Numerical Determination of Effective Material Properties of Porous Media

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ABSTRACT

The properties of porous media and composite materials depend strongly on the geometric distribution of the constituent materials. The GEODICT software permits to compute material properties based on three-dimensional computer-tomography (CT) images or virtually created structure models. In either case, the property is computed by solving a partial differential equation on the 3d mesh and postprocessing the solution. Thus, by varying the geometric parameters in the computer it is possible to design new porous media and composite materials with improved properties.

1. Introduction

Improving an existing material to achieve better performance or lower production costs is a challenge often encountered by material scientists. In case of porous materials, the "performance" of the material is usually related to certain effective properties of the medium, e.g. permeability, diffusivity or conductivity. Typical problems are e.g. to raise the conductivity of the material without lowering the permeability too much or to achieve the same conductivity with less material.

In order to achieve this goal, computer simulations can be useful. The basic idea behind them is to create a model of a new porous material first in the computer, predict its properties numerically and - by iterating this process - find a better material. The advantage of this process is that it allows to analyze porous materials before actually producing them.

However, to make this *virtual material design* possible, three steps are necessary:

In the first step, the ability of the numerical algorithms to predict the effective properties of the existing material has to be proved. To do so, a tomography image of the material is used. Then, using the segmented (and probably noise filtered) image as voxel mesh, the effective material properties like e.g. pore size distribution, diffusivity, permeability and conductivity are determined numerically. These results are then compared to measurements performed on the same material.

In the second step, the ability to produce realistic structure models virtually has to be shown. For this purpose a representative structure model is created virtually (often by a random process) using a small set of input parameters. For example, for fibrous structures these input parameters are fibre diameter and cross sectional shape, fibre length, directional distribution (anisotropy) and the porosity. It then has to be checked that the effective properties calculated for this model are the same as those calculated for the tomography image before.

Only if those first two steps are successful, we can in a third step study new materials. Starting point is the model created in step 2. Now, by changing the input parameters of the virtual model generator, the effect of for example different fibre diameters or porosities can be studied.

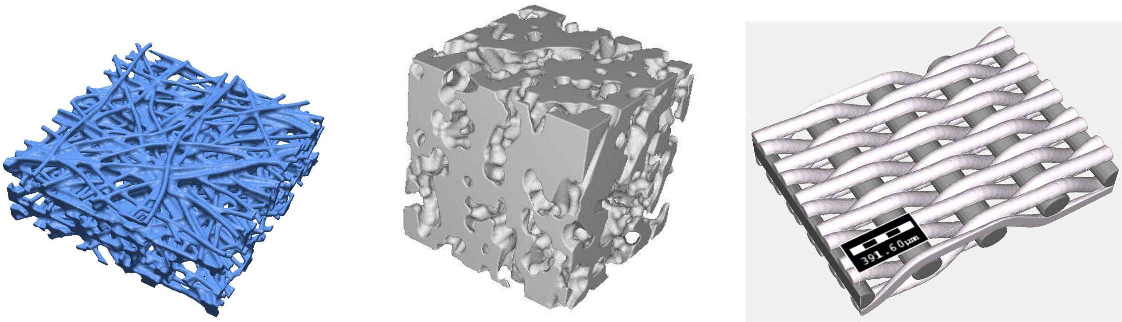

Figure 1: Examples of virtually created media, from left to right: fibrous gas diffusion layer, sintered ceramics filter, twill dutch weave metal wire mesh.

So a software tool enabling virtual material design necessarily has to have the abilities to a) import tomography images, b) create structure models virtually and c) determine the effective material properties numerically. These abilities are combined in GeoDict[1] and are explained in more detail in the following two chapters.

2. Virtually Created Structure Models

There are many different types of porous structures used in various fields of applications. Obviously, there are also many different approaches needed to create models of these structures. An often used porous medium is a fibrous nonwoven and the method used to create the structure model shows a very typical approach: the algorithm starts with an empty box into which fibres are then placed randomly until the desired porosity is reached. Random placement means that the actual fibre added is the result of a random process: the centre may be distributed uniformly in space, the direction distribution may follow a prescribed anisotropy[2], the fibre radius may be Gaussian distributed. In this way, the resulting 3D model is a random realisation of the underlying stochastic algorithm.

Similar approaches are used to model sintered materials. In this case spherical, rectangular or multiangular particles are used instead of fibres. A different approach is needed for woven structures[3]. Here, the structure is defined by the weave pattern and randomness may only enter if perturbances of the weave are to be modeled or in case of multi-filament fibres. Additional steps needed may be the addition of binder or adding different layers to form a composite material.

Independent on the method of creation, GeoDict uses a rectangular voxel mesh as discretisation. This allows to apply the same numerical algorithms on tomography images and on virtually created structures, which simplifies the comparison between imaged real and constructed virtual media.

3. Determination of Material Properties

Once the voxel mesh is created, the properties of the medium can be calculated numerically. For this it is important, that the structure model is representative of the porous medium. Only in this case, the properties are independent on the choice of cut-out imaged in the tomograph or the random realisation of the virtually created medium. This requires the structure model to be large enough to exhibit all characteristic features of the porous medium, which may demand

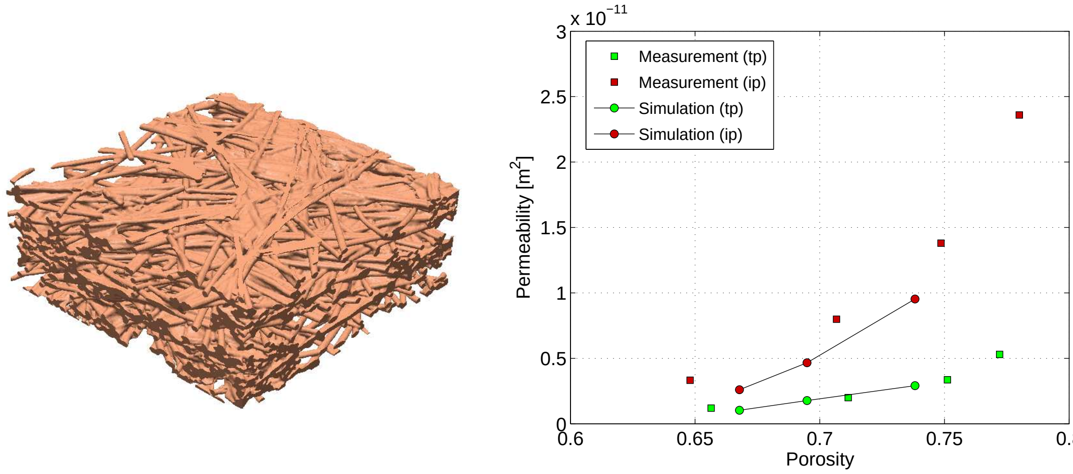

Figure 2: Left: tomography image of an uncompressed fuel cell gas diffusion layer. Right: calculated permeability compared to measurements performed on the same layer. Measurements were done under various levels of compression. The simulations were performed on three tomography images taken at different compression levels. The chart shows the anisotropy between in-plane (ip) and through-plane (tp) results and a good agreement between simulated and measured values. See Becker et al[4] for more details

models to have 500^3 or even 1000^3 grid points.

Determinating the effective properties often requires to solve a partial differential equation. To determine the permeability, the flow of the fluid through the medium has to be simulated, i.e. Stokes' equation

$$-\mu\Delta u + \nabla p = 0, \quad \text{div}\ u = 0 \tag{1}$$

has to be solved in the pore space. The resulting velocity field u allows to determine the average velocity $\bar{u}$, which, together with Darcy's law

$$\bar{u} = -\frac{\kappa}{\mu}\nabla p \tag{2}$$

can be used to determine the permeability κ.

A similar approach can be used to determine the effective diffusivity. In this case the Laplace equation has to be solved in the pore space and Fick's first law is then used instead of Darcy's law to determine the diffusivity. Effective conductivity can be determined using the same ideas.

Solving (1) or other PDE's on the aforementioned huge voxel meshes is on the one hand demanding, but on the other hand the simplicity of the voxel mesh allows to reduce the amount of CPU time and memory extremely in comparison to more general finite element approaches. Therefore, GeoDict uses solvers developed specifically for large voxel meshes (e.g. the FFF-Stokes solver[5] or the EJ-Heat solver[6]) and thus allows to find the solution in reasonable time.

4. Fields of Application

Porous materials appear as natural materials like soil, sand and rock, wood or cellulose fibres and membranes. They also include artificially created media like fibrous filters, sintered ceramics or woven meshes. Analysis of porous materials and virtual material design is therefore often needed.

GeoDict and the methods described in the previous chapters have successfully been applied to a variety of problems. Gas diffusion layers of PEM fuel cells have been analyzed[4,7] and the results have been compared with measurements as shown in Fig 2. Furthermore, these tools were applied to predict the properties of metal wire meshes[3], to simulate the thermal conductivity of wood fibre networks[8] and of cast iron[9].

References

[1] A. Wiegmann. GeoDict virtual micro structure simulator and material property predictor. 2001–2010. http://www.geodict.com.

[2] K. Schladitz, S. Peters, D. Reinel-Bitzer, A. Wiegmann, and J. Ohser. Design of acoustic trim based on geometric modeling and flow simulation for non-woven. *Comp. Mat. Science*, 38(1):56–66, 2006.

[3] E. Glatt, S. Rief, A. Wiegmann, M. Knefel, and E. Wegenke. Struktur und Druckverlust realer und virtueller Drahtgewebe. *Filtrieren und Separieren*, 23(2):61–65, 2009.

[4] J. Becker, R. Flückiger, M. Reum, F.N. Büchi, F. Marone, and M. Stampanoni. Determination of material properties of gas diffusion layers - experiments and simulations using phase contrast tomographic microscopy. *J. Electrochem. Soc.*, 156:B1175–B1181, 2009.

[5] A. Wiegmann. Computation of the permeability of porous materials from their microstructure by FFF-Stokes. Technical Report 129, Fraunhofer ITWM Kaiserslautern, 2007.

[6] A. Wiegmann and A. Zemitis. EJ-HEAT: A fast explicit jump harmonic averaging solver for the effective heat conductivity of composite materials. Technical Report 94, Fraunhofer ITWM Kaiserslautern, 2006.

[7] A. Pfrang, D. Veyret, F. Sieker, and G. Tsotridis. X-ray computed tomography of gas diffusion layers of pem fuel cells: Calculation of thermal conductivity. *International Journal of Hydrogen Energy*, 35(8):3751 – 3757, 2010.

[8] H. Thoemen, T. Walther, and A. Wiegmann. 3d simulation of macroscopic heat and mass transfer properties from the microstructure of wood fibre networks. *Composites Science and Technology*, 68:608–616, 2007.

[9] A. Velichko, A. Wiegmann, and F. Mücklich. Estimation of the effective conductivities of complex cast iron microstructures using FIB-tomographic analysis. *Acta Materialia*, 57: 5023–5035, 2009.