

Calculation of material properties and modelling of material geometry based on CT-scans

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Abstract

CT-scans in combination with recent hardware and software developments establish new possibilities for the engineering of materials with the computer. Using CT-scans one can calculate material properties via geometrical analyses and numerical simulations. Furthermore, CT-scans can be the basis for the development of geometry models for a material. Using a realization of such a model one again can simulate the relevant material properties, what allows for the optimization of the geometry. In a next step one tries to produce the new material and a CT-scan can now help to proof if the optimal geometry was achieved.

This ansatz is applied to a multitude of projects at the Fraunhofer ITWM. The main applications are the design of filter media, the optimization of PEM fuel cells and the simulation of felts for the dewatering of paper. For these applications we calculate pore size distributions, one and two phase flows, the efficiency and life-time of filters, the electrical and thermal conductivity, and the effective elastic properties. To assure the reusability of the knowledge, which was obtained in many public and industrial projects, all the options for the computer aided engineering are included in the GeoDict software. This software is also usable for partners of the ITWM (see www.geodict.com).

Keywords: material properties, simulation, geometry analyses, material modelling

1 Material property calculation based on CT-scans

For the material property analyses on a CT-scan one has to segment the gray-scale image. The result of the segmentation is a mesh, in our case a voxel-mesh, in which the different materials are distinguished. For the calculations each material can have certain characteristics (permeability, conductivity, contact angle, ...).

Two types of methods are used for the calculation of material properties on the segmented image. The first type is based on the direct analyses of the geometry. Examples demonstrating such methods are presented in Chapter 1.1. For the second type one has to solve a partial differential equation (PDE) on the segmented CT-scan, where examples are shown in Chapter 1.2. From the three-dimensional solution of a PDE, one can approximate a material property by calculating the according mean value.

1.1 Geometry-based property analyses

1.1.1 Bubble point and pore size distribution for knitted wire meshes

One geometry-based method is the computation of the bubble point. First one has to find the largest through pore of a geometry. This largest through pore is shown in Figure 1(b) for the CT-scan of a knitted wire mesh, which is displayed in Figure 1(a). The diameter of this pore and the contact angle of the material define the bubble point pressure. A comparison of the bubble point pressure, in dependency on the contact angle, for three knitted wire meshes is shown in Figure 1(c).

The pore size distribution of a material can also be computed using a geometry-based method presented in [1]. The result of such a calculation, for the same knitted meshes, is shown in Figure (1)d.

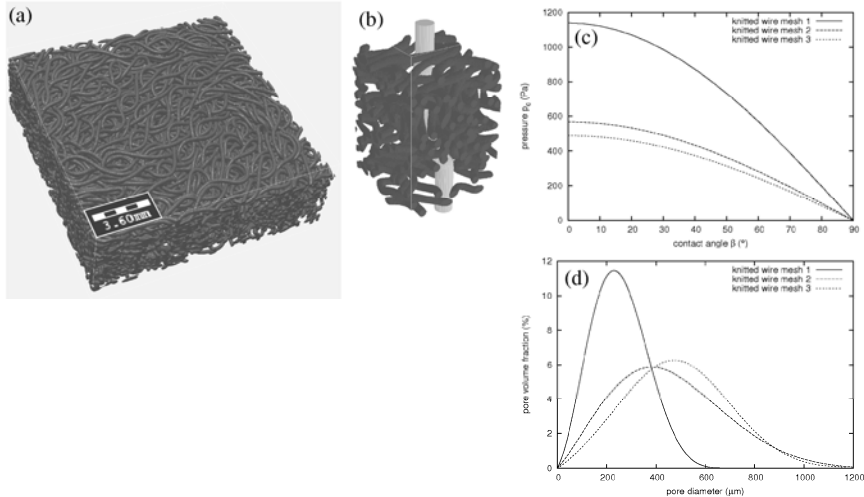


Figure 1. (a): The CT-scan of a knitted wire mesh. (b): The largest through pore of the knitted wire mesh from (a). (c): The bubble point pressure in dependency on the contact angle for three knitted wire meshes. (d): The pore size distribution for three knitted wire meshes.

1.1.2 Pressure saturation relationship for gas diffusion layers of PEM fuel cells

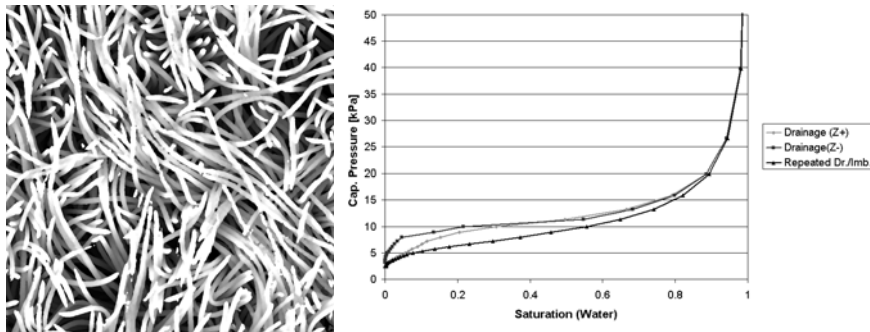


Figure 2. Left: tomography image of a gas diffusion layer. Right: corresponding capillary pressure curves for drainage from top (Z+), bottom (Z-), and repeated drainage/imbibition. Images taken from [2].

The gas diffusion layer (GDL) of a PEM fuel cell is located between the flow field on one side and the catalyst layer on the other side. It has to provide good electronic conductivity while at the same time allowing oxygen to diffuse from the flow field channels to the catalyst layer and allowing the product water to pass from the catalyst layer to the flow field. State-of-the-art GDL are fibrous non-wovens of about 200 μm thickness. When the fuel cell is under operation, the GDL is always partially saturated with water. Thus the relation between capillary pressure and water saturation is an important material property. Under the assumption that all fiber surfaces inside the GDL have the same wetting properties, the pore morphology method of Hilpert and Miller [3] can be applied to model drainage and imbibition and find the corresponding capillary pressure curves. Fig. 2 shows a tomography image of a GDL and its calculated capillary pressure curves.

1.2. Partial-differential-equation-based property analyses

1.2.1 Velocity dependent pressure drop for knitted wire meshes

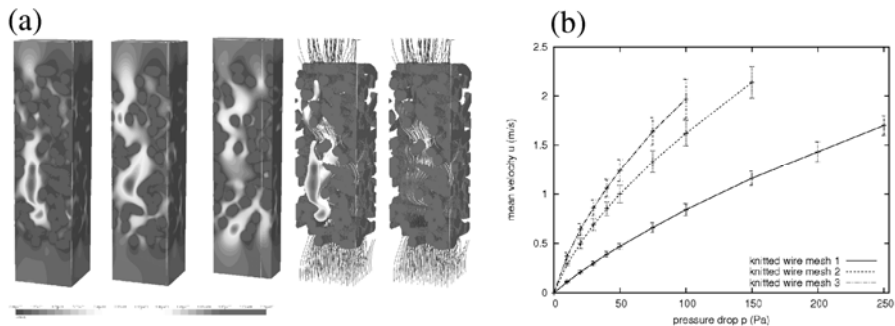


Figure 3. (a): Visualization of the flow simulation for a knitted wire mesh. (b): The velocity dependent pressure drop for three knitted wire meshes.

An example of a PDE based method is the calculation of the permeability or the pressure drop. To get these quantities one has to compute the flow through the medium, which is described by the Stokes or Navier-Stokes equation. In Figure 3 the results of such flow simulations are displayed. Figure 3(a) shows the visualization of a flow field in a part of the knitted wire mesh from Figure 1(a). In Figure 3(b) one sees the comparison of the velocity dependent pressure-drop for three knitted wire meshes.

1.2.2 Saturation dependant transport properties for gas diffusion layers

As described in Chapter 1.1.2 the GDL has to allow for oxygen transport to the catalyst layer, for water transport to the flow channel and electric conductivity between catalyst layer and backing layer. Thus diffusivity, permeability and conductivity of the layer influence the performance of the cell. But not only the properties of the dry medium are important here, but also those of the partially saturated medium. To obtain those saturation dependant values, the methods of Chapter 1.1.2 are combined with single-phase simulations: The distribution of air and water is determined with the pore morphology method. Then, this distribution is assumed to be fixed. Now air permeability can be determined by solving the Stokes equation in the air phase, air diffusivity by solving Laplace's diffusion equation in the air phase. Relative conductivity is obtained by solving the conduction equation with different coefficients for air, water and fibers. Fig. 4 shows some exemplary results.

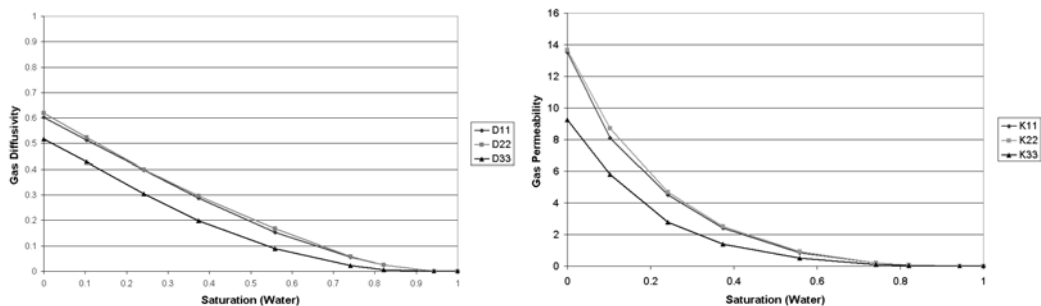


Figure 4. Left: Relative permeabilities, K11 and K22 are in-plane directions, K33 is through-plane. The permeabilities are given in 10^{-12} m^2 . Right: Relative diffusivities, D11 and D22 are in-plane, D33 is through-plane direction. Images taken from [2].

1.2.3 Virtual compression for a gas diffusion layer of PEM fuel cells

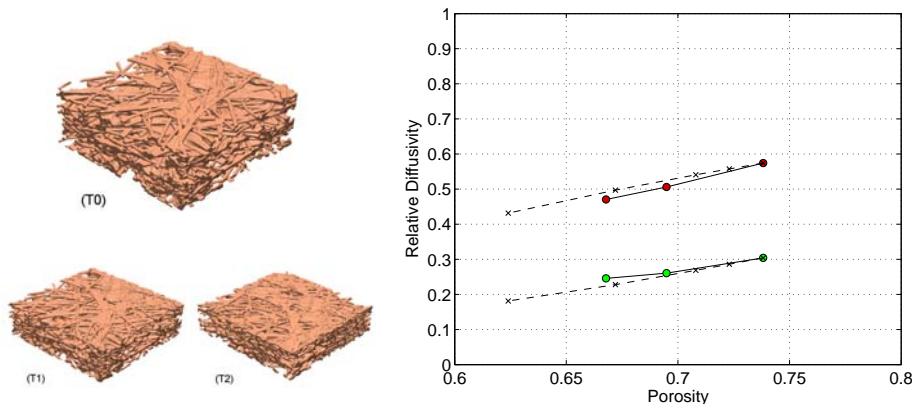


Figure 5. Left: 3D structure of a Toray TGP H060 gas diffusion layer, CT-Scans of the same sample at three different compression levels. Right: Diffusivity values, the dotted lines show the numerical results for the virtually compressed (T0), the circles the numerical results for (T0), (T1) and (T2). The light markers are through-plane and the dark markers in-plane results. Images taken from [5].

CT scans of GDLs usually image the layer ex-situ and in uncompressed state. Due to the clamping pressure of the fuel cell stack, the GDL is compressed when built into the fuel cell. Thus the material properties of the compressed layer are more interesting than those of the uncompressed layer. To obtain the properties of the compressed medium based on an uncompressed CT scan, a reduced compression model was introduced in [4]. Fig. 5 shows a comparison between the diffusivity values determined for a virtually compressed layer with diffusivity values calculated from tomography images of compressed layers.

2 Modelling of the material geometry based on CT-Scans

CT-scans give an accurate depiction of the material geometry as far as the resolution and the contrast of the material are sufficient. However, to design a new material, one needs a material model, where the geometrical properties are described by a few parameters. Varying these parameters the material geometry can be optimized. To obtain such a model the accurate information provided by CT-scans is needed or at least very helpful. In our group we model fiber structures (nonwovens), components of PEM fuel cells, ceramics, woven textiles, metal wire meshes and felts. In this chapter it is shown how CT-scans help to model fiber structures (nonwovens), metal wire meshes and felts.

2.1 Fiber structures

A simple model for fibrous structures was introduced by Schladitz et al. in [6]. The intersection of infinitely long straight and possibly overlapping fibers of circular diameter with a given box geometry is computed based on three input parameters: The porosity, the fiber diameter distribution, and the fiber orientation. All three parameters can be estimated from CT-scans, in our case after it has been converted into a mesh. For the porosity, one simply counts the empty cells and relates to the total number of cells. Schladitz et al. [6] describe a procedure how a one-parameter distribution of fiber orientations can be estimated from 2d cross sections of a CT-scan. If the fiber diameter distribution is not known from the manufacturing process, it may be estimated from a CT-scan by inverting the image and conducting a geometric pore size analysis (see Chapter 1.1.1) on the inverted mesh, e.g. viewing the space covered by the fibers as pore space. Figure 6 gives an example of this procedure, in this case

applied to a virtual fibrous structure. At the moment, the method works best if the fiber diameter is close to an even number of voxels. An improvement of the method for diameters close to an odd number of voxels is in the works.

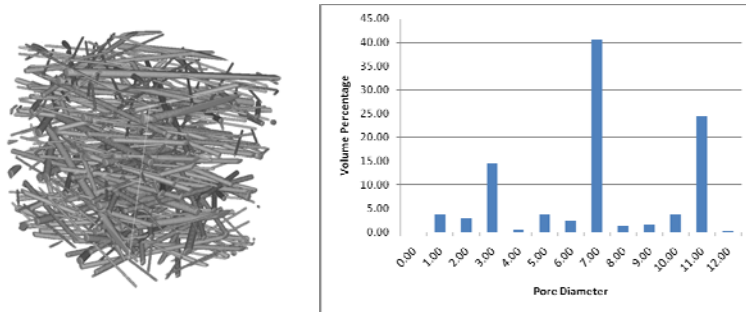


Figure 6. Left: Visualization of a virtual fibrous structure with 20% fibers of 3.5 μm diameter, 40% of 7.5 μm diameter and 30% of 11.5 μm diameter. Right: Analysis of the geometric pore diameter of the inverted structure. The peaks are identifying the diameters, and also the relative distribution of diameters is correct.

2.2 Metal wire meshes

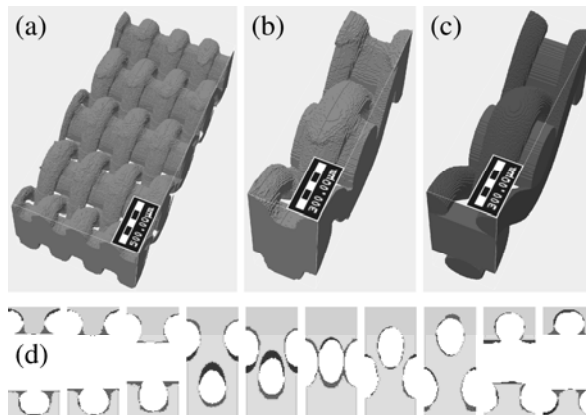


Figure 7. (a): The CT-scan of a metal wire mesh. (b): A unit cell from the CT-scan. (c): A unit cell of the weave modelled with GeoDict. (d): Comparison between the CT-scan and the model geometry.

The structure of a weave is determined by the interlace of the warp and weft wires, which is usually given by the weave diagram. However real weaves exhibit a wide range of shape variations, which can be seen in CT-scans. These variations have to be included in the weave model to get a better approximation of real structures. The shape variations included in the GeoDict software, which are explained in detail in [7, 8], are the broadening of the threads, the lateral and vertical deformation of the threads, the different bending behaviour of warp and weft threads and the stiffness of the threads. In Figure 7 a tomography of a plain Dutch weave and the corresponding model are shown. The model was developed with the help of the CT-scan. Hence the agreement between the two structures is very good, what is displayed in Figure 7(d). The white color shows where the geometries match.

2.3 Paper Machine Clothings: Felts and fabrics

In modern paper machines, forming fabrics, dewatering felts and drying fabrics are highly sophisticated multilayered structures which guarantee high performance in many respects. Durability,

non-marking forming, high dewatering levels and efficient drying are some requirements being constantly optimized.

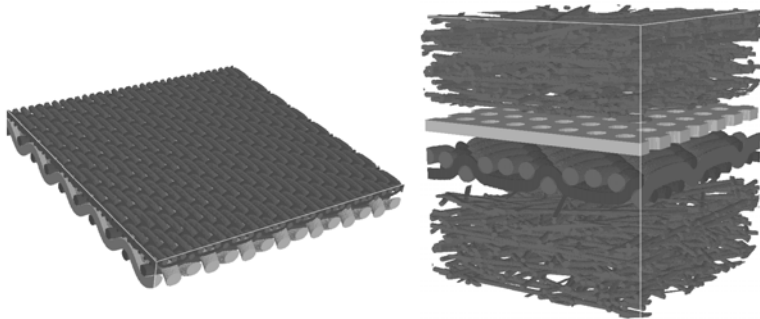


Figure 8. Left: Geometry model of a forming fabric. Right: Geometry model of a dewatering felt.

For this optimization process one has to design corresponding models, where CT-scans help to reveal the complex structure. Such models, composed of woven and nonwoven layers, are displayed in Fig. 8.

3 Conclusions

CT-scans can be used to analyse material properties. To calculate these properties a segmentation of the greyscale image, which results in a (voxel) mesh, is needed. The mesh can be analysed directly or it can be the basis to solve partial-differential-equations. Both methods help to gain an understanding of the complex influence of the underlying geometry on the material properties.

Secondly the CT-scan can be used to develop or improve models of the material geometry. Varying model parameters one can design new materials with improved features.

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