Computer Based Design Study of Porous Transport Layers of PEFC

ModVal 2012, Sursee

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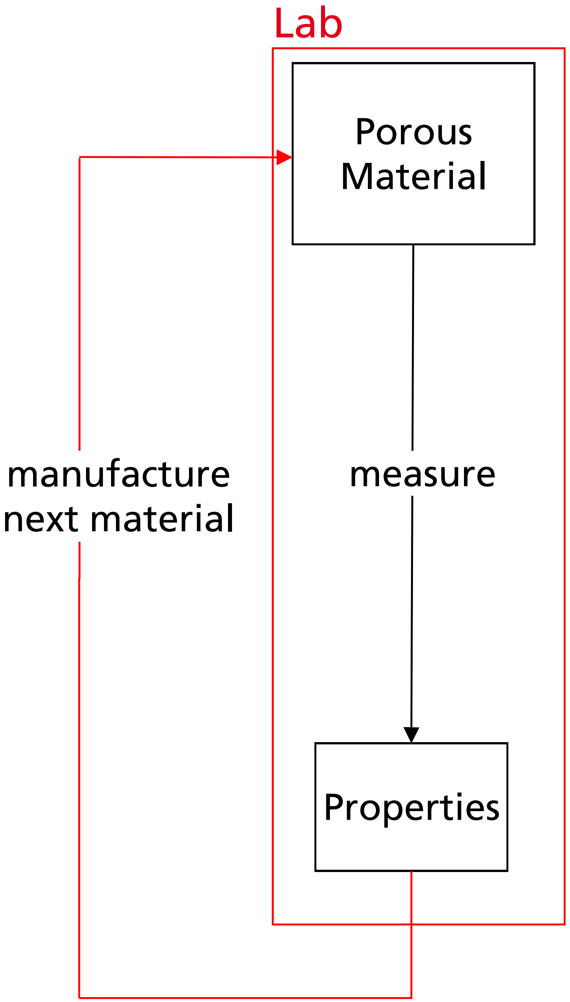
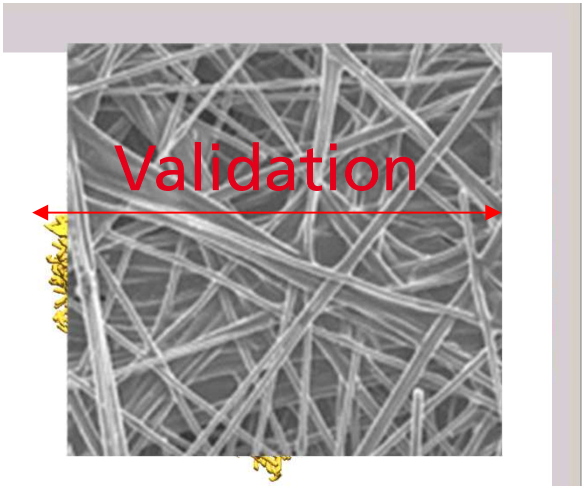
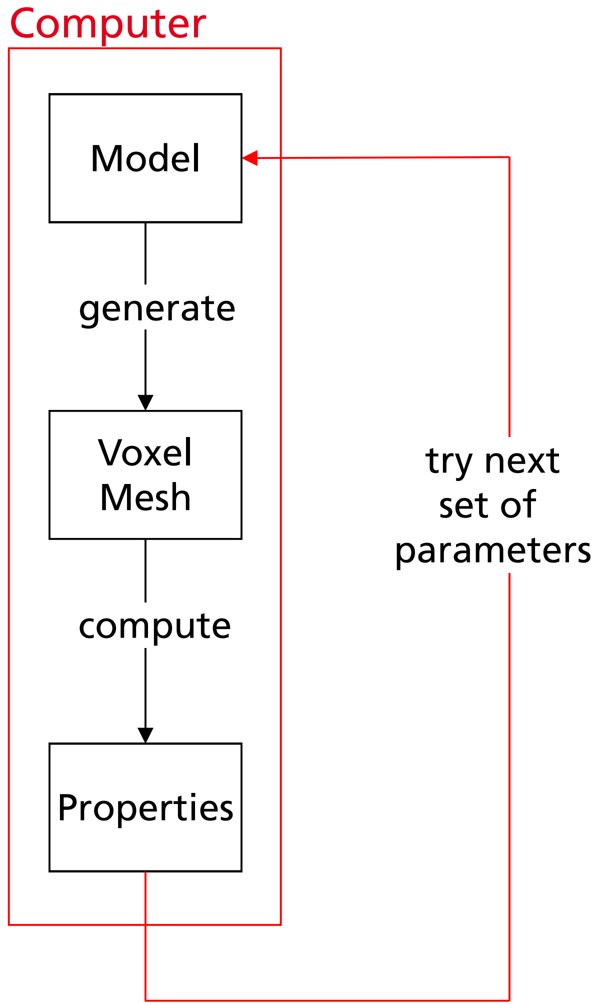
The General Approach: Computer Aided Material Engineering



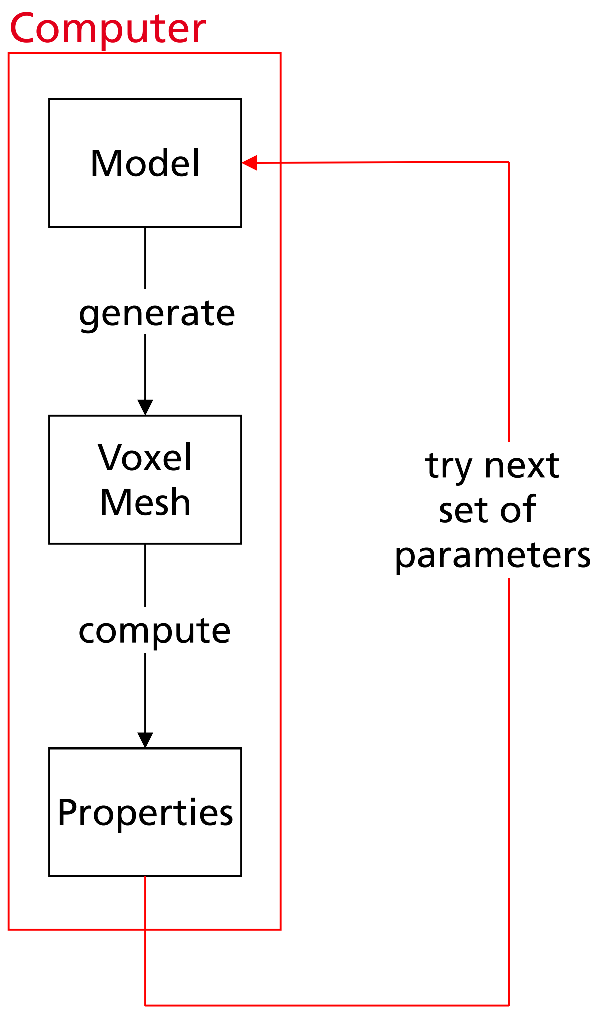


Properties are:
- pore size distribution
- permeability
- diffusivity
- capillary pressure curve
- ...



Overview

1. 3D structure model
2. Property computations
3. Parameter study
   - GDL
   - MPL



3D Models: Gas Diffusion Layer (GDL)

Nonwoven fibres

Input:
- Porosity
- Fibre diameter and type
- Anisotropy

Agorithm:
- Poisson line process

- Production process not modeled

3D Models: Gas Diffusion Layer (GDL)

Nonwoven fibres (entangled)

Input:
- Porosity
- Fibre diameter and type
- Anisotropy

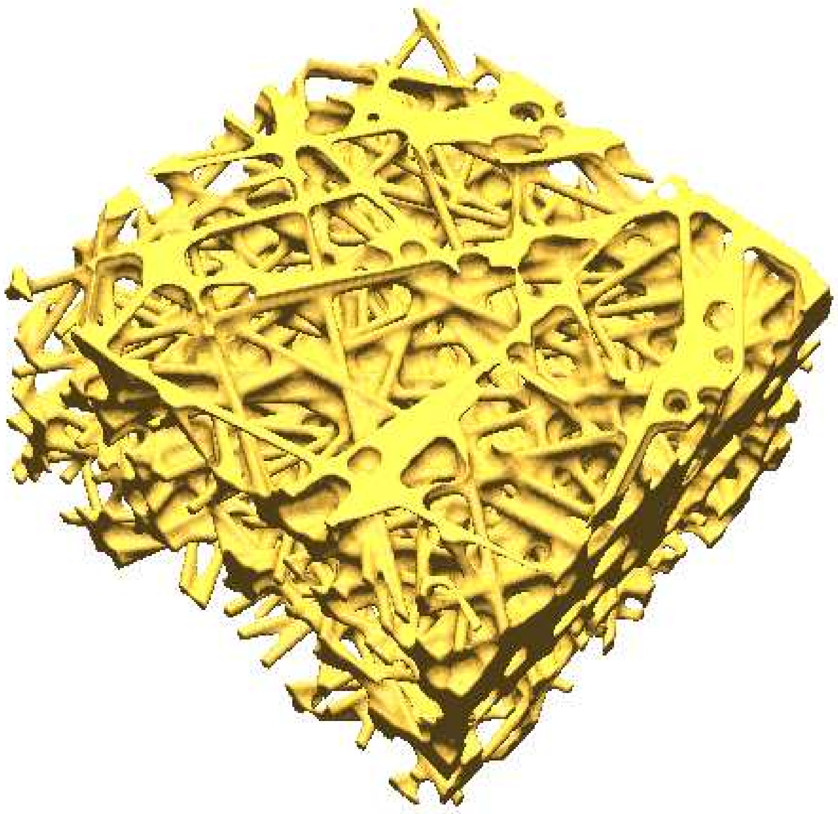
- Fibre crimp

3D Models: Gas Diffusion Layer (GDL)

Nonwoven fibres plus binder

Input:
- Porosity
- Fibre diameter and type
- Anisotropy

- Weight% binder

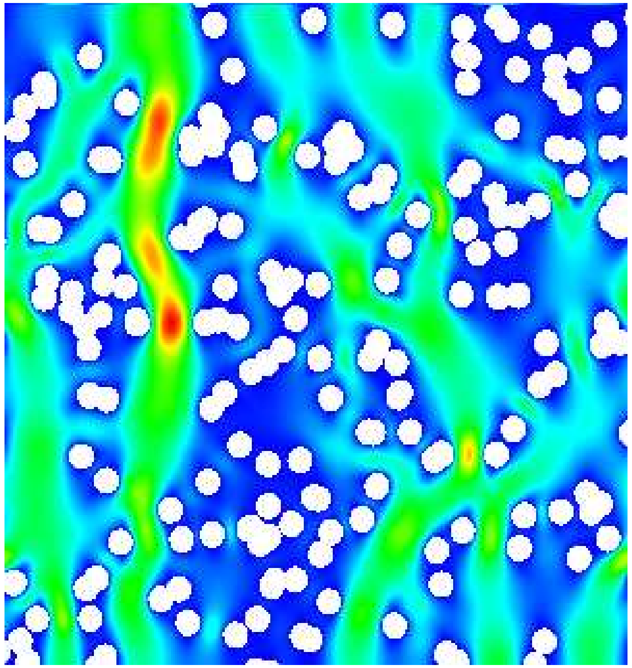


Permeability

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!

Diffusivity

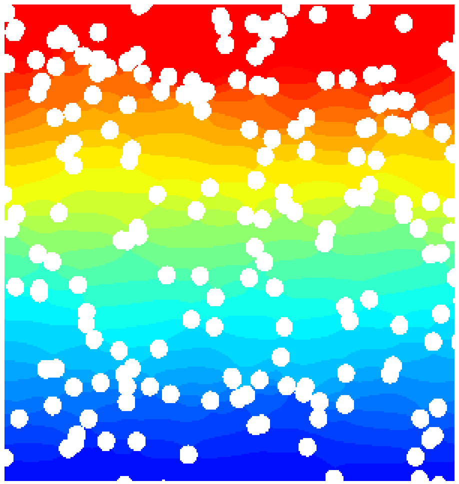
Macroscopic description
(homogenized porous media model)
Fick's first law: $j = -D^* \nabla c$

D^* : effective diffusivity [m²/s] ***unknown***
j : diffusion flux [mol/m²/s]
c : concentration [mol/m³]

Microscopic description (pore structure model)
Laplace equation: $-\Delta c = 0$

Boundary conditions: no-flux on fibre surface, concentration drop

D^* can be determined from the solution!



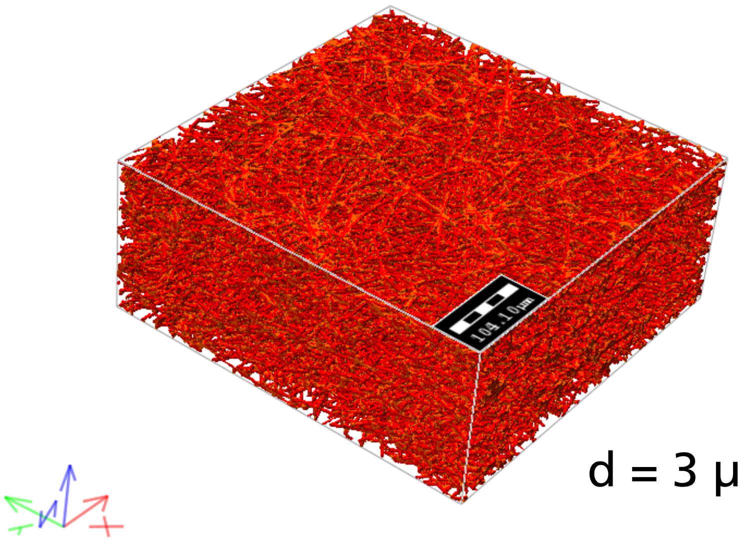
GDL Design Study

1. Create 3D structure with X vol% fibers with diameter X µm
2. Add binder until X wt% is reached

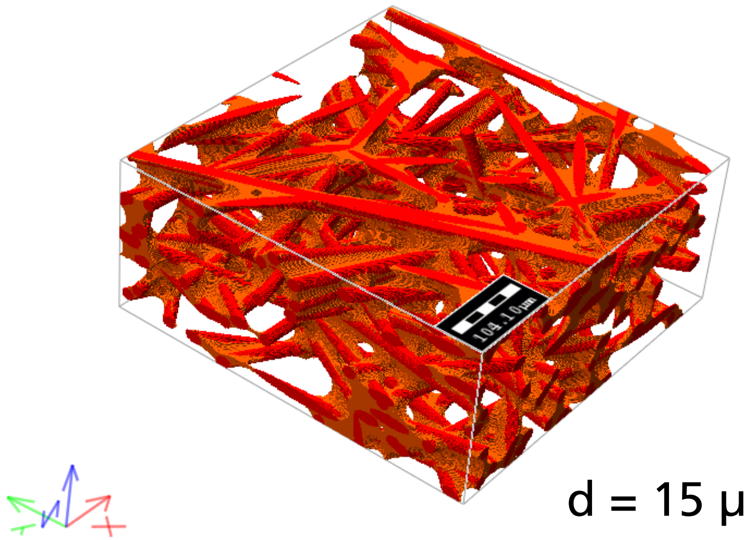
3. Determine in-plane and through-plane diffusivity and permeability

Fiber Diameter

- 12 vol% fibers
- binder content 40 wt%   (leads to porosity 80%)

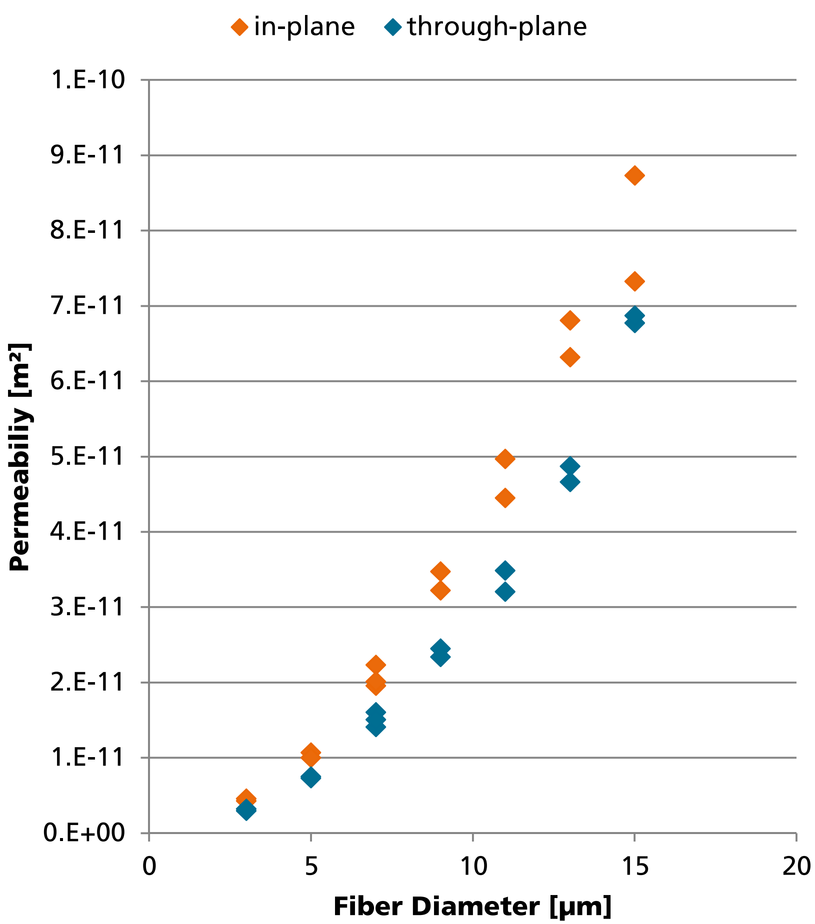


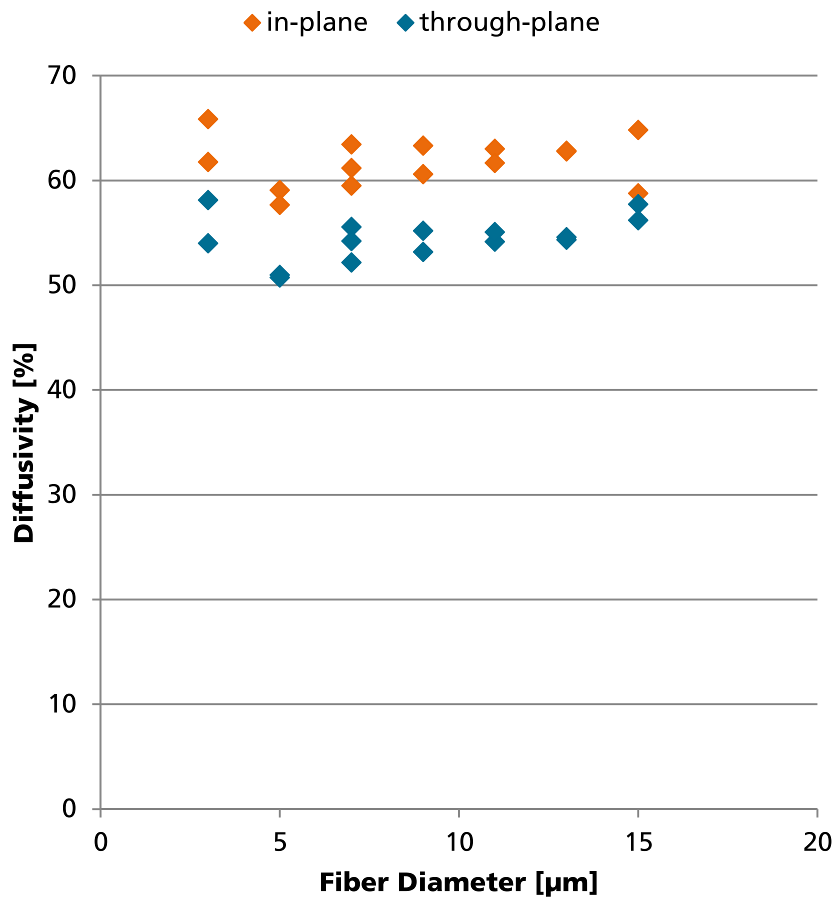
d = 3 µm



d = 15 µm

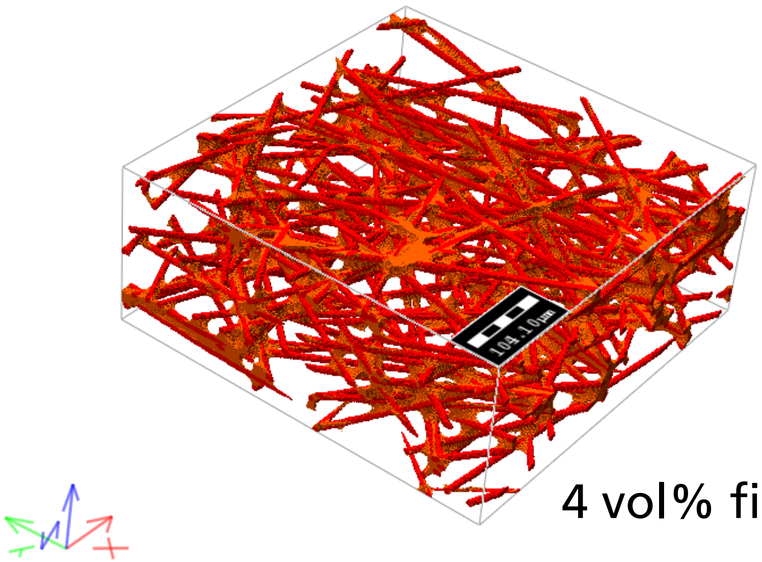
Fiber Diameter



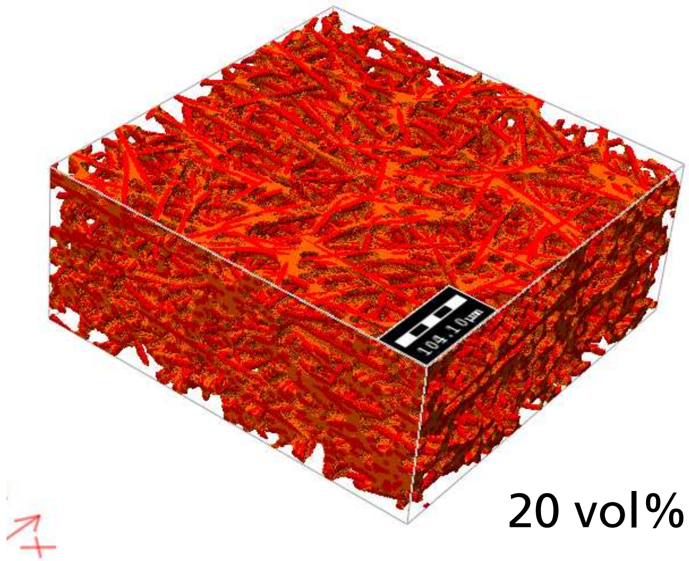


Porosity

- 7 µm fiber diameter
- 40 wt% binder content

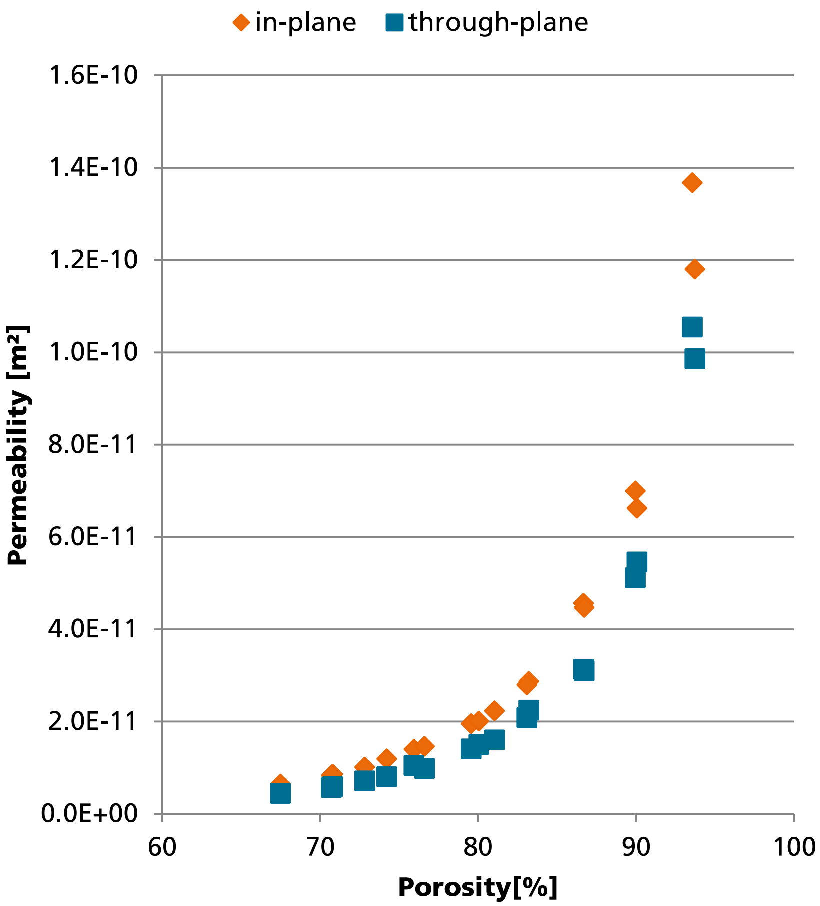


4 vol% fibers

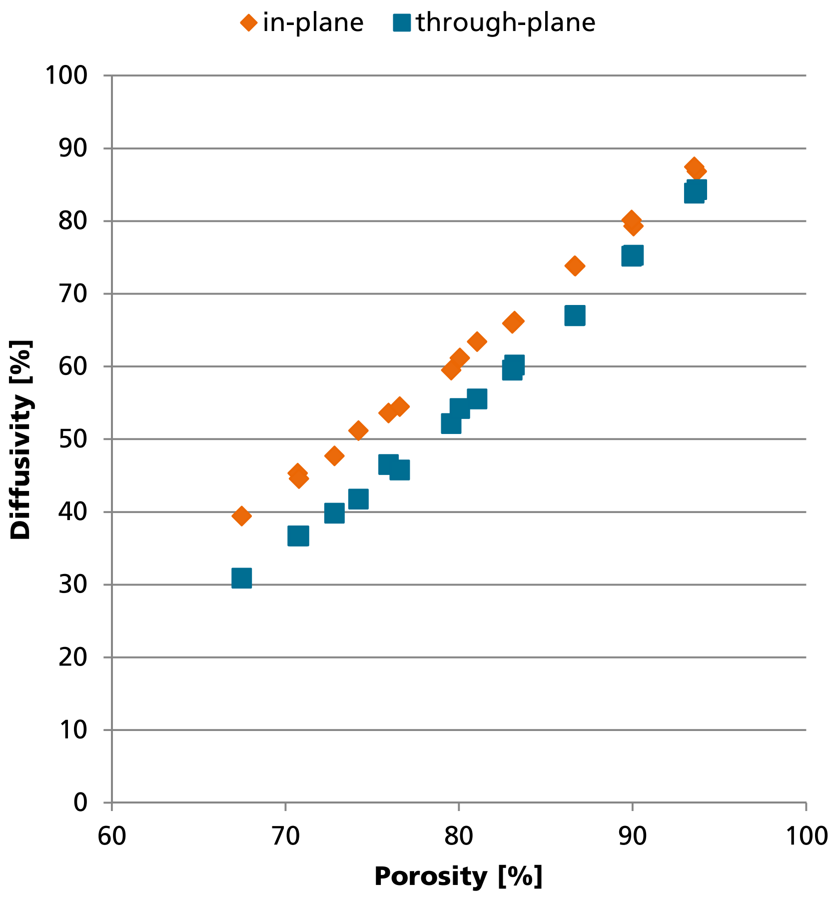


20 vol% fibers

Porosity



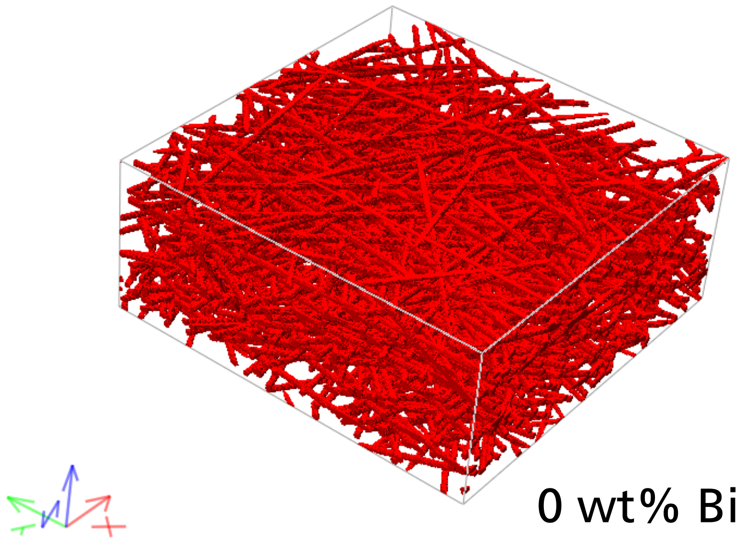
in-plane
through-plane
1.6E-10
1.4E-10
1.2E-10
1.0E-10
8.0E-11
6.0E-11
4.0E-11
2.0E-11
0.0E+00
Permeability [m²]
60
70
80
90
100
Porosity[%]



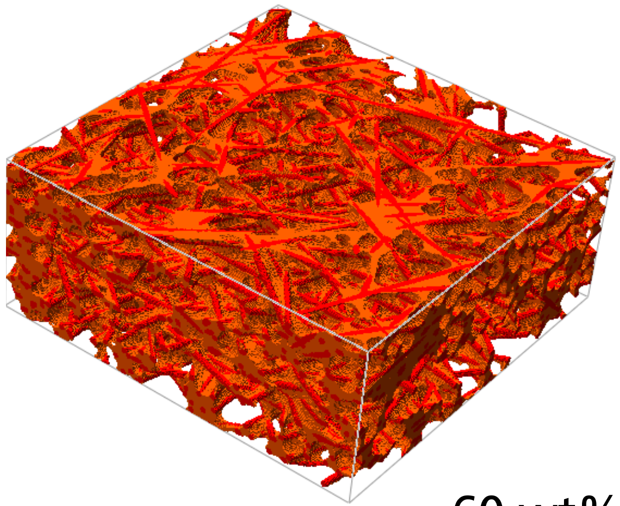
in-plane
through-plane
100
90
80
70
60
50
40
30
20
10
0
Diffusivity [%]
60
70
80
90
100
Porosity [%]

Binder content

- 7 µm fiber diameter
- 12 vol% fibers

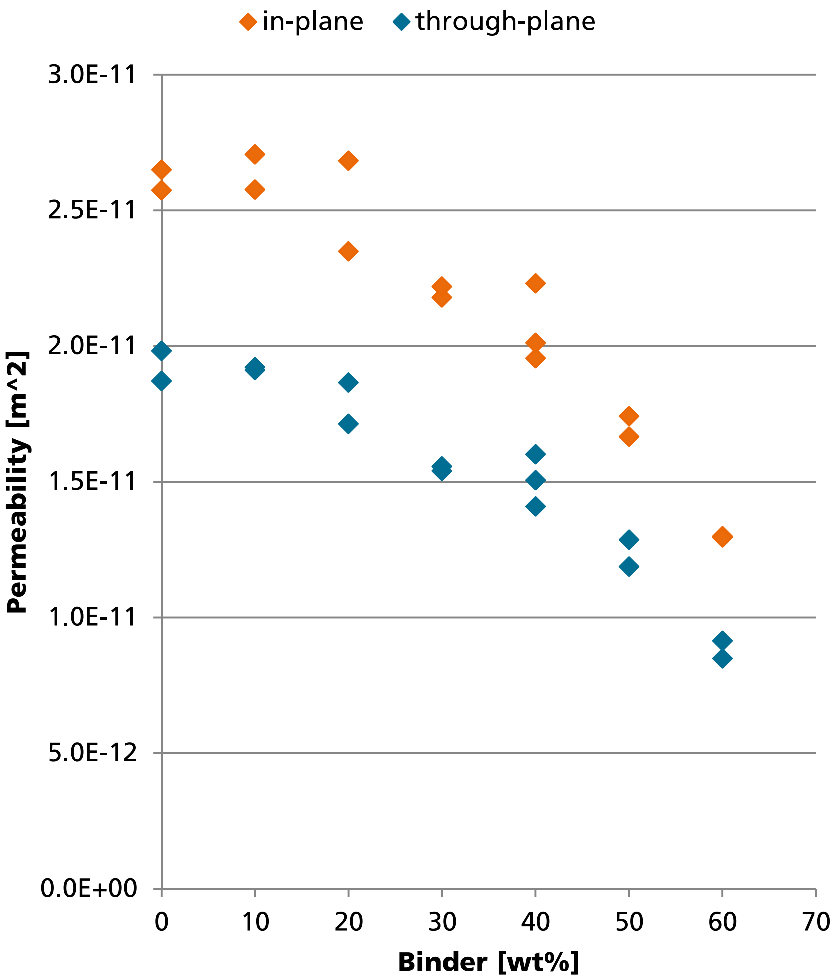


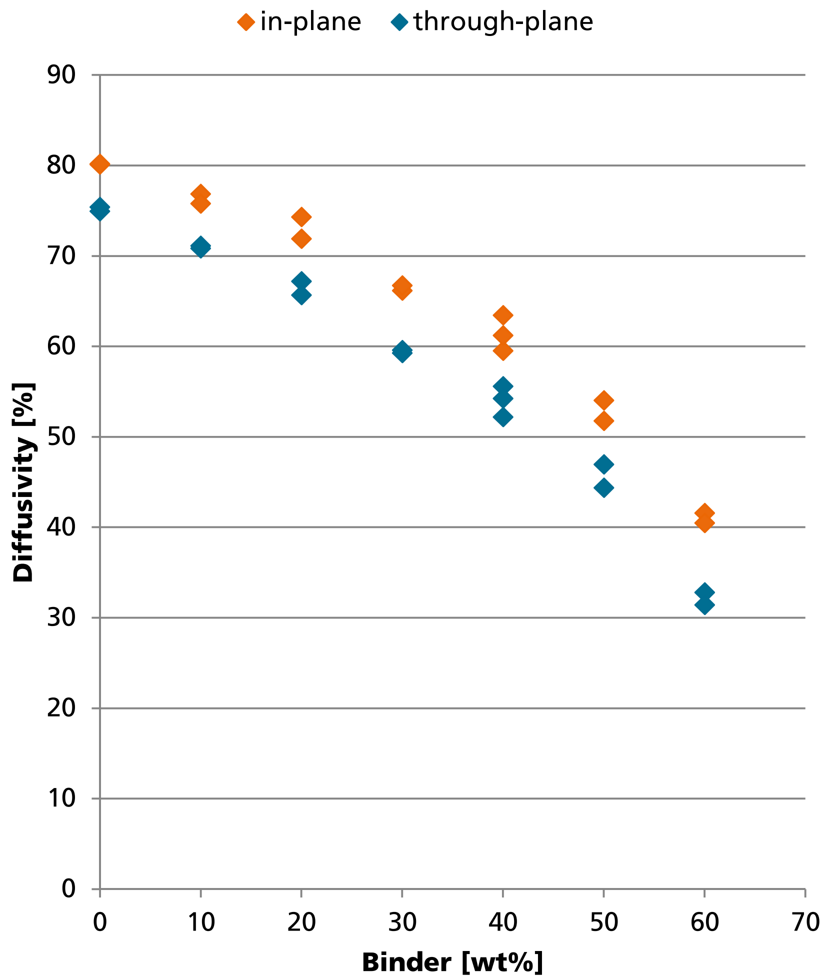
0 wt% Binder



60 wt% Binder

Binder Content

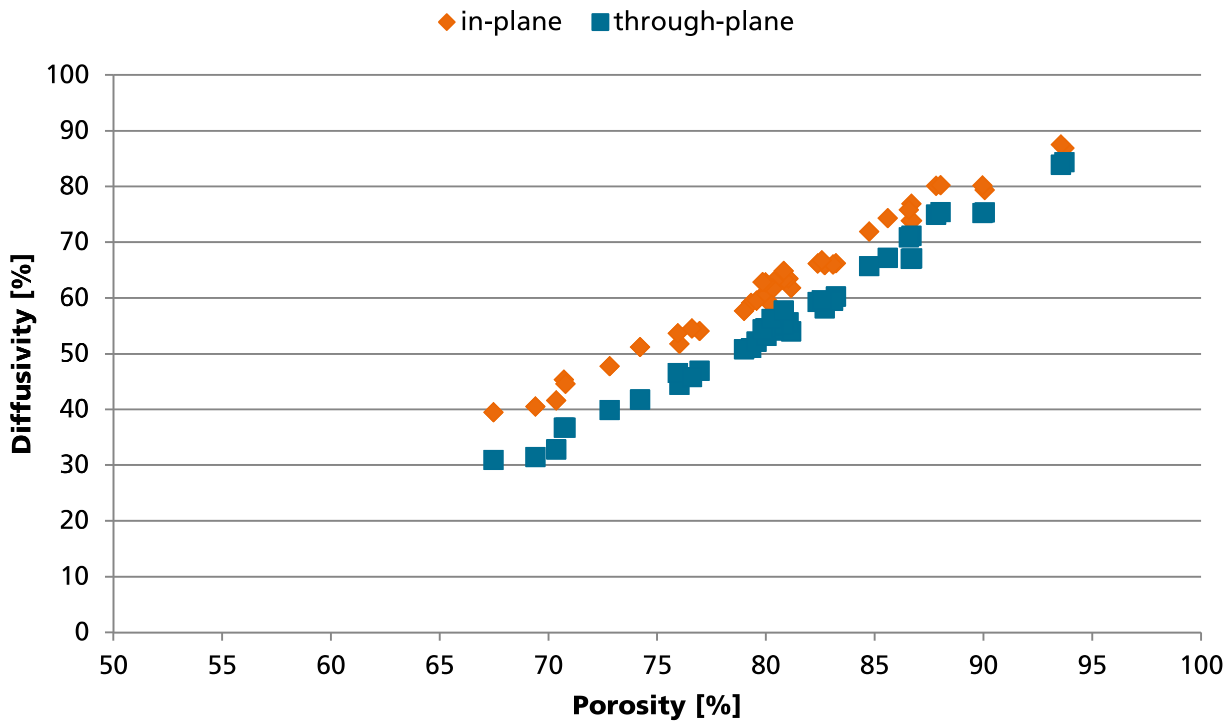




MATH 2 MARKET

Fraunhofer ITWM

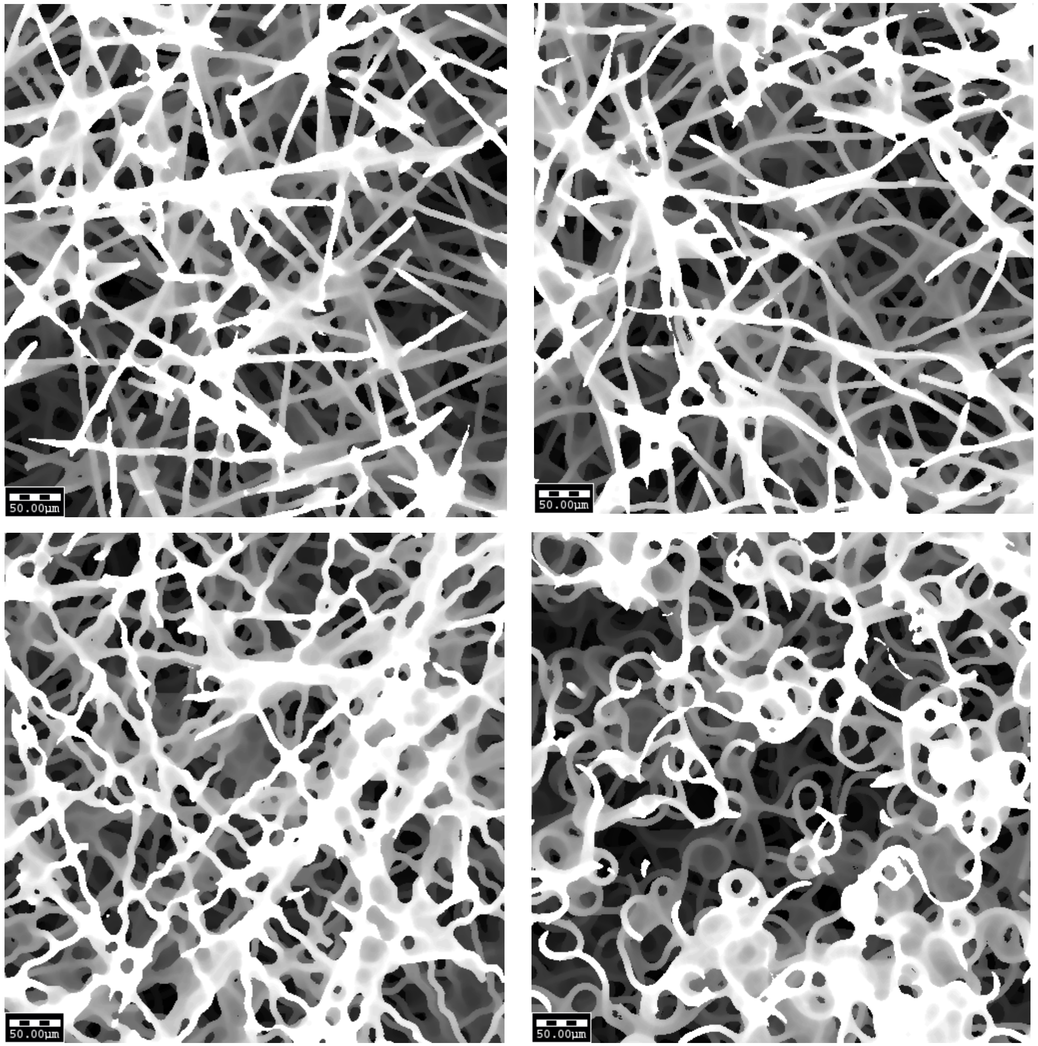
Diffusivity vs Porosity (all structure models)



Diffusivity only depends on porosity !

(all structures are similar enough)

Curl



- No direct influence on diffusivity and permeability
- Indirect influence by:
  - anisotropy
  - clustering

MPL Design Study

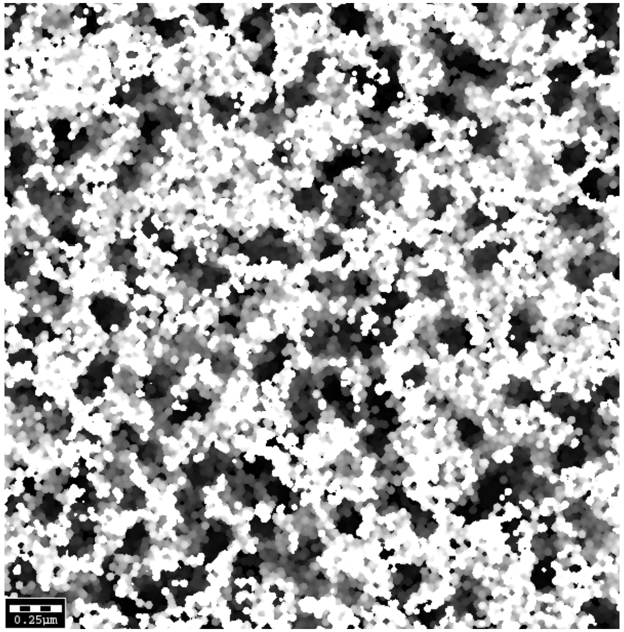
- Step 1: Create model of MPL structure, determine effective parameters for MPL alone
- Step 2: Create model for GDL+MPL, determine diffusivity and conductivity of combined layer
- Step 3: What changes when we change MPL design parameters?

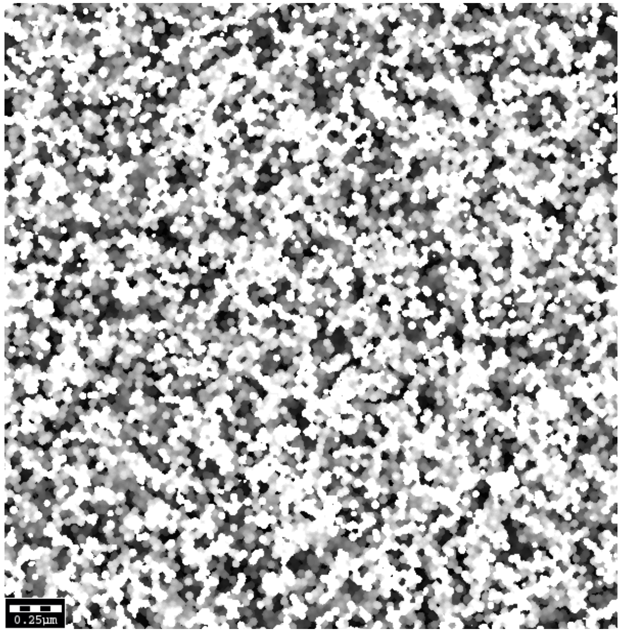
Work done by N. Zamel

Comparison of Different MPL

Create MPLs with

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

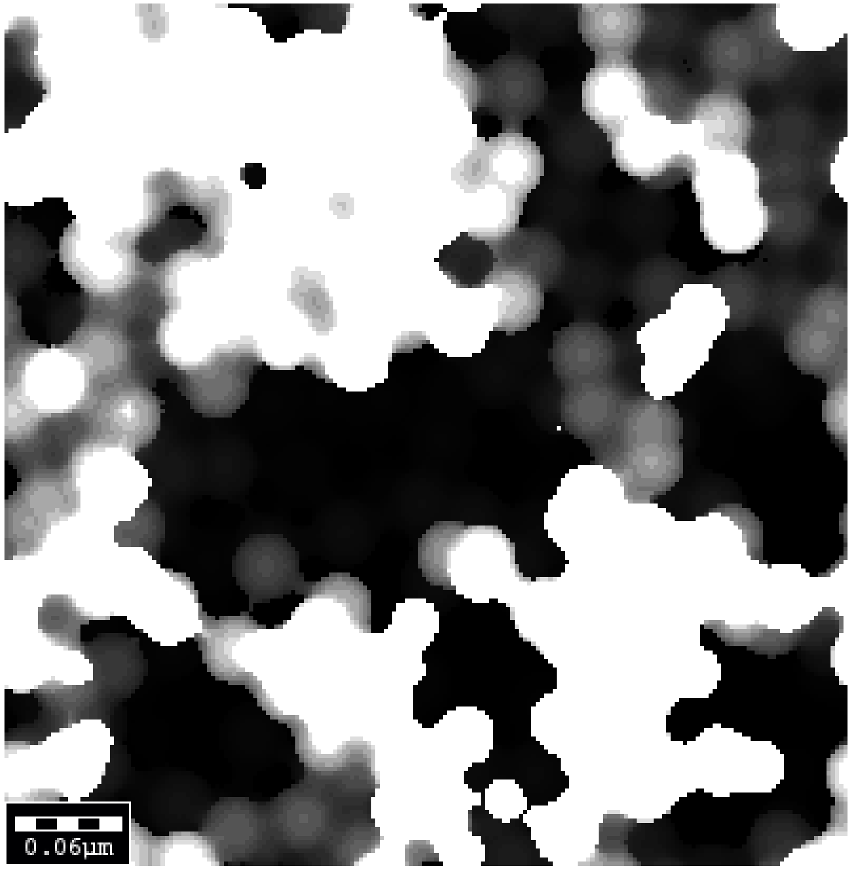




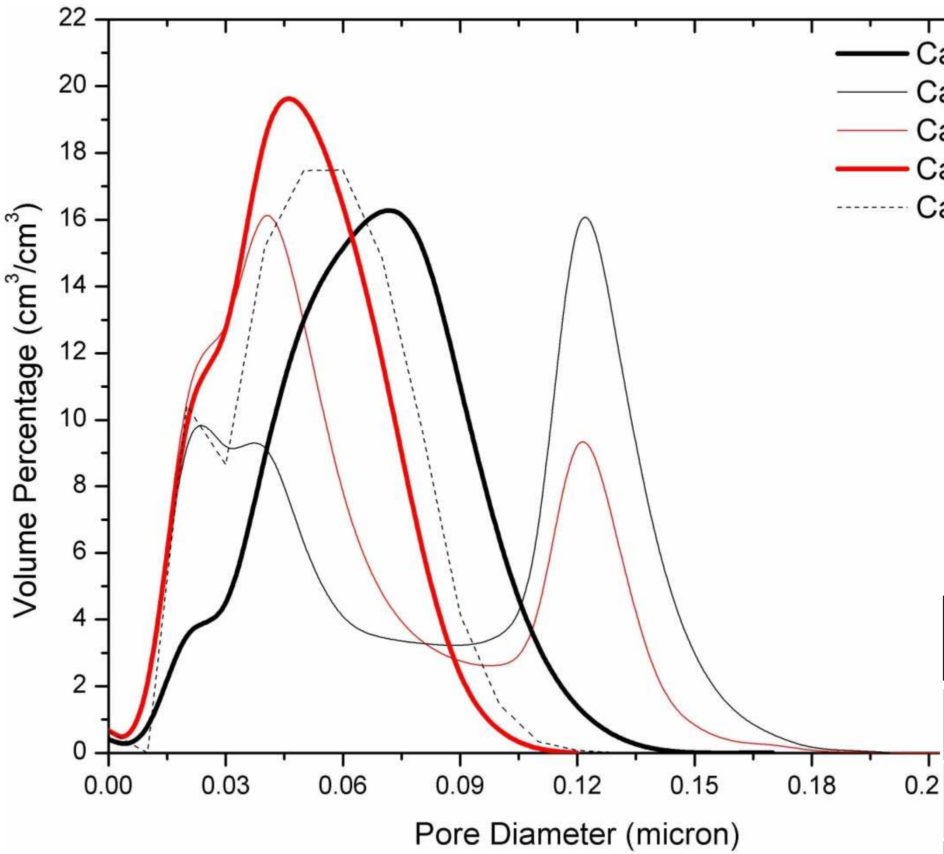
MPL Model

1. Create large pores
   (distribute spheres randomly)
2. Create carbon particles
   (distribute spheres in white area)
3. Glue
   (fill small pores)

Parameters: radii, volume fractions



Comparison of Different MPL



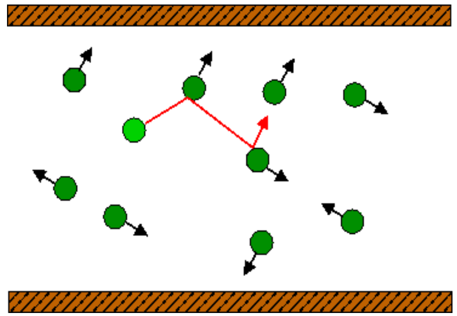
Diffusivity:
Becker, Wieser, Fell, Steiner, Int. J. Heat and Mass Transfer 54, 2011.

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

Knudsen Diffusivity

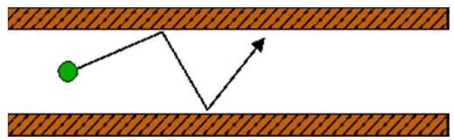
Macroscopic description
(homogenized porous media model)
Fick's first law: $j = -D^* \nabla c$



D^* : effective diffusivity [m²/s] ***unknown***
j : diffusion flux [mol/m²/s]
c : concentration [mol/m³]

Diffusion mechanisms

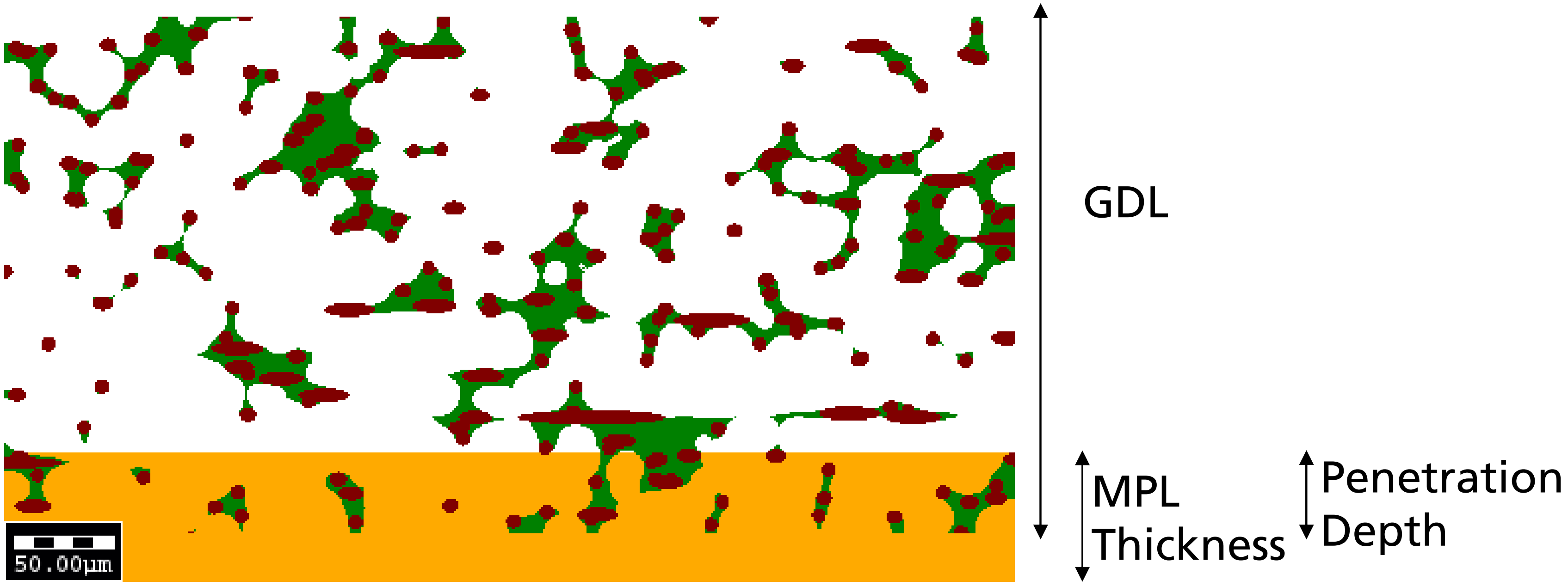
1. Kn << 1 (bulk diffusion)
   - Diffusion by particle-particle collisions
   - Mathematical model: Laplace equation
2. Kn >> 1 (Knudsen diffusion)
   - Diffusion by particle-wall collisions
   - Mathematical model: random walk methods
3. Kn ~ 1 (transition regime diffusion)
   - Both mechanisms are present, Bosanquet:



$$D_{Kn} = \frac{\varepsilon}{2t} E[(x_t - x_o)(x_t - x_o)^T]$$

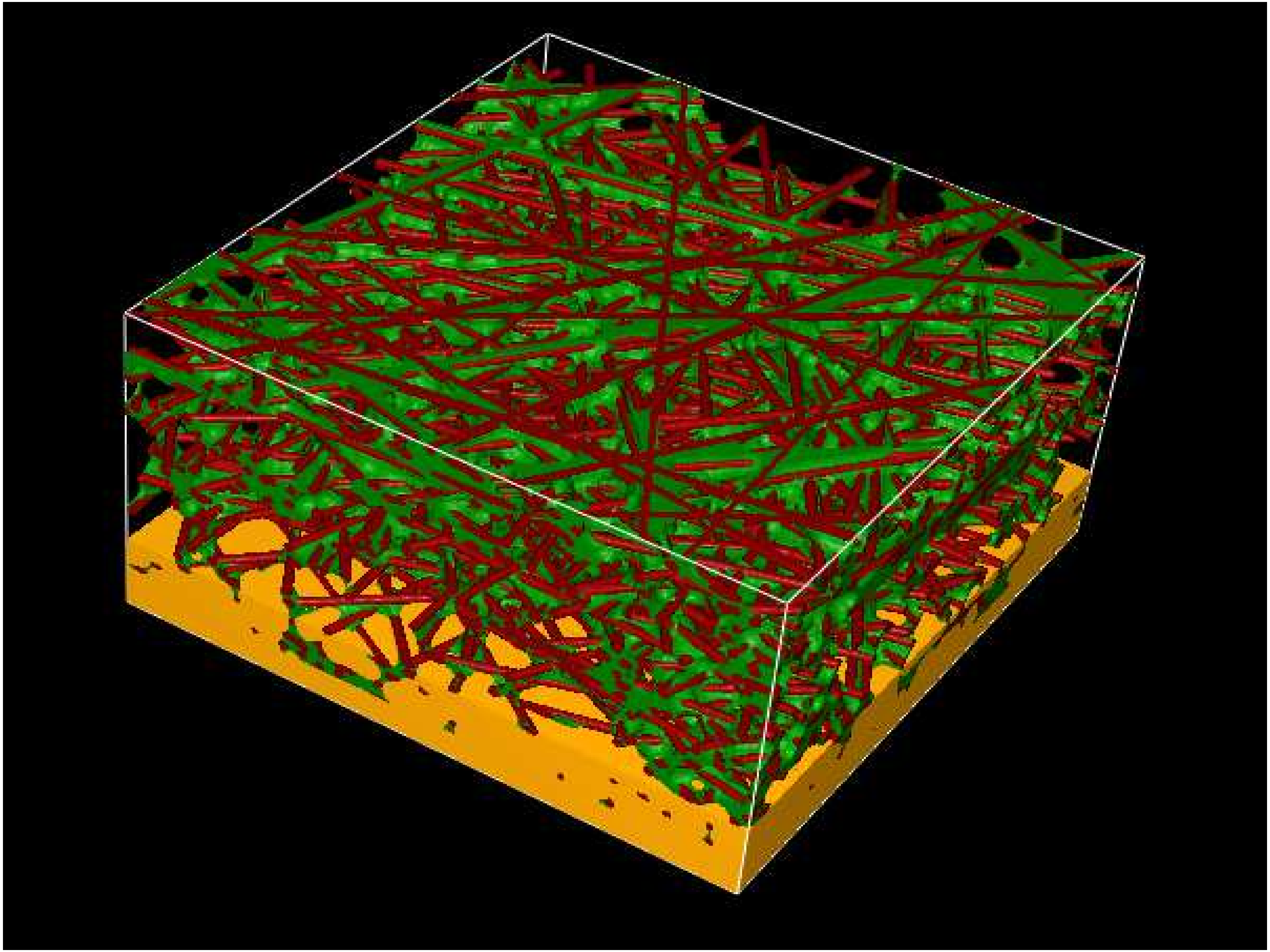
$$D = \left(D_{bulk}^{-1} + D_{Kn}^{-1}\right)^{-1}$$

GDL / MPL Assembly

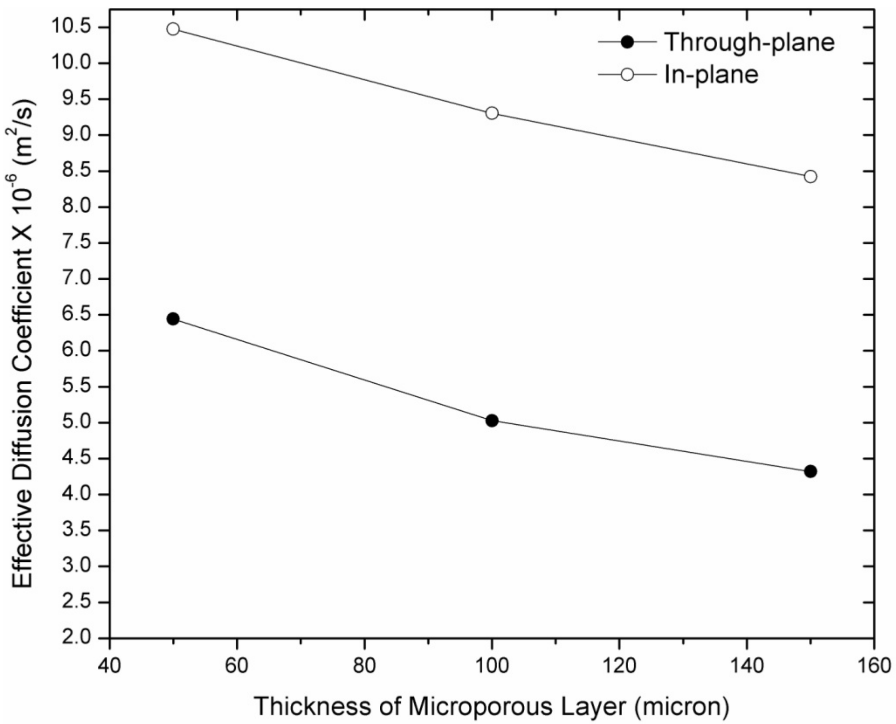


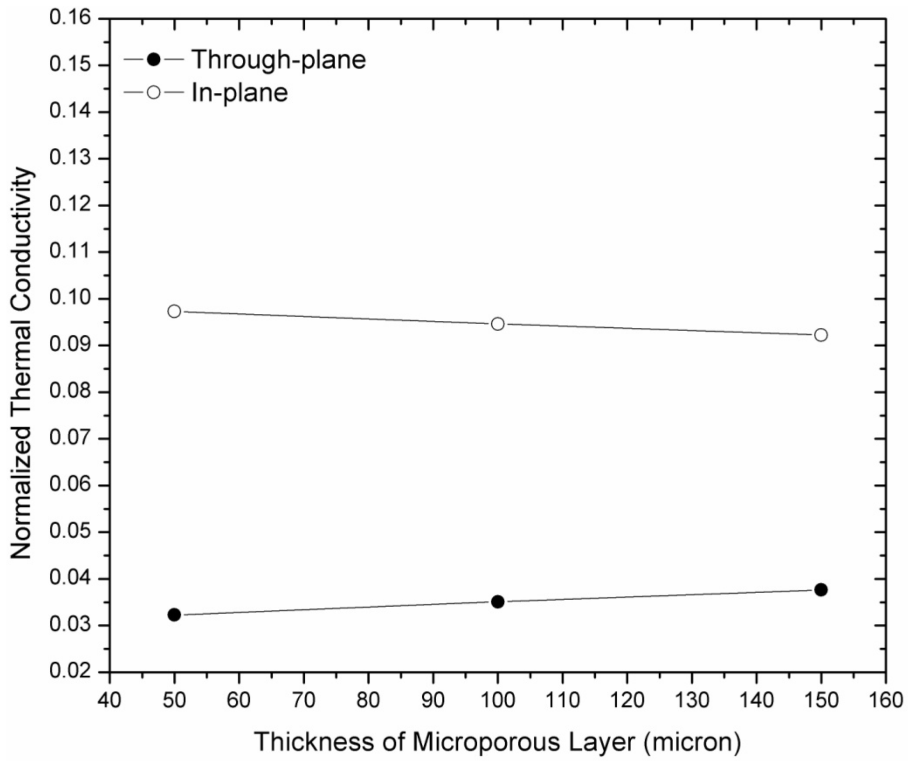
2D Cross Section

Red: Fibers
Green: Binder
Orange: MPL

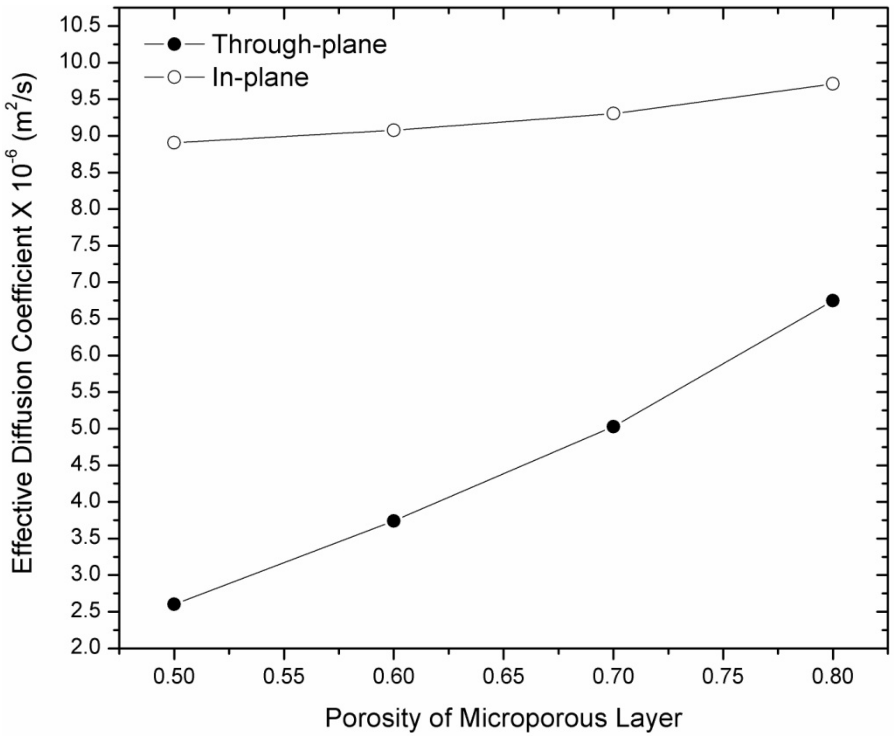


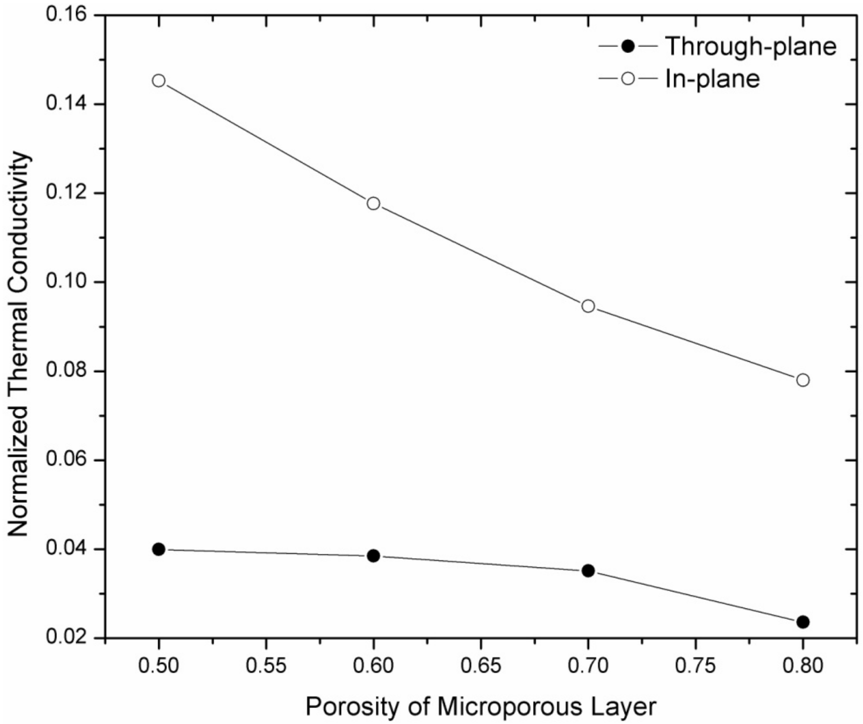
Variation of MPL Thickness



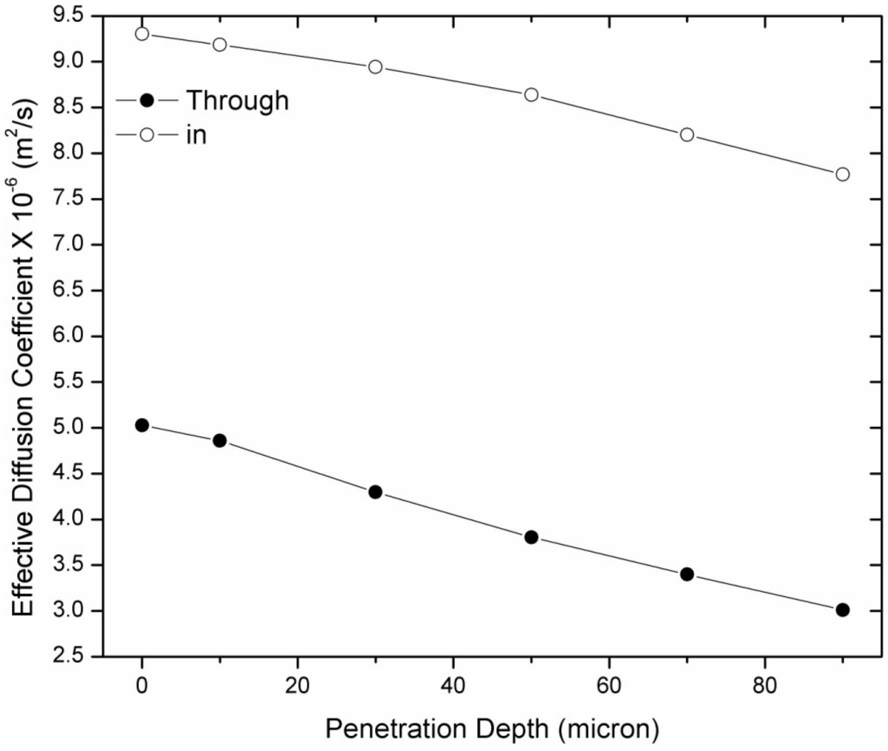


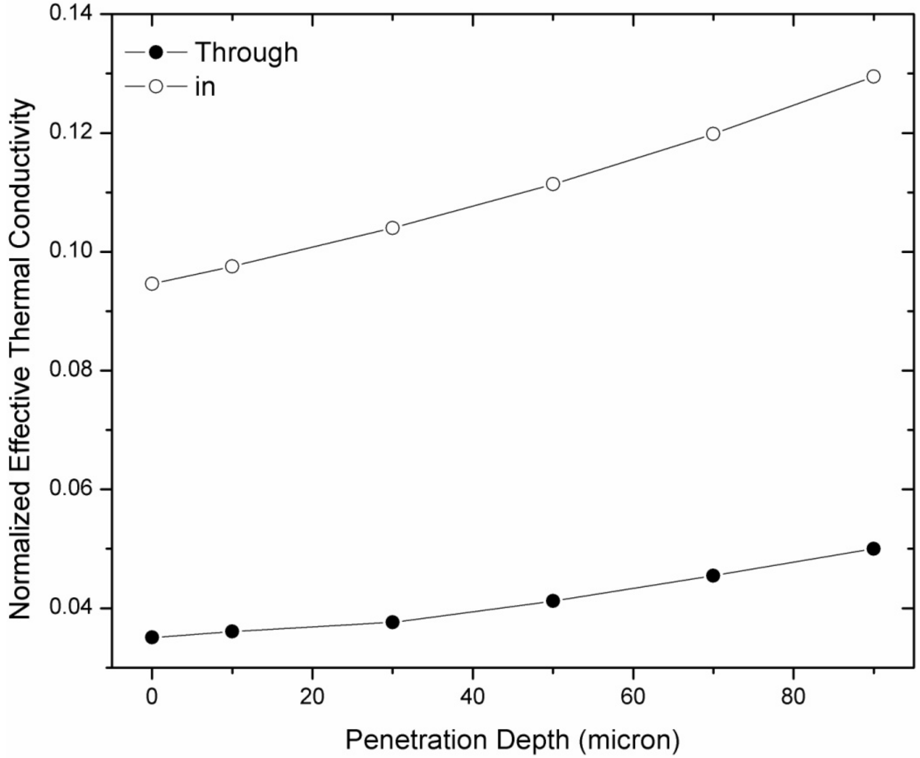
Variation of MPL Porosity





Variation of MPL Penetration Depth





Design Studies Summary

- GDL structure
  - fiber diameter, porosity, binder content, curl
- MPL micro structure
  - pore size distribution, porosity
- MPL macro structure
  - thickness, penetration depth

Thank You !

Geometry generator, property predictor and virtual material designer

www.geodict.com

BMBF project PemCaD