the details of fibrous filter media. One can try to understand them by performing detailed 3-dimensional simulations of the filter media, air flow, particle motion, particle capture and filter clogging.

As the starting point, one must create a geometric 3D model of the filter media in the computer. This can be achieved using scanning electron microscopes (SEM) or ideally Micro X-ray Computed Tomography (µCT) of the filter media. After image enhancement and segmentation, a 3D array of millions of solid and empty cubic cells is created. The 3D images allow engineers to see the details of the material's interior and to get a much better impression about the samples than ever before.

On such an array, filtration process simulations can be performed, but it is not feasible to modify the structure in a media design step. To do so, geometric properties such as porosity, fiber diameters, fiber orientation, etc. must be determined. This information can be used to create structure models like the one from µCT. To achieve this, automatic algorithms to determine porosity, local orientation and local fiber diameters were developed. The toolkit, named FilberGuess, has been implemented into the digital material laboratory software, GeoDict.
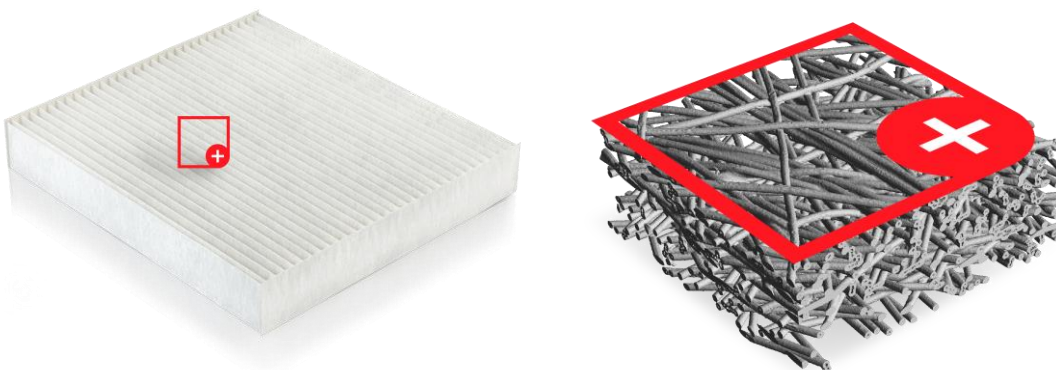
2. Method

Fig 1. A filter and its computed tomography image

As a way to find the input parameters needed to recreate the fibrous structure, the diameter and orientation of fibers in three-dimensional models are analyzed from segmented computed tomography (or FIB/SEM) images of the material.

2.1 Estimation of Fiber Diameters

A three-dimensional model has been obtained from segmented (µ)CT (or FIB/SEM) images of the material. A region of interest (ROI) is then defined and a domain is cropped in it. The analysis is done on this domain of the material's region of interest. The domain is divided into one or multiple sub-blocks. The fiber diameter distribution is computed for each block.

2.2 Estimation of Fiber Orientations

The fiber orientation tensor result shows the probability of fiber alignment in the specified principal direction. A high probability of fiber alignment in the specified principal direction will be indicated by a value of close to 1 on the result scale, whereas a low probability is indicated by a value close to 0. The fiber orientation tensor in the first principal direction is the most useful result to view.

Eigenvectors and eigenvalues are used as a method by which a mass of information of orientation and dip can be summarized in a 3-D space by six numbers. The fiber orientation tensor is expressed in the global coordinate system. The diagonal components of a fiber orientation tensor represent the strength of alignment in the respective directions. The values of diagonal components range between 0 and 1, and the sum of all three diagonal components is 1. Fig 2 shows the structure with the aligned fibers, planar randomness, and 3D randomness, respectively. They corresponds to the tensors with the diagonal components of [1/3,1/3,1/3], [1/2,1/2,0], [0.9,0.05,0.05], and all zeros for the off-diagonal components.

Fig 2. Structures with aligned fibers, planar randomness, and 3D randomness

The off-diagonal components of a fiber orientation tensor represent the amount that alignments vary from the coordinate axes, and they are zero when coordinate axes coincide with the principal directions of the orientation tensor. The off-diagonal tensor values reflect the symmetry of the composite material and the orientation with respect to the direction of conduction.

The principal directions are numbered in the order of the respective principal values, from the largest to the smallest. The first principal direction represents the direction along which the most fibers are aligned, and the third principal direction represents the one along which the fewest fiber are aligned. The larger the principal value in a given direction, the stronger the alignment.

To compute fiber orientations, two algorithms have been developed:

Principal Component Analysis (PCA):

The domain is cut into blocks of a given size. For each block, all connected components are found. Ideally, these connected components correspond to segments of individual fibers.

For each component, it is assumed that the voxels of the component form a point cloud. An ellipsoid which best approximates this point cloud is computed using the PCA method (Principal Component Analysis) and provides the principal orientation. These principal orientation vectors are averaged to get an orientation for each block. Per-block orientations are averaged to obtain the desired number of orientation tensors.

In summary, the method cuts the fibers into segments and determines the local average of the orientation of these segments to obtain an orientation tensor and a histogram.
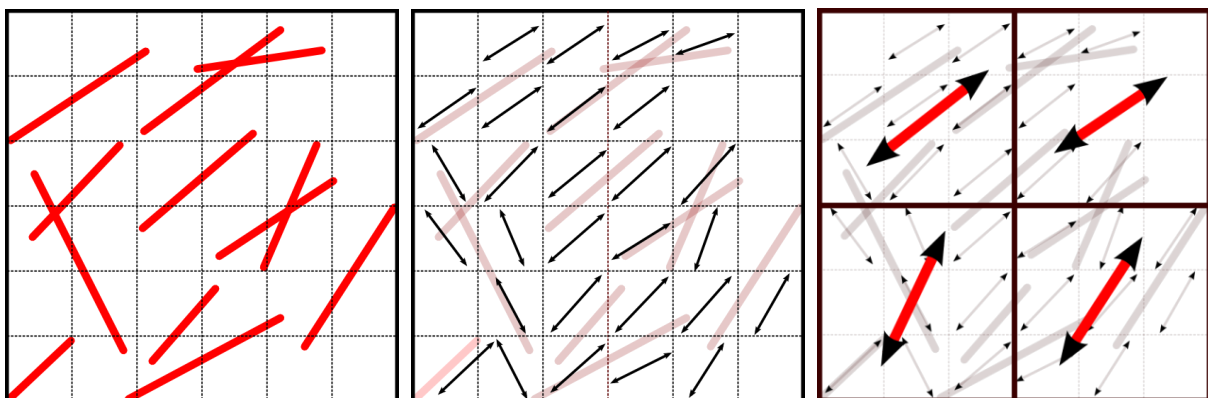

Fig. 3 PCA algorithm for fiber orientation estimation

Star Length Distribution (SLD):

Analysis is done on a per-voxel basis. For each voxel, the algorithm analyzes chord lengths through the voxel for a pre-defined set of directions. When using the SLD algorithm, the anisotropy (e.g. transverse isotropic) of the fibrous structures can be analyzed. In case of transverse isotropy, the material properties in fiber direction differ from the material properties in the direction perpendicular to the fiber.
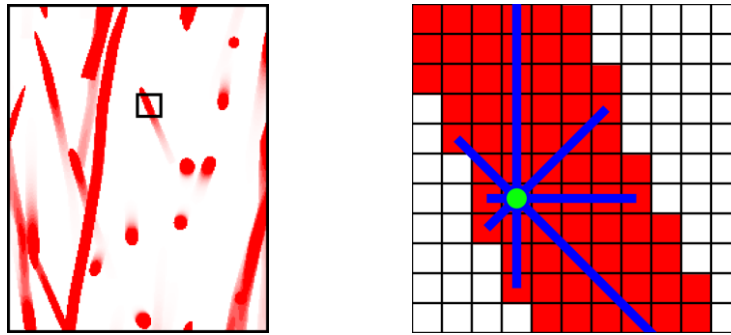

Fig. 4 SLD algorithm for fiber orientation estimation

3. Results

As a test case, a virtual CT is made and taken for the estimations of fiber diameters and orientations. The obtained parameters of diameters and orientations are used as input for FiberGeo to regenerate the structure. The generated structure can then be compared with the original virtual CT data to validate the estimations. After the validation, the estimated parameters can be modified to design new materials.

The virtual CT is loaded and segmented with ImportGeo module, which converts the image into segmented voxel data. After the region of interest (ROI) is determined, the domain is cropped to limit the analysis to the actual material region. The domain size of the example in Fig. 5 is cropped to 640 x 640 x 1024.
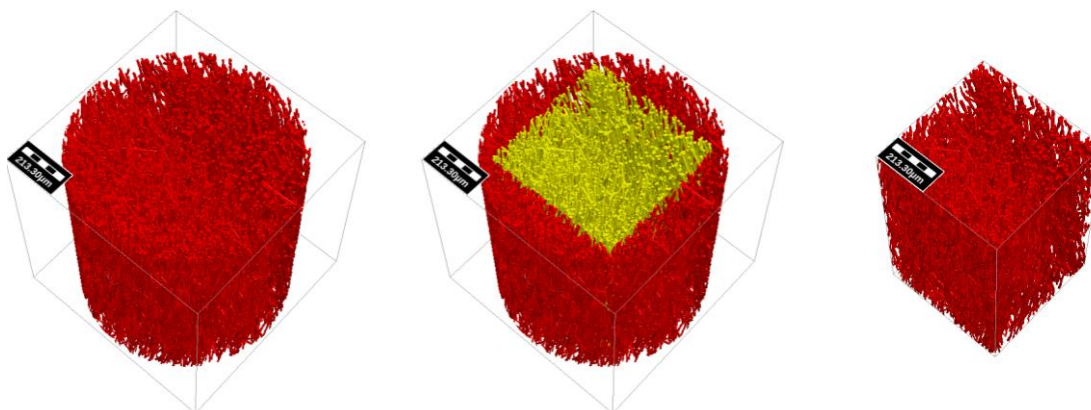

Fig. 5 Importation of µCT and selection of region of interest

At first, the fiber orientation is studied with the PCA method. The domain is subdivided into 2x2x3 blocks.

The arrows in Fig. 6 indicate the main fiber orientation for each block. Long arrows correspond to strong preference in orientation. It is observed that the orientation is quite uniform in x and z direction. In y direction (Fig.6 middle), two main orientations of the fibers are observed.
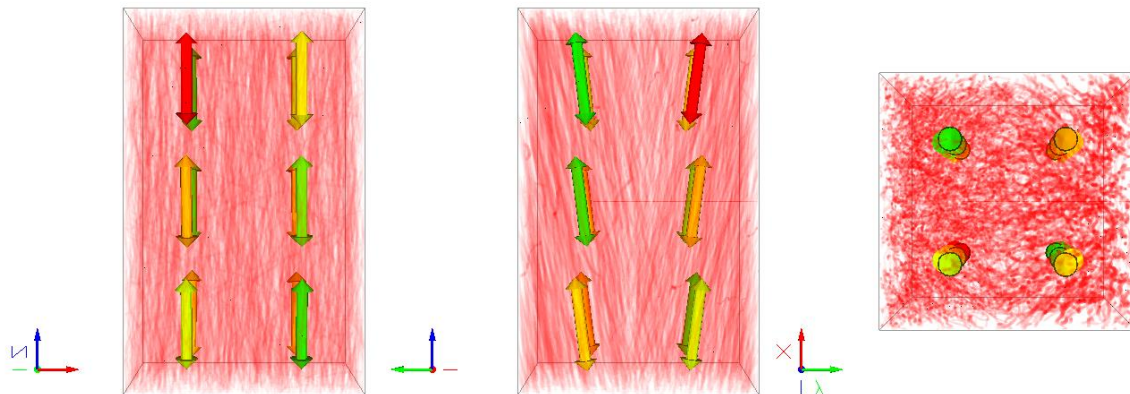

Fig. 6 Fiber orientation in y-z (left), x-z (middle), and x-y (right) plane

The fiber diameter distribution can then be computed for each block. Gradient from 8μm to 11μm is computed in the Y-direction from the cross-sectional view in Fig.7.
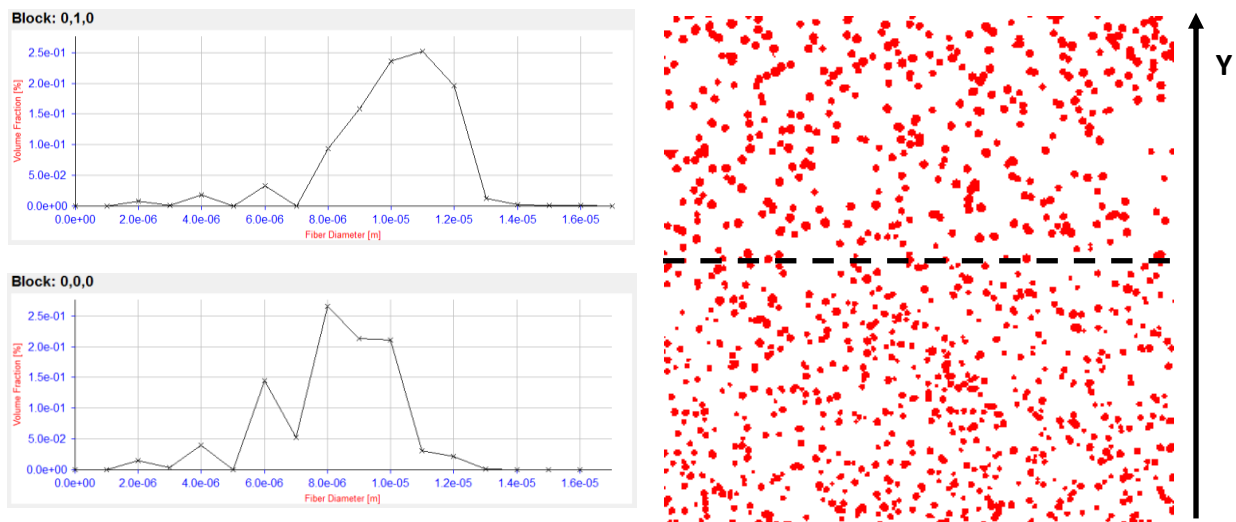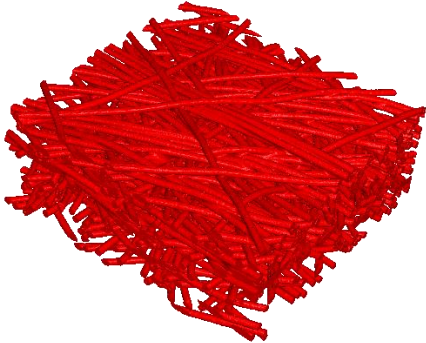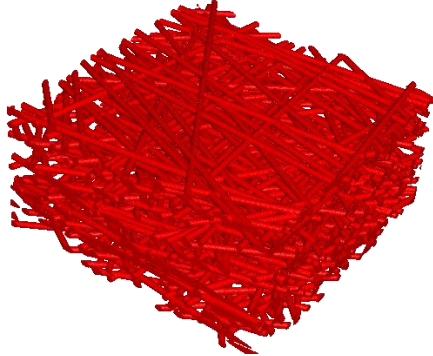

Fig. 7 Fiber diameter distributions

The parameters taken from the analysis of the scanned structure are listed in Table 1. The parameters are fed into ImportGeo to generate a new computer model. The clogging lifetime filtration simulations then are carried on both the reconstructed model from CT scanning and the new generated model. The pressure drop evolutions during the clogging filtration are plotted in Fig. 8 for the CT scanned structure and the

generated model.

CT Scan	Model
Input parameters found by CT-Scan analysis: ▪ media thickness ▪ porosity ▪ fiber diameter ▪ in-plane anisotropy	Input parameters taken from assumptions: ▪ straight fibers ▪ fibers oriented in-plane ▪ homogeneous distribution ▪ circular cross section

A deviation around 10% can be observed. One of the reasons is that curved fibers exist in the filter medium while in the current status, the curvatures cannot yet be analyzed; therefore only straight fibers are modeled. Another reason may be that the computer model uses homogeneous distribution, but the inhomogeneity to some extend can be observed.
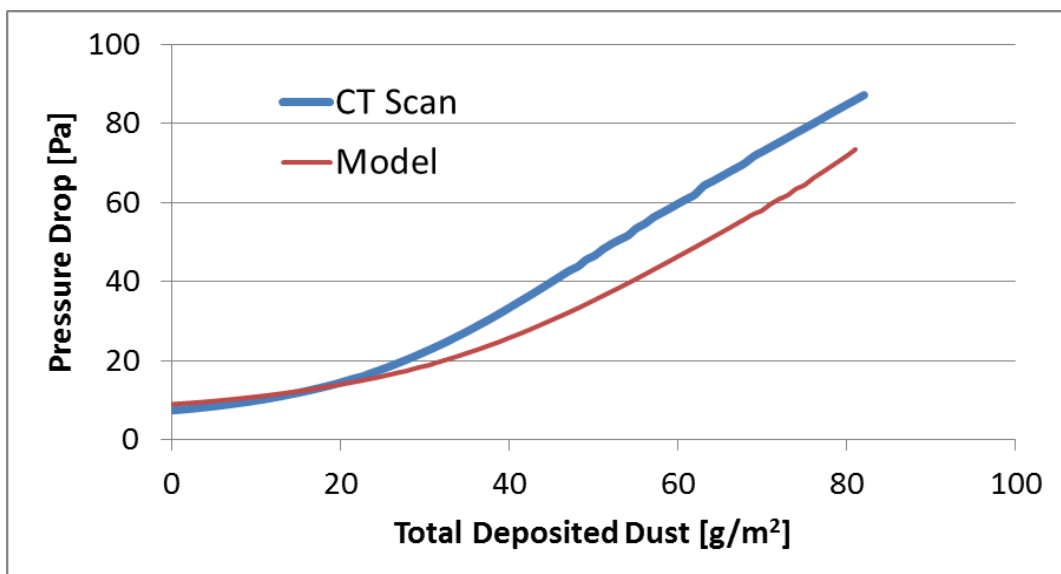

Fig. 8 The comparison of lifetime filtration simulations on CT scan and computer model

4. Conclusion

µCT scans and SEM images can be used to investigate existing materials. But for material design and development, structure models are required. To create realistic structure models, the µCT scans are analyzed to find matching input parameters. FiberGuess can estimate fiber orientation and fiber diameters. It is particularly well suited for the analysis of diameter and orientation of fibrous structures made of long non-hollow fibers with circular cross-section. It is the starting point to reproduce fibrous structures with FiberGeo, the module to model and generate nonwovens and fiber-reinforced composite. Then, the user can modify parameters in FiberGeo and observe the effect of these changes in the modelled structure. For the future, more work needs to be done on the analysis of the fiber curvatures and inhomogeneity.