Numerical Determination of Transport Properties of Catalyst Layer, Micro-porous Layer and Gas Diffusion Layer

Jürgen Becker, Math2Market GmbH, Kaiserslautern

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- M2M was founded in Sep. 2011 by 3 developers of the GeoDict software.
- M2M has aquired all rights for marketing and developing GeoDict from Fraunhofer.
- M2M is located in the „Innovationszentrum Westpfalz“ at Kaiserslautern.
- Close cooperation with Fraunhofer ITWM.

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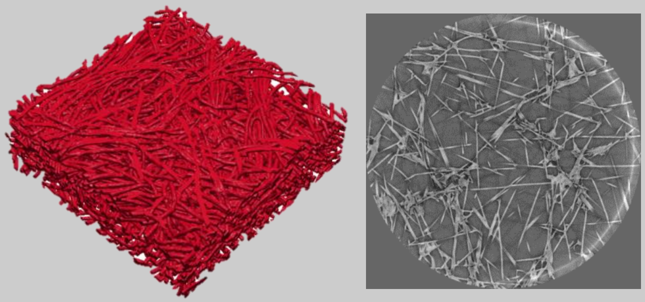
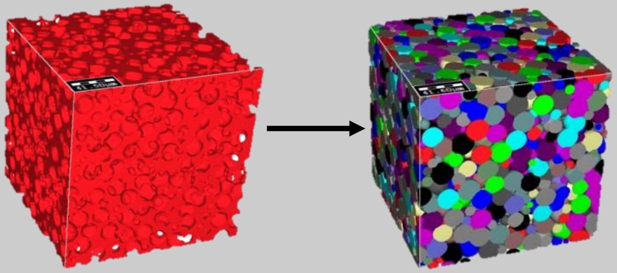
GeoDict: The Virtual Material Laboratory ...

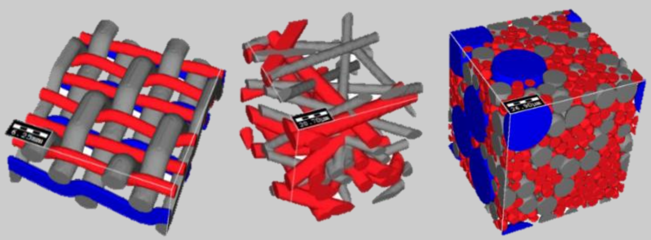
Import



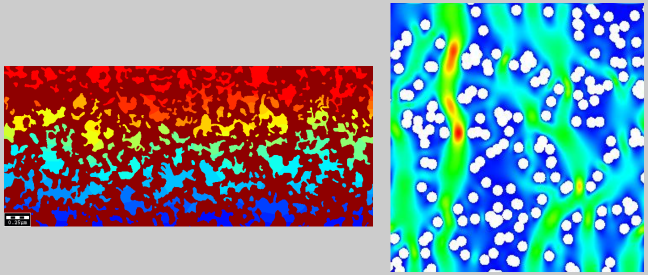
Analyze Geometry



Create



Determine Properties



... Applied to Porous Transport Layers of PEFC

1. Determine Transport Properties from 3D Images
   a. GDL Analysis Based on Tomography Image
   b. Catalyst Layer Model Based on FIBSEM Images

2. Create 3D Structure Models Virtually
   a. GDL Model: Fibers, Binder, Compression
   b. MPL Design Study

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1. Determine Transport Properties from 3D Images

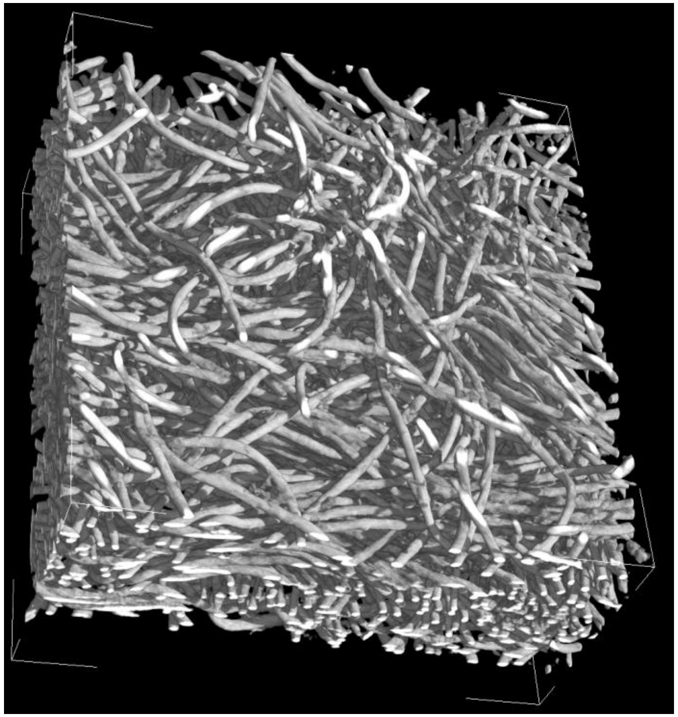
a. GDL Analysis Based on Tomography Image

Tomography Image

Input: tomography image

- Carbon fibres of diameter ~ 7 μm
- Hydrophobic PTFE coating
- Porosity 78%
- Layer thickness ~ 200 μm

- Picture shows area of size 717x717 μm
- Resolution: 0.7 μm/voxel



Aim:

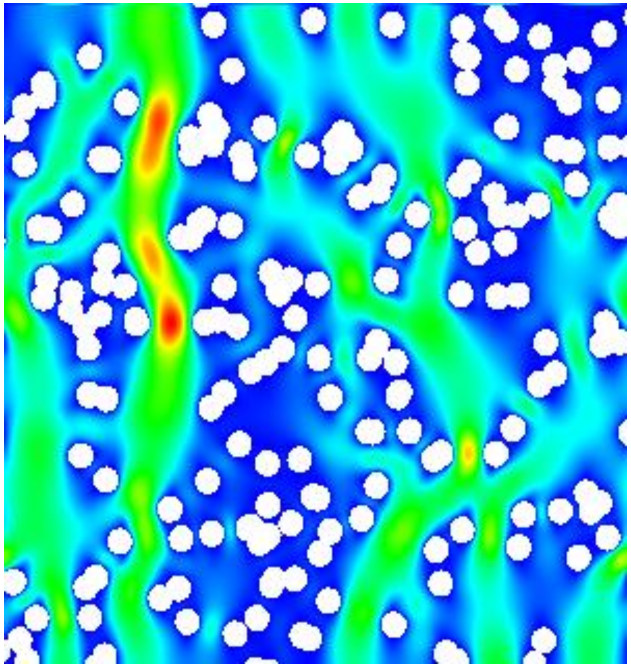
- Find capillary pressure curve, relative permeability, relative diffusivity

Permeability

Macroscopic description
(homogenized porous media model)

Darcy's law : $u = -\frac{1}{\mu} \kappa \nabla p$

u : average flow velocity
κ : permeability tensor ***unknown***
μ : viscosity
p : pressure



Microscopic description
(pore structure model)

Stokes equation: $-\mu \Delta u + \nabla p = 0$

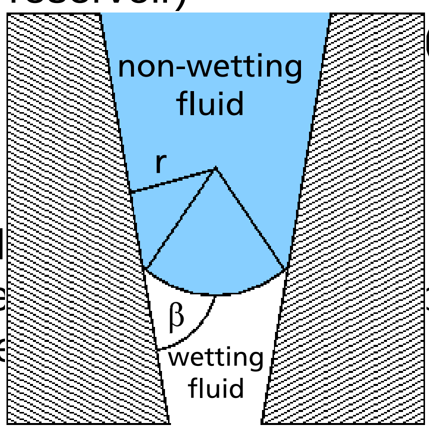
Boundary conditions: no-slip on fibre surface, pressure drop
κ can be determined from the solution!

Relative Permeability

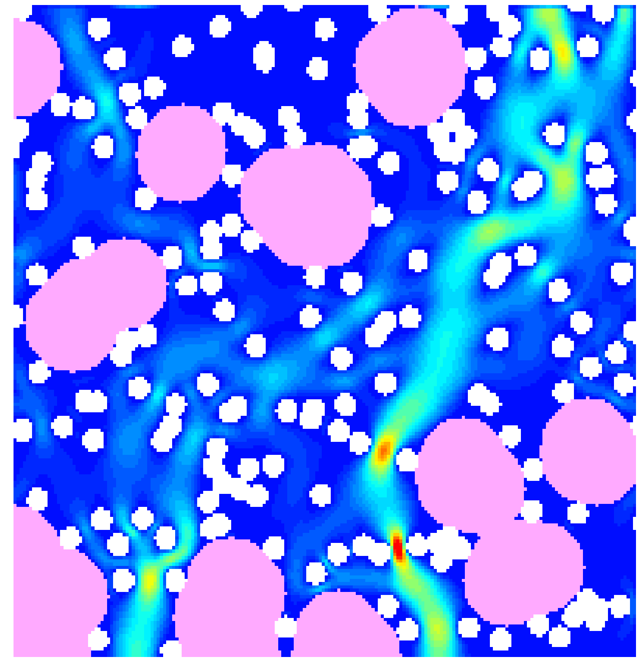
Two-step approach:

1. Use pore morphology method (Hilpert, 2001) to determine distribution of air and water phase.

- Idea: a pore is filled with the non-wetting fluid (=water), if $p_c \geq \frac{2\sigma}{r}\cos\beta$
- Drainage and imbibition (connectivity to reservoir)
- (connectivity of pores)



2. Sol the remaining pore space phase (=air) perme



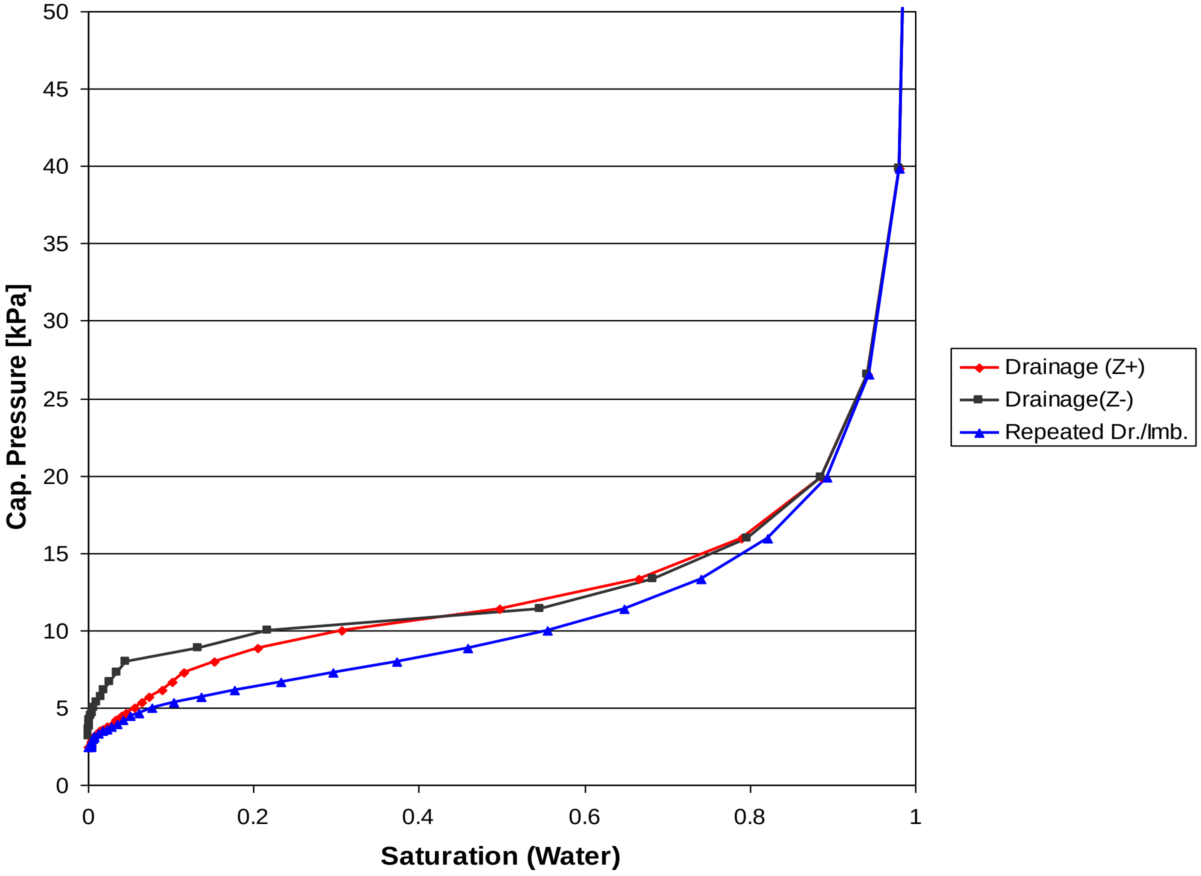
Capillary Pressure Curve

Parameters:

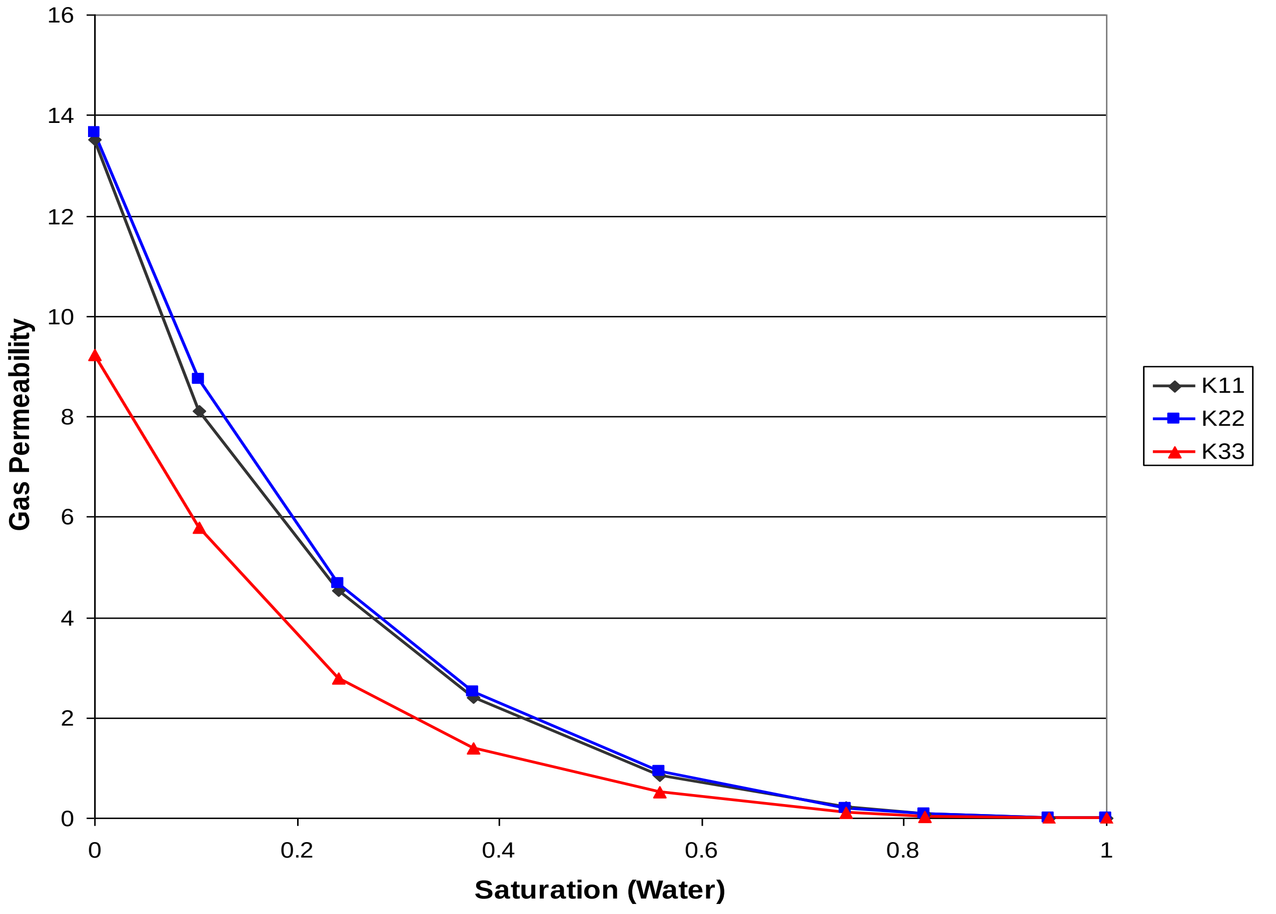
- Contact angle: 140

Results:

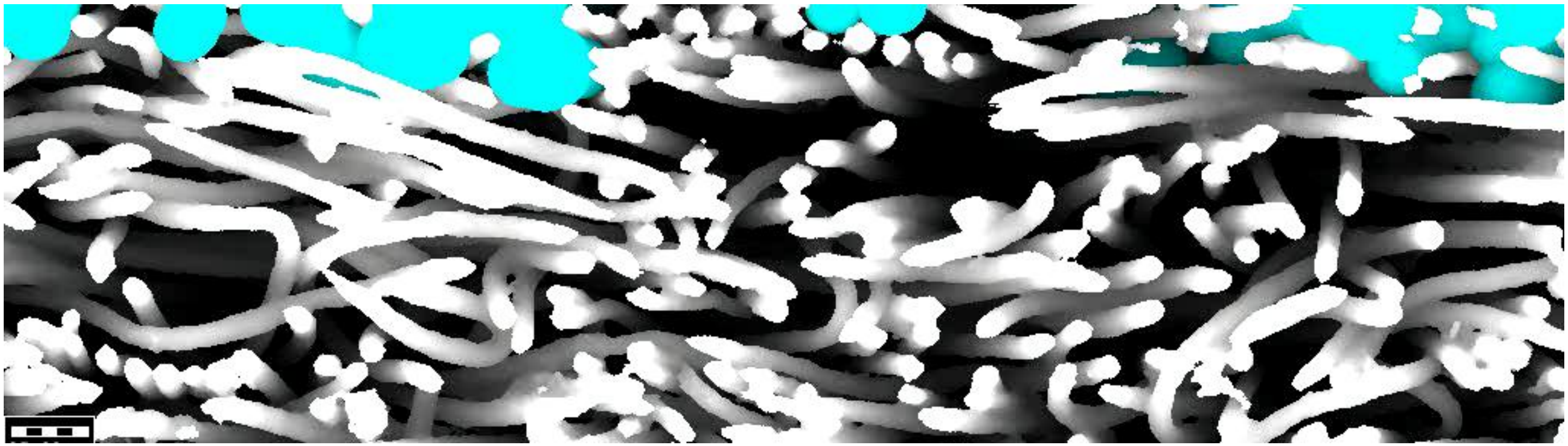
- Bubble point (drainage): 8.8 kPa
- Saturation at bubble point: 20.8%



Relative Permeability



Water Distribution at Bubble Point



p = 10.6 kPa   (r=10.5 mm)

1. Determine Transport Properties from 3D Images

b. Catalyst Layer Model Based on FIBSEM Images

i. Reconstruction
ii. Simulations on 3D data

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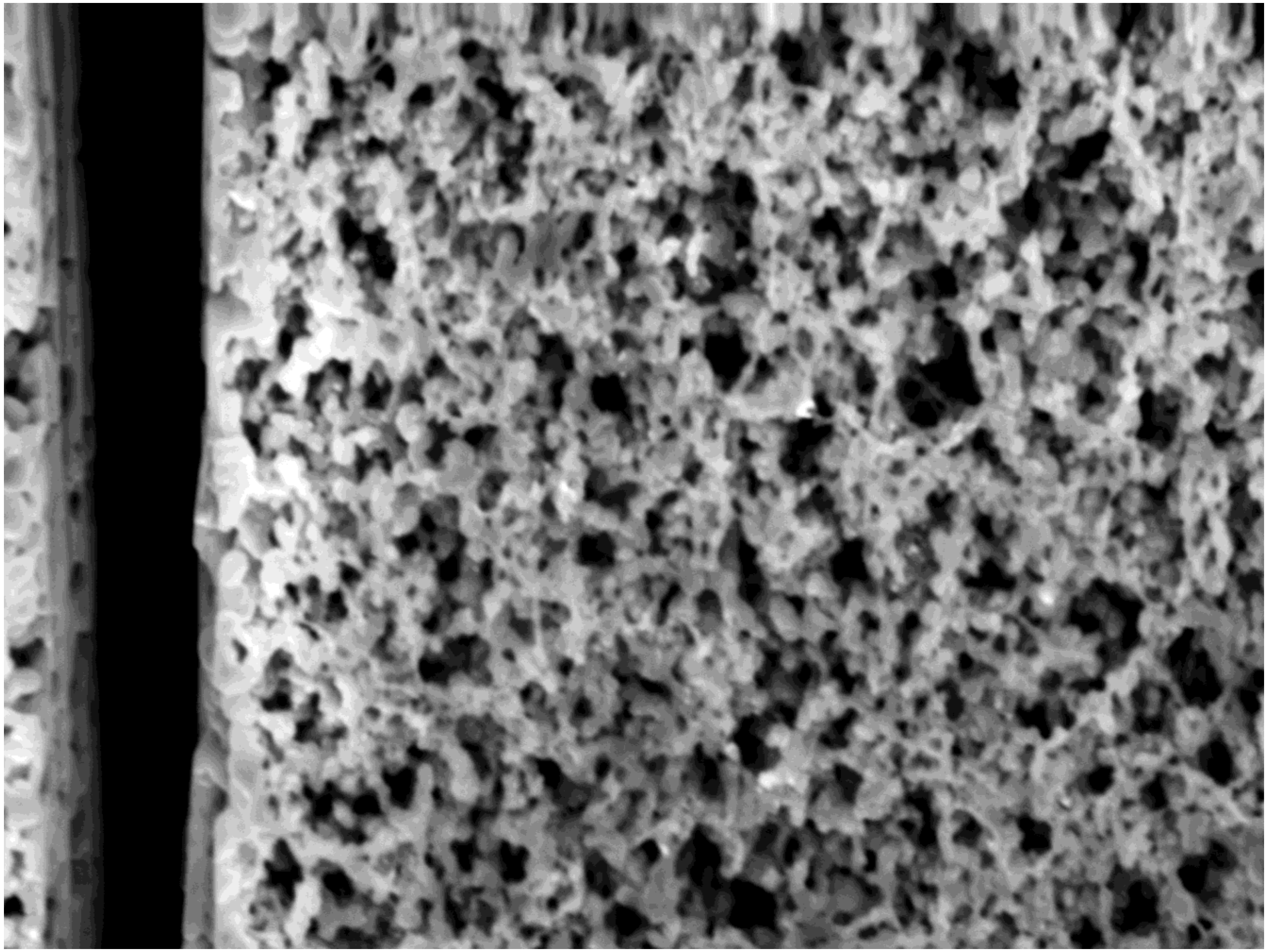
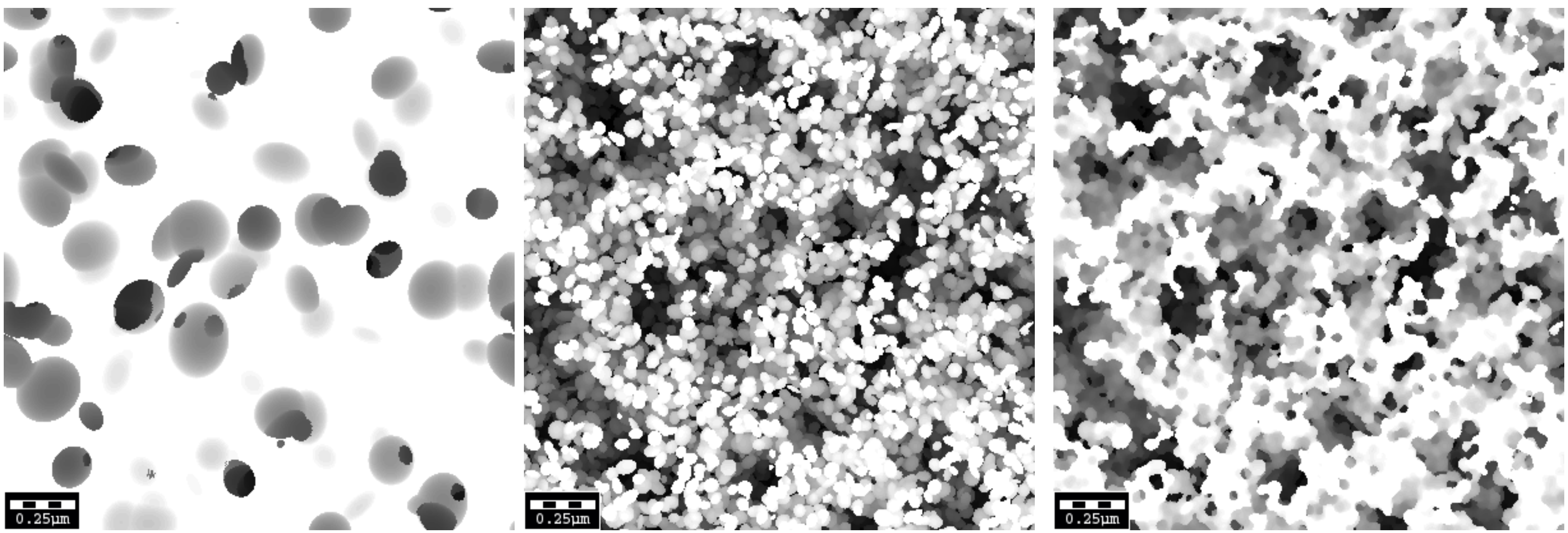
i. Reconstruction from SEM Images

SEM by IMTEK,
Uni Freiburg

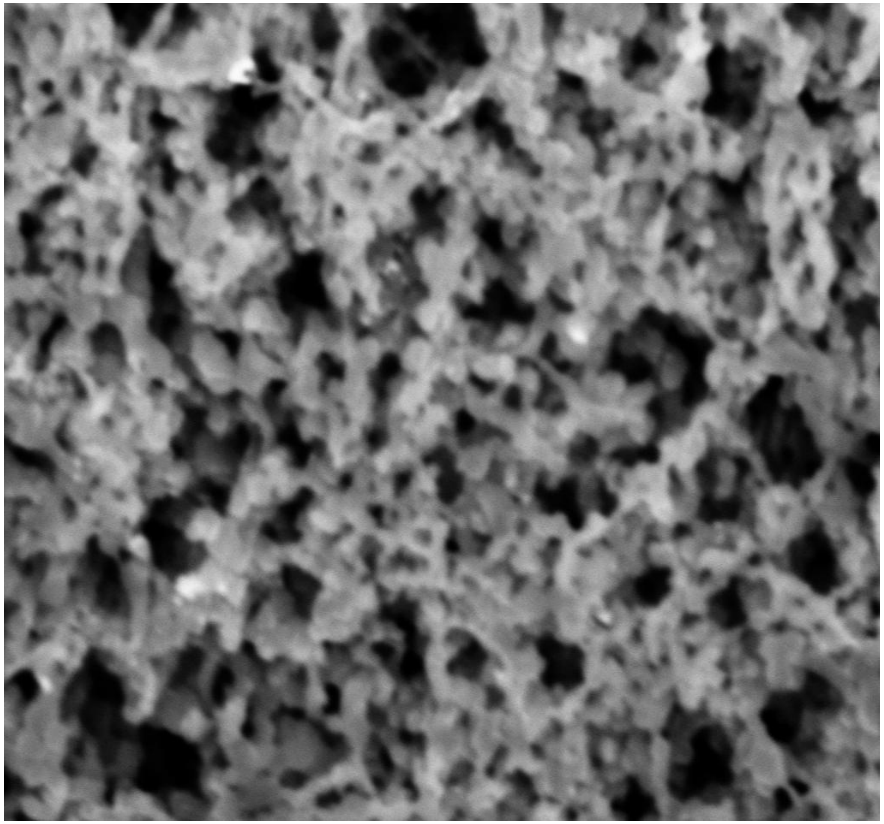


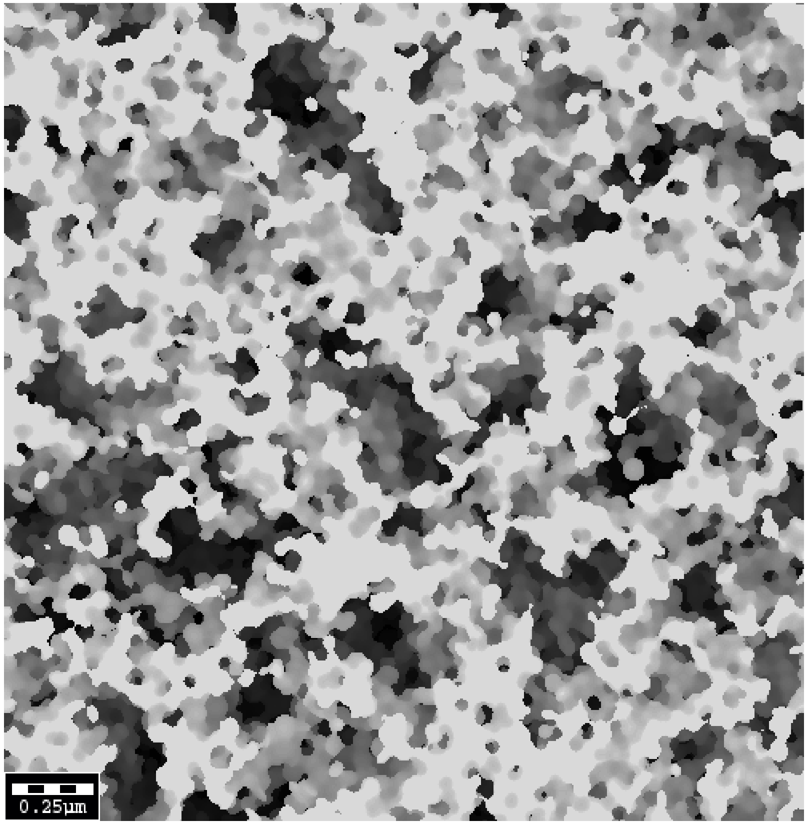
Reconstruction Algorithm

1. Place holes randomly
2. Place particles randomly (not inside holes)
3. Fill small pores between particles

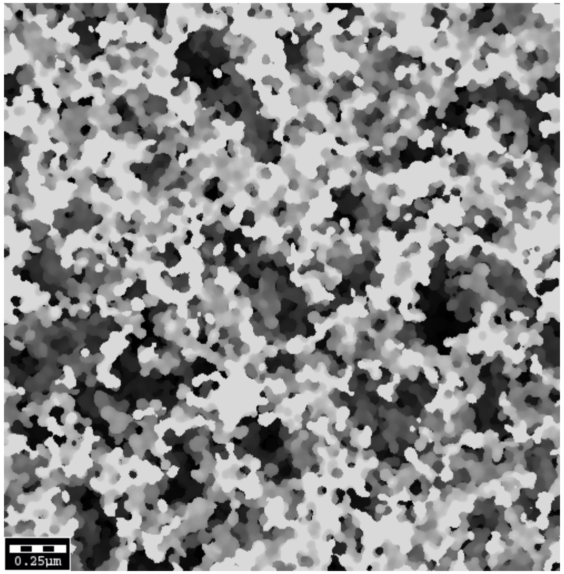


Optical Comparison

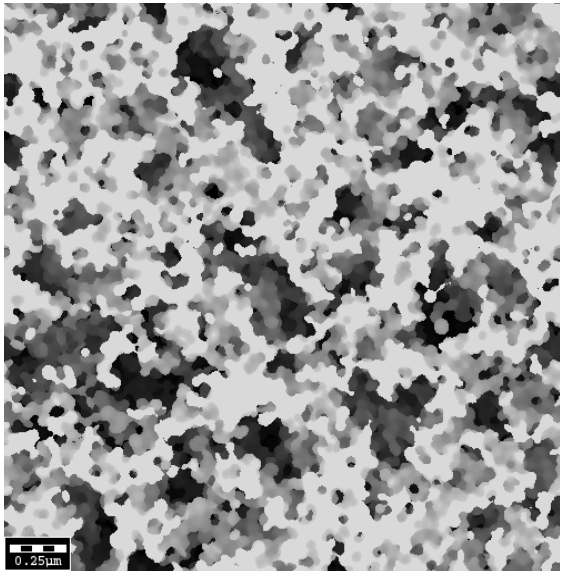




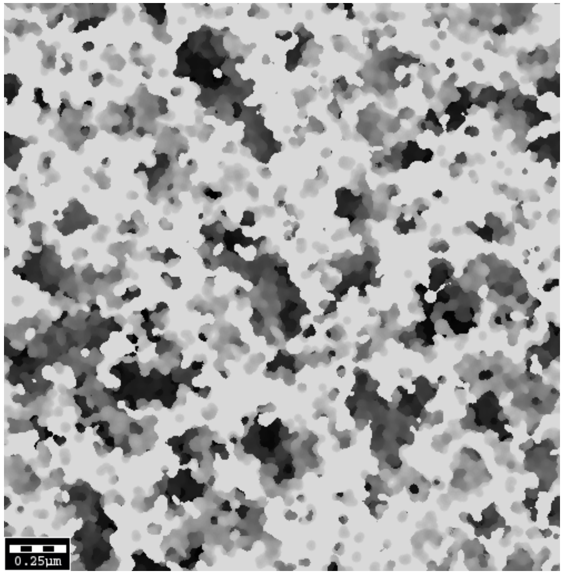
Variation of Porosity



73%



65%



57%

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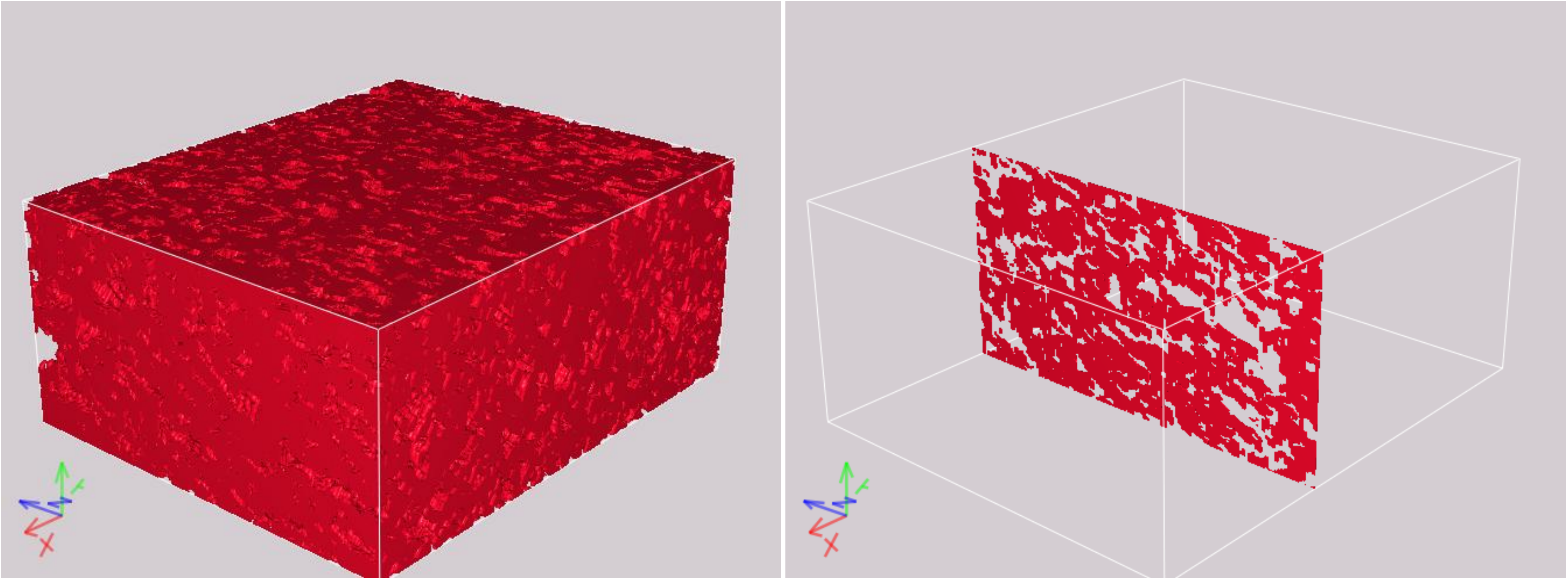
Conductivity and Diffusivity

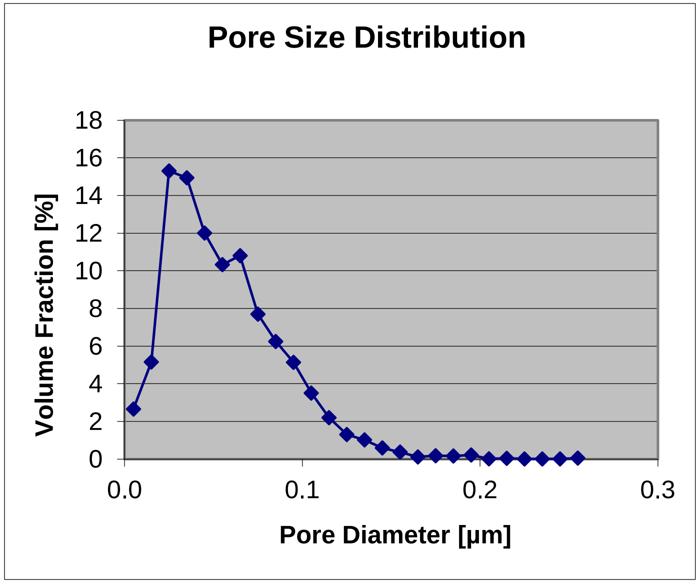
Porosity	Relative Diffusivity	Relative Conductivity
73 %	51.8 %	7.1 %
65 %	38.1 %	13.4 %
57 %	25.6 %	21.1 %

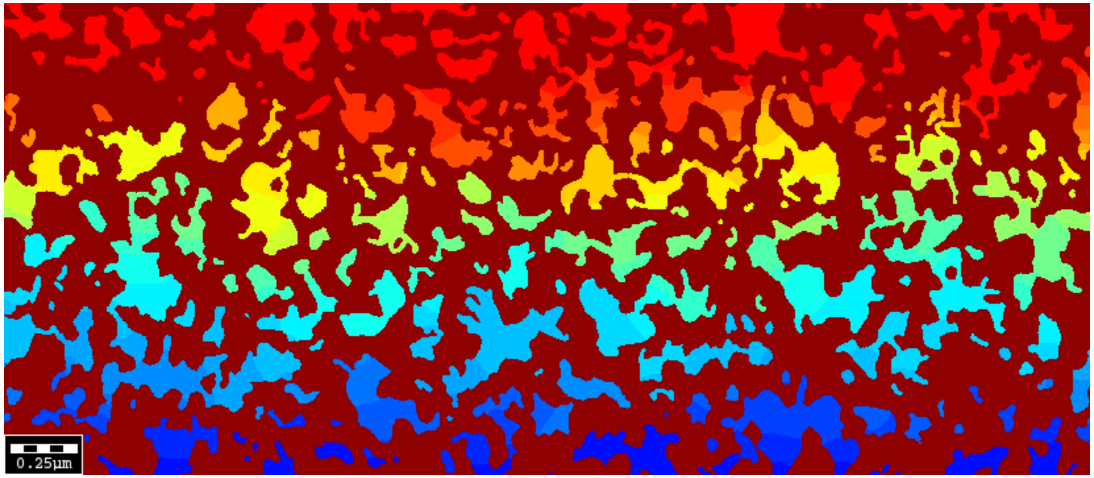
ii. Simulations on 3D FIBSEM Data

- Pore Structure obtained from FIBSEM Data (IMTEK, Uni Freiburg)
- Cannot distinguish between Ionomer and Carbon



Results





Concentration field from diffusion simulations

Determine:

- Pore size distribution, diffusivity

T. Hutzenlaub, J. Becker, R. Zengerle und S. Thiele, Modelling the water distribution within a hydrophilic and hydrophobic 3D reconstructed cathode catalyst layer of a PEMFC, J. Power Sources 227, pp 260-266, 2013.

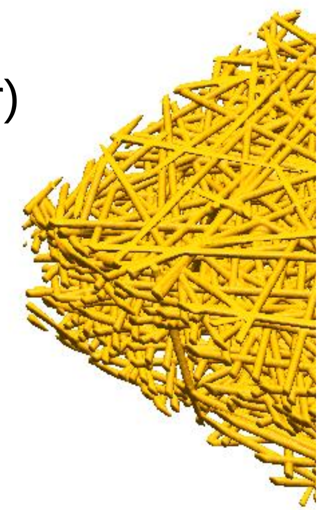
2. Create 3D Structure Models Virtually

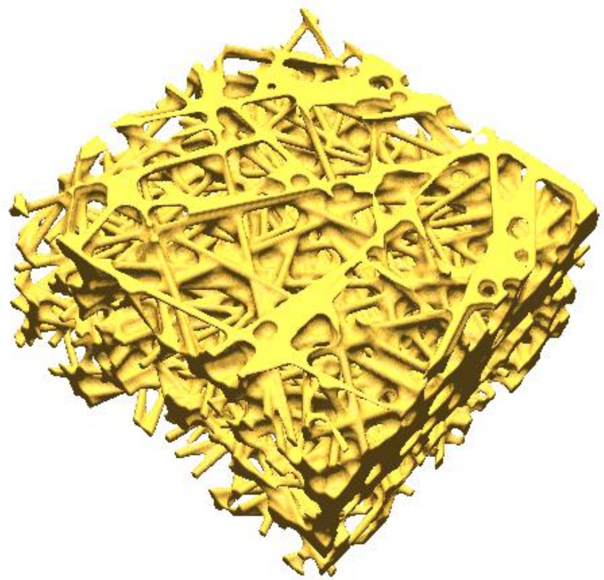
a. GDL Model: Fibers, Binder and Compression

Gas Diffusion Layer Model

Created with a stochastic process

Input:
- Porosity
- Fiber diameter and type
- Anisotropy
- (Fiber crimp)
- (Weight% binder)





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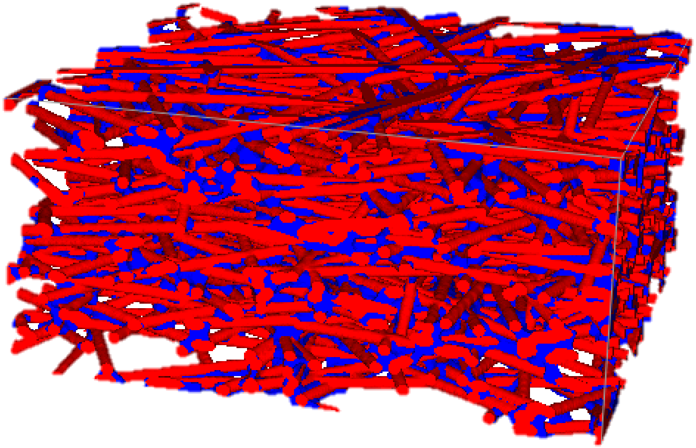
Compression

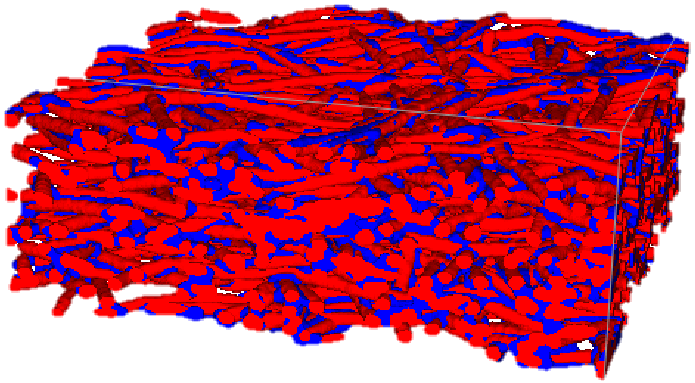
Aim: how does the structure change due to clamping pressure?

Current development together with Fraunhofer

- transverse isotropic elastic modulus for fibers
- isotropic elastic modulus for binder
- 30% compression



10 min on Laptop
13.5 mio grid points



2. Create 3D Structure Models Virtually

b. MPL Design Study

MPL Design Study

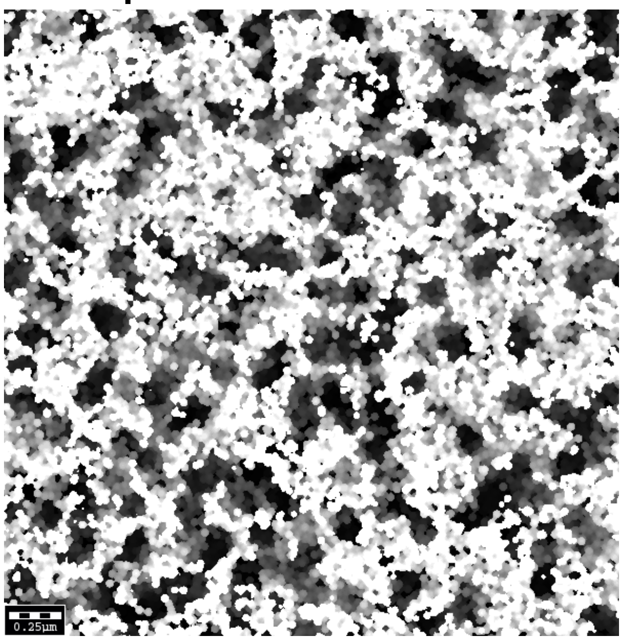
- Step 1: Create model of MPL structure, determine effective parameters for MPL alone
- Step 2: Create model for GDL+MPL, determine diffusivity and conductivity of combined layer
- Step 3: What changes when we change MPL design parameters?

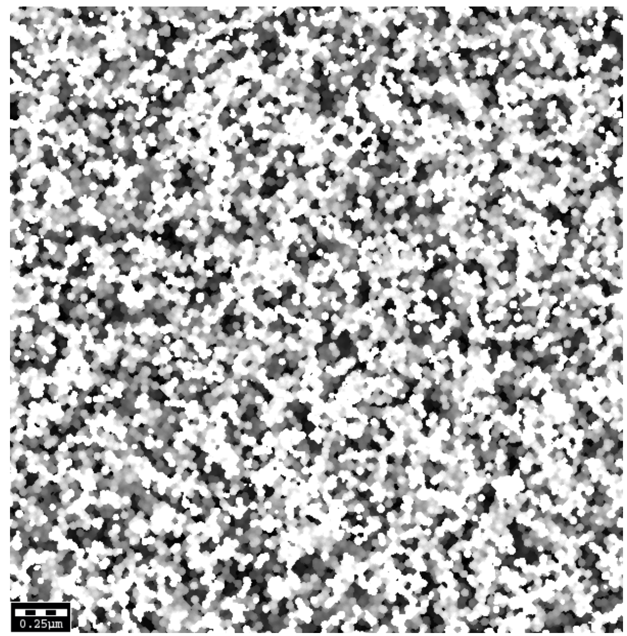
Zamel, Becker, Wiegmann, J. Power Sources 207, 2012.

Comparison of Different MPL

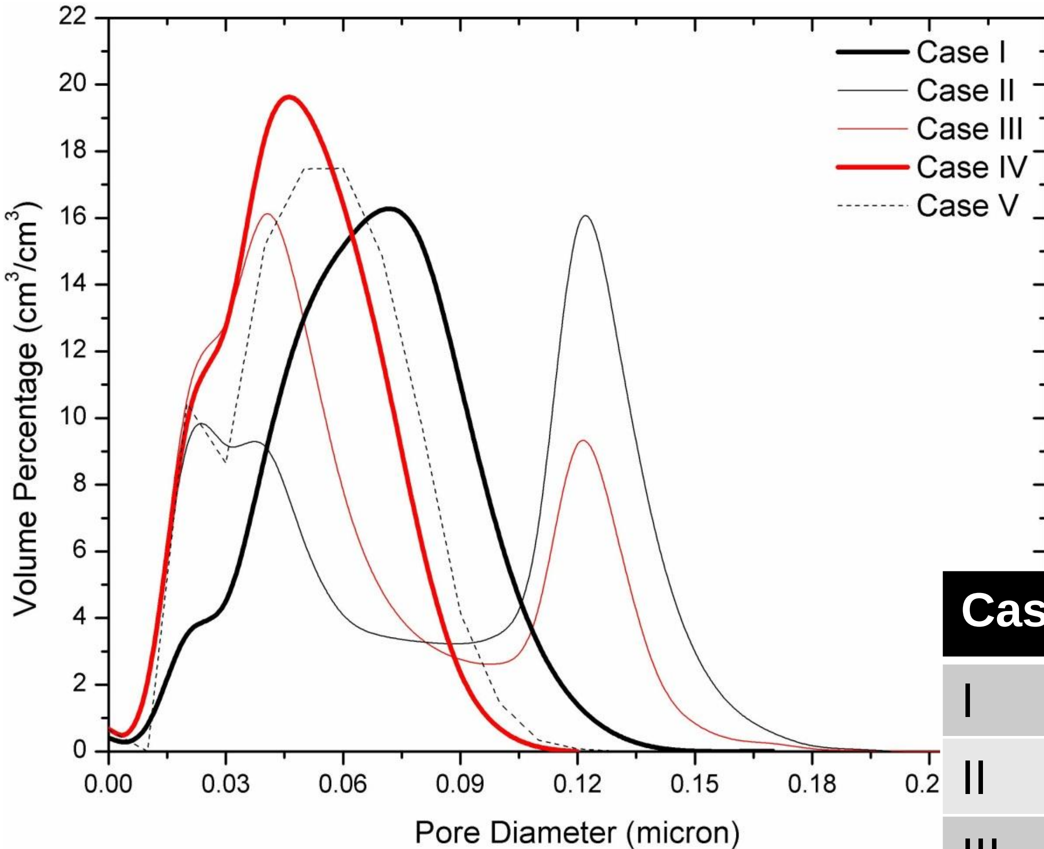
Create MPLs with

- same porosity & carbon particle sizes
- different pore size distributions





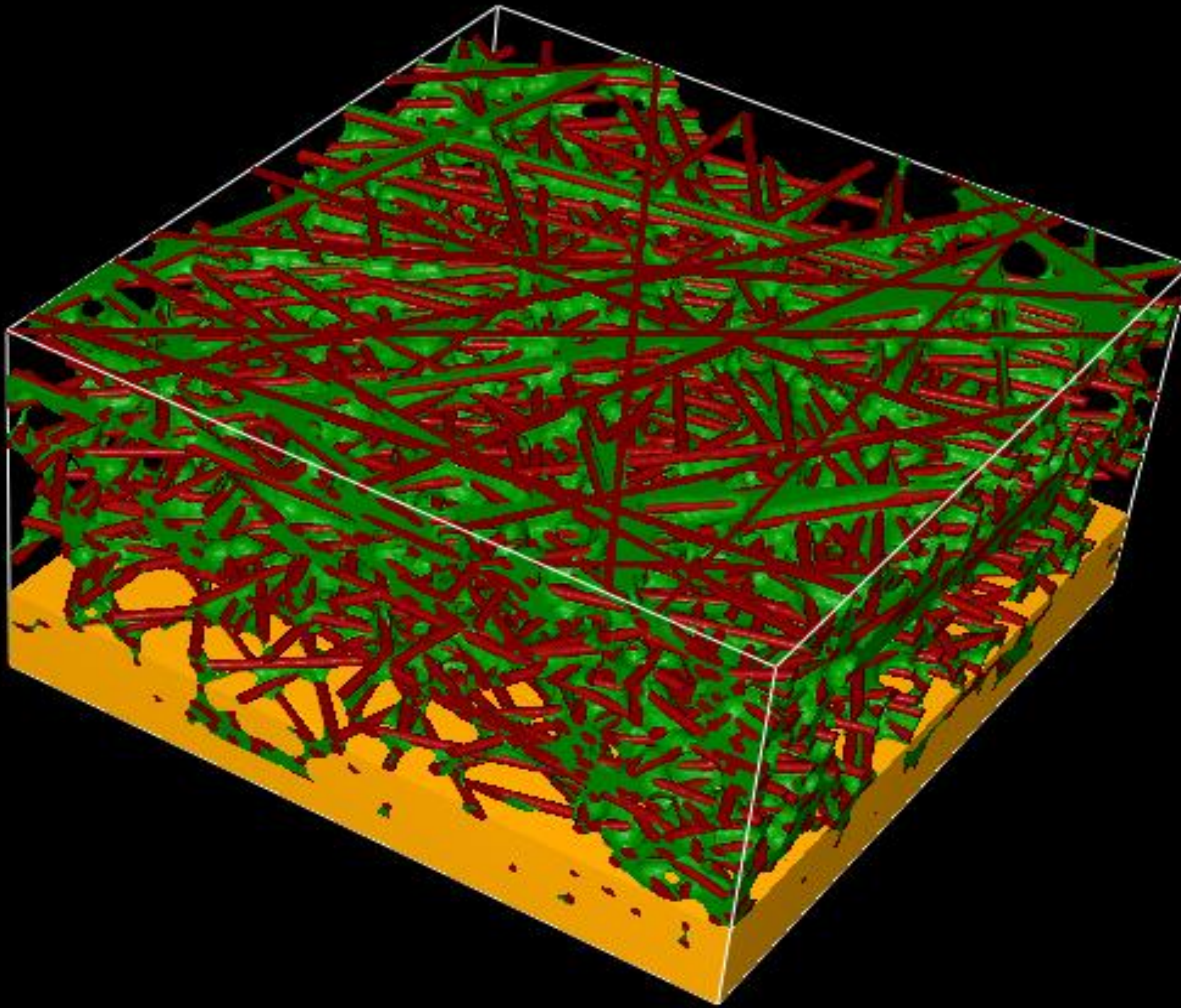
Comparison of Different MPL



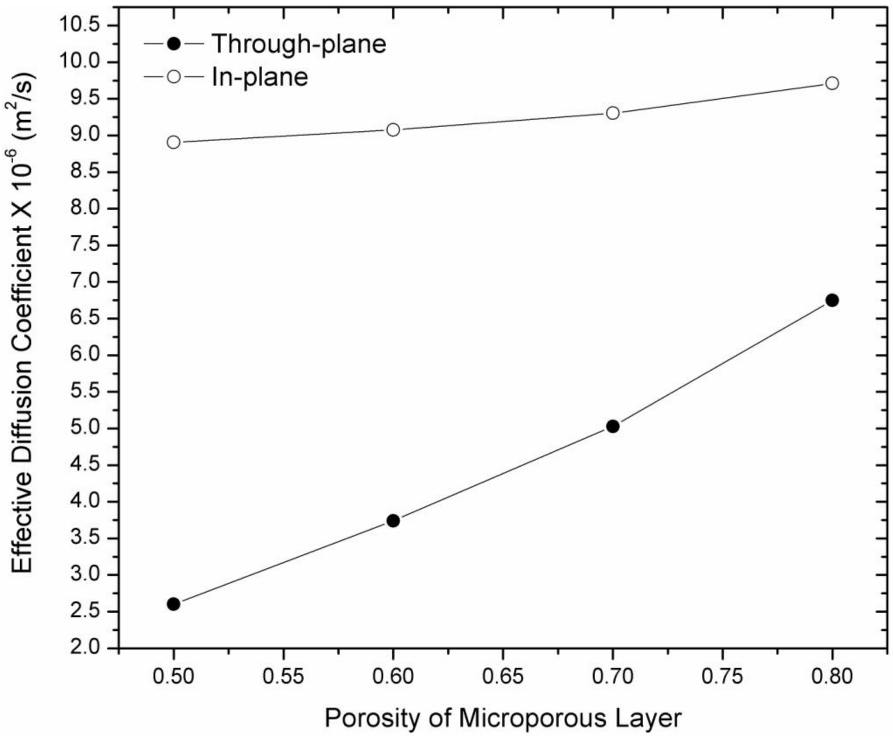
Diffusivity:
Becker, Wieser, Fell, Steiner, Int. J. Heat and Mass Transfer 54, 2011.

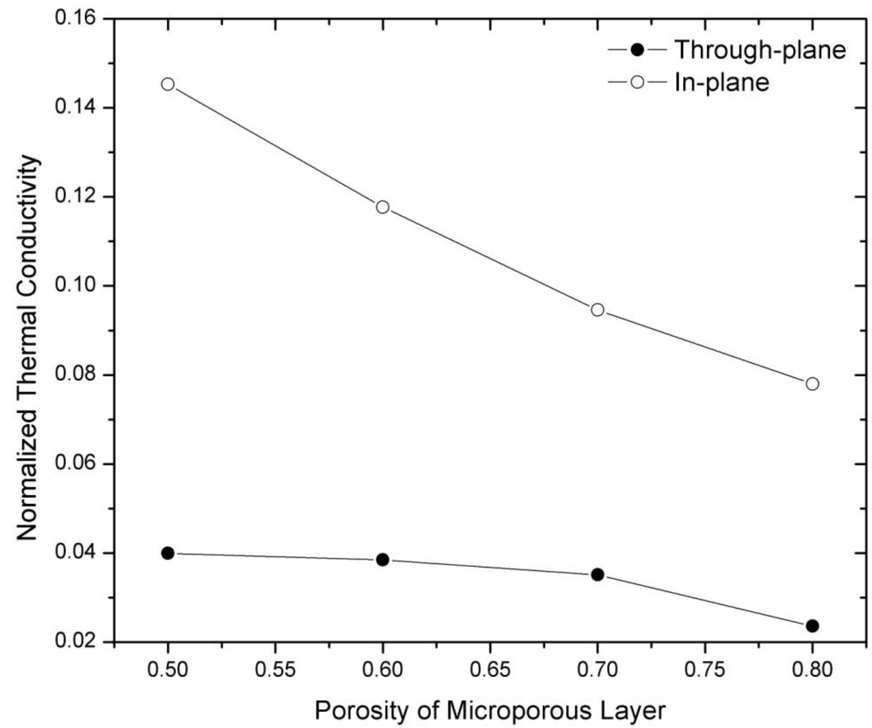
Conductivity:
Wiegmann, Zemitis, Tech Report 94, ITWM, 2006.

Case	Conductivity	Diffusivity
I	0.094	1.92
II	0.120	1.78
III	0.104	1.65
IV	0.092	1.59
V	0.095	1.67



Variation of MPL Porosity





Summary: Material Properties

GDL:
- (saturation dependent) diffusivity, (saturation dependent) permeability, electric conductivity, heat conductivity
- pore size distribution, capillary pressure

MPL:
- (Knudsen) diffusivity, electric conductivity, heat conductivity
- pore size distribution

CL:
- pore size distribution, surface or contact areas, contact lines
- protonic conductivity, electronic conductivity, (Knudsen) diffusivity

Caveat: Results cannot be better than the 3D structure model permits.

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Thank You !

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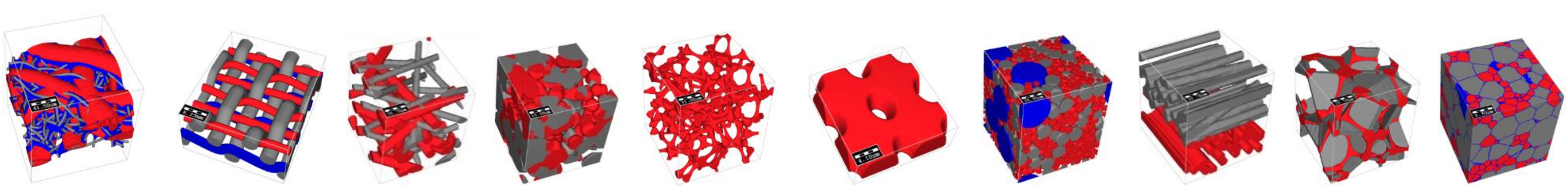
www.geodict.com



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