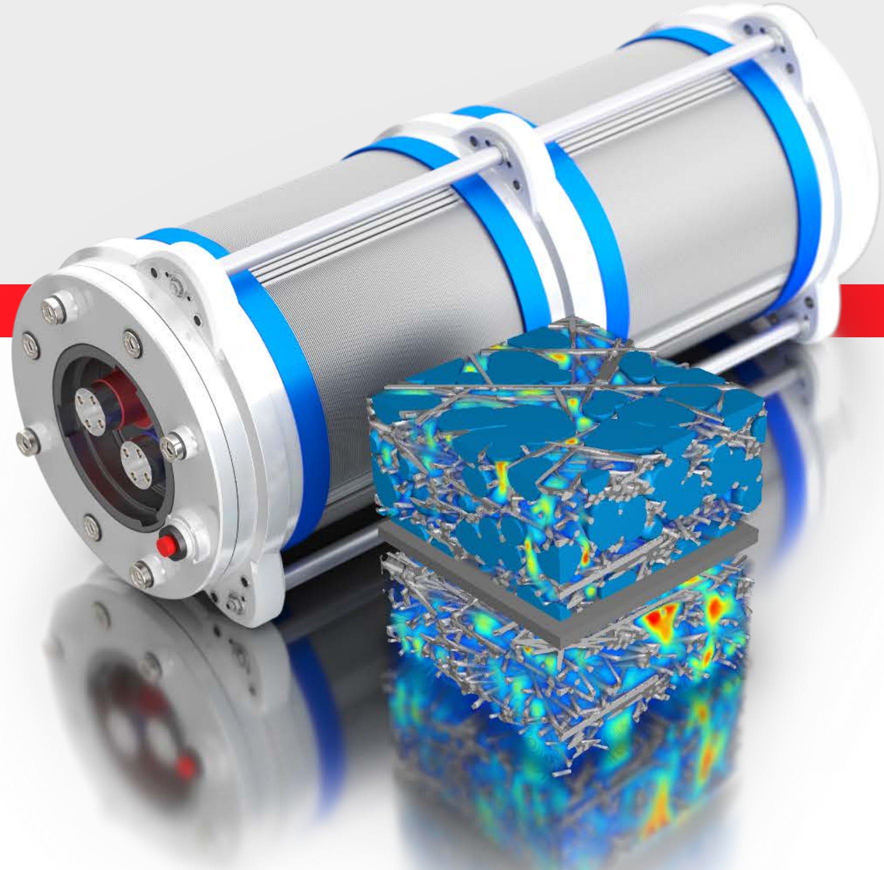
Computer Based Design of Porous Transport Layers of PEM Fuel Cells

Dr. Jürgen Becker

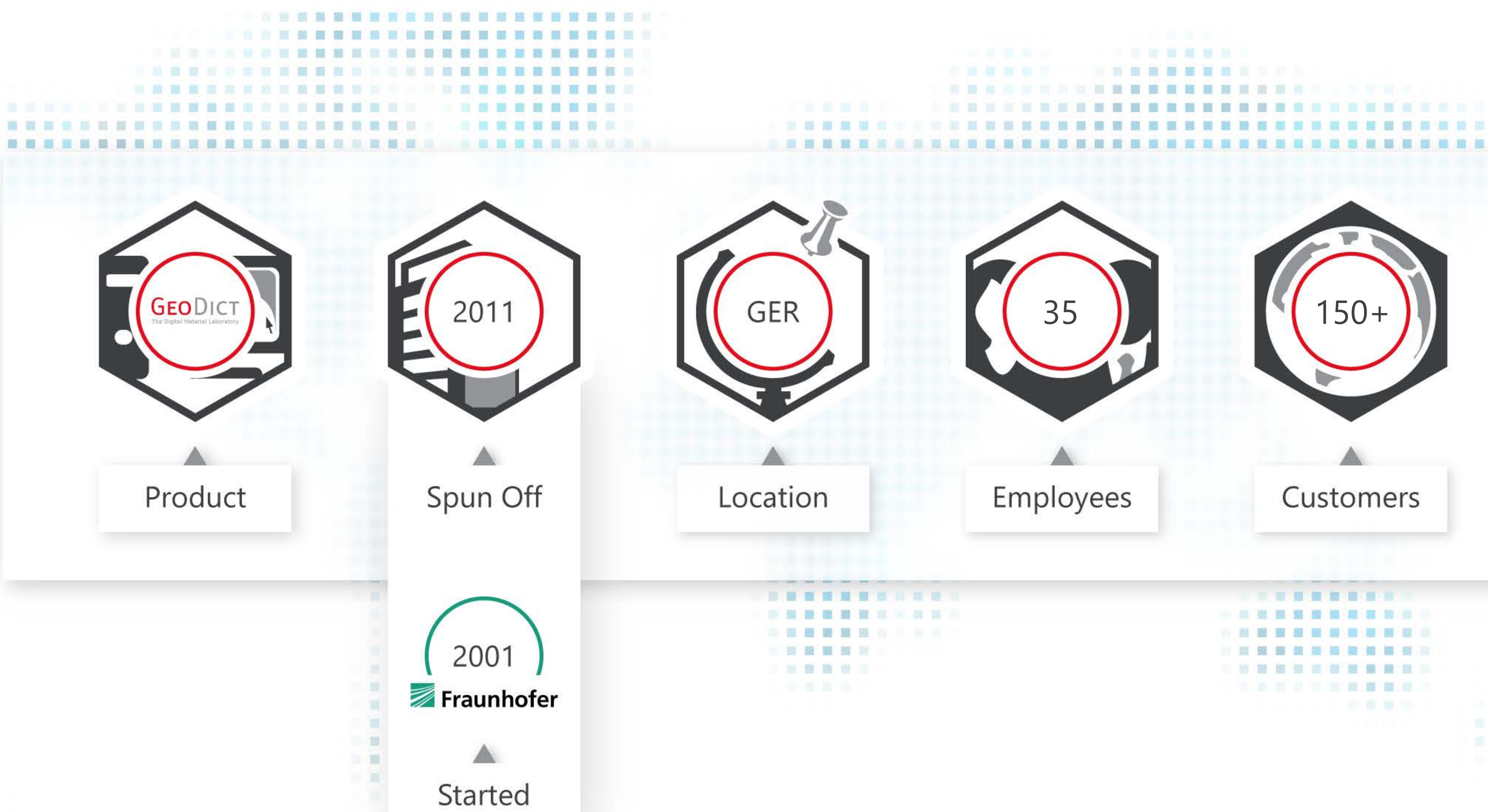
EVS30 / f-cell

Stuttgart

11.10.2017



Math2Market GmbH Company Overview



MATH 2 MARKET

GeoDict The Digital Material Laboratory

We help our clients to profitably
engineer better materials and processes
through
digital solutions.

We believe that to understand is to improve.

GeoDict The Digital Material Laboratory

Filtration

Mostly automotive, filter media & filters for water, sludge, oil, air and fuel

Electrochemistry

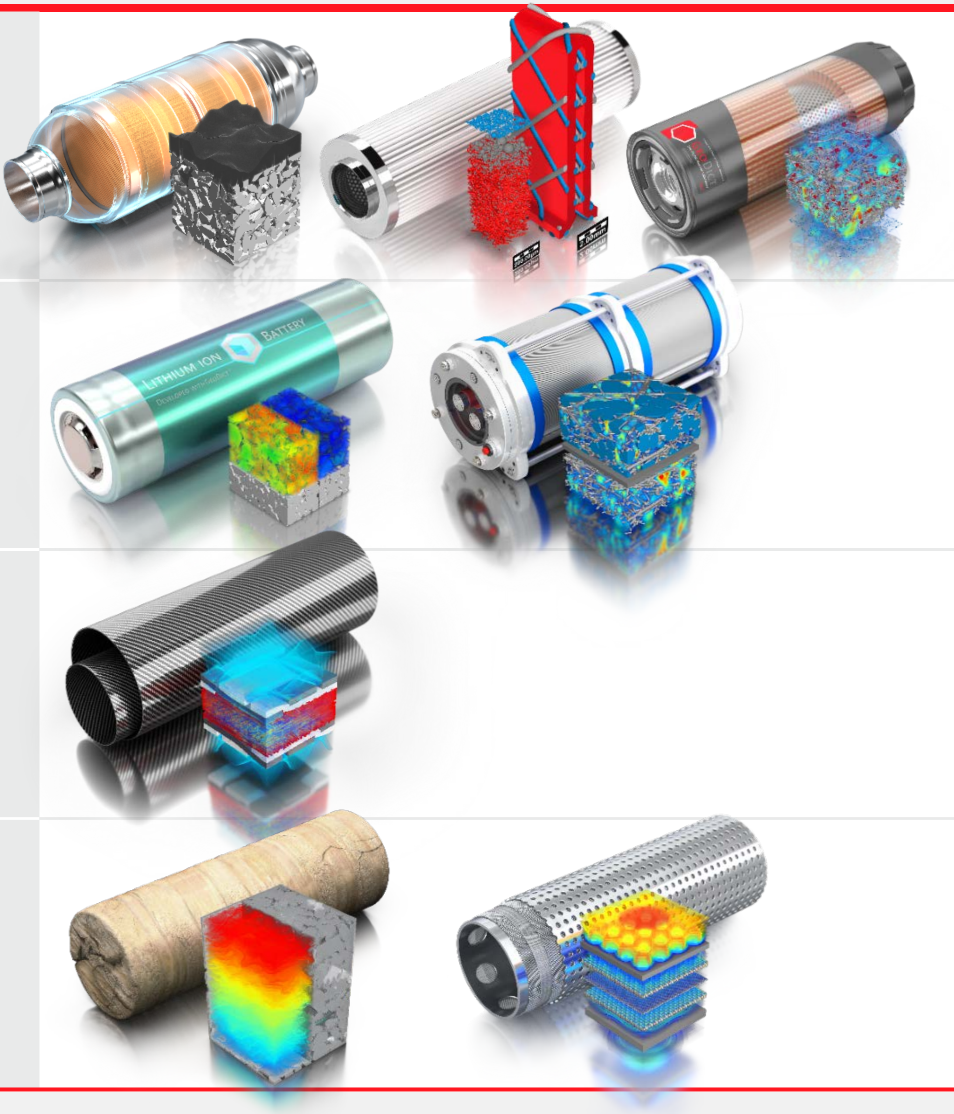
Fuel cell media & battery materials, catalyst materials

Composites

CFRP, GFRP, mostly automotive, lightweight materials

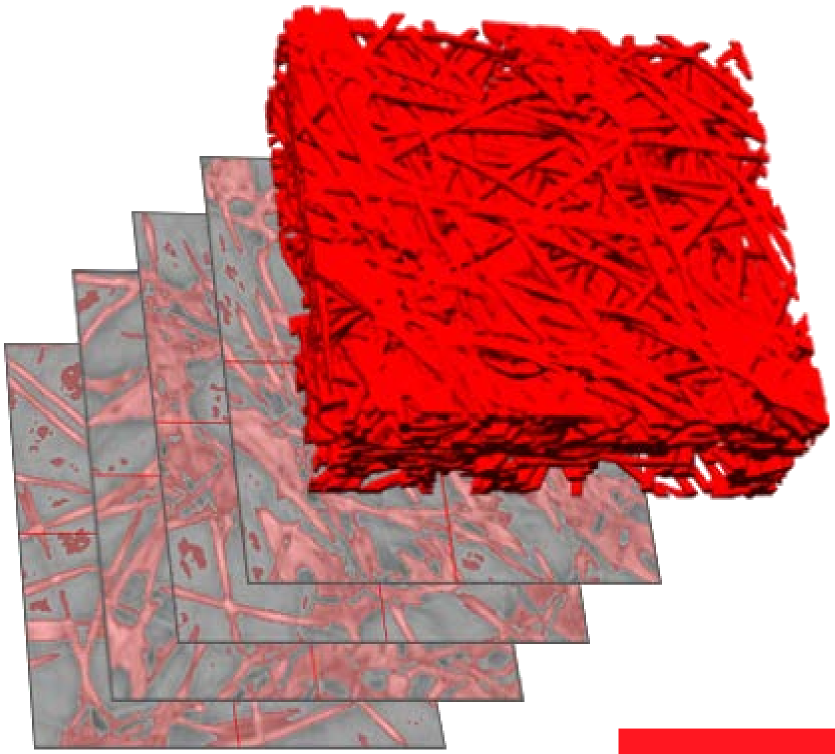
Oil and Gas

Digital rock physics, digital sand control



Development of Materials

Development of Materials by Digital Material Design



- Import CT scans
- Import FIB-SEM data

Image Acquisition

Development of Materials

Development of Materials by Digital Material Design

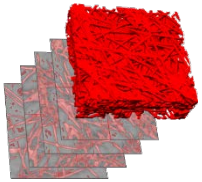


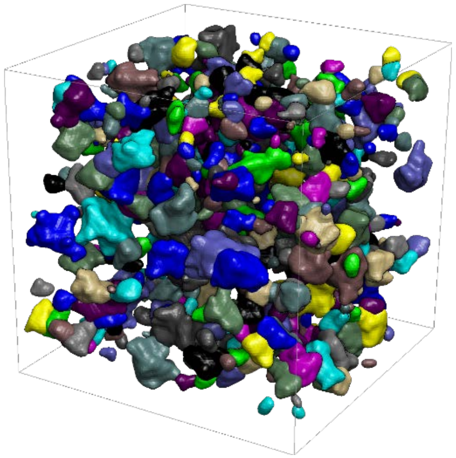
Image Acquisition

Development of Materials

Development of Materials by Digital Material Design

Determine:

- Pore size distribution
- Fiber size and orientation
- Grain size and shape



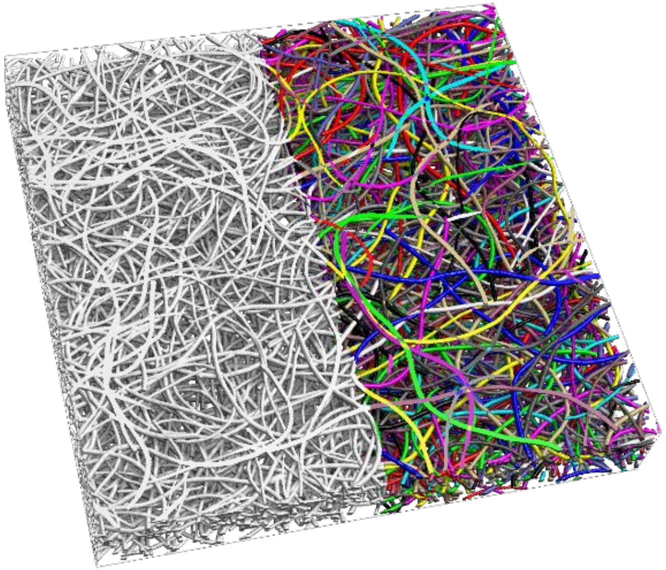


Image Analysis

Development of Materials

Development of Materials by Digital Material Design

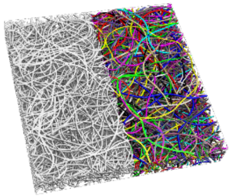


Image Analysis

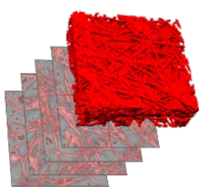


Image Acquisition

Development of Materials

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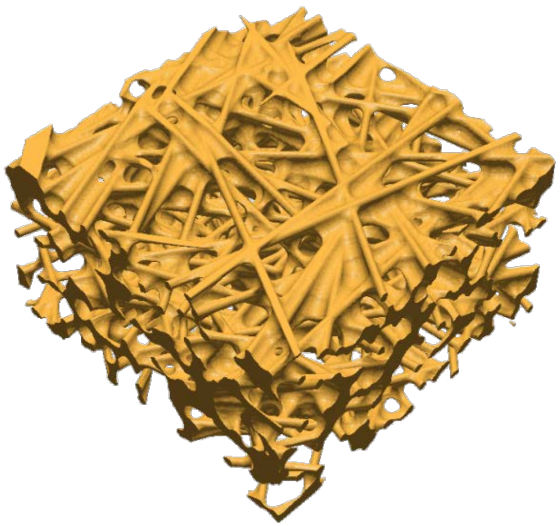
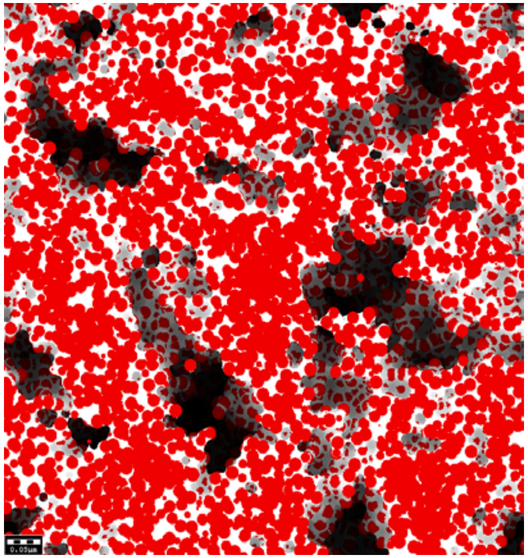


Gas diffusion layer

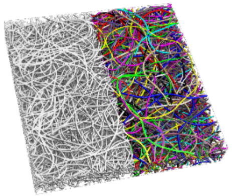


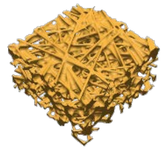
Catalyst layer

Modelling Microstructures

Development of Materials

Development of Materials by Digital Material Design





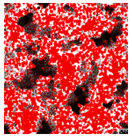


Image Analysis ▶ Modelling Microstructures

▲

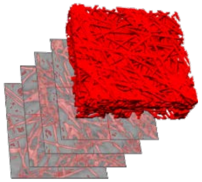


Image Acquisition

▲

Development of Materials ▶

Development of Materials by Digital Material Design

Capillary Pressure

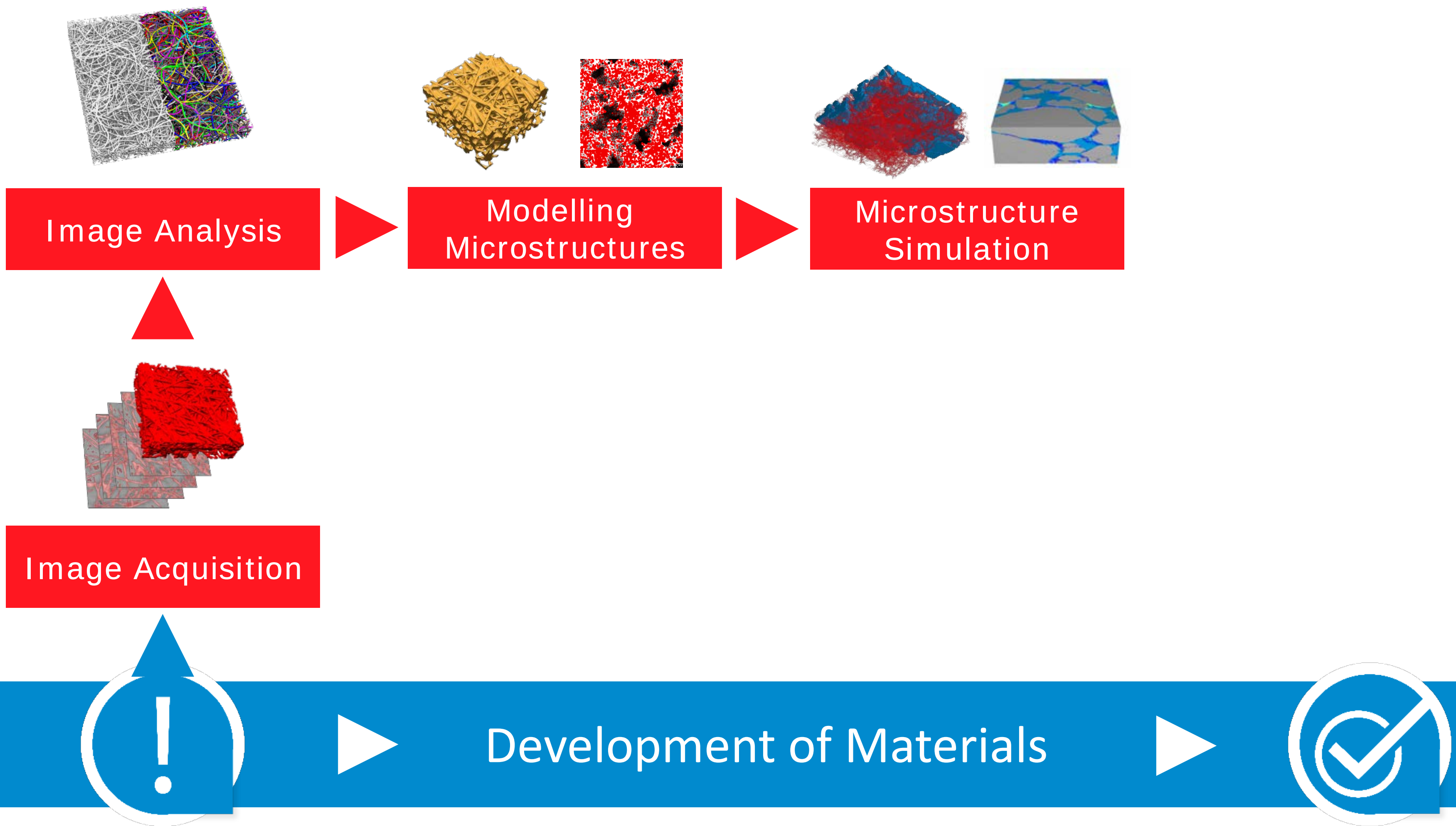
Flow

Diffusion

Microstructure Simulation

Development of Materials

Development of Materials by Digital Material Design



Development of Materials by Digital Material Design

Permeability tensor / (m^2)

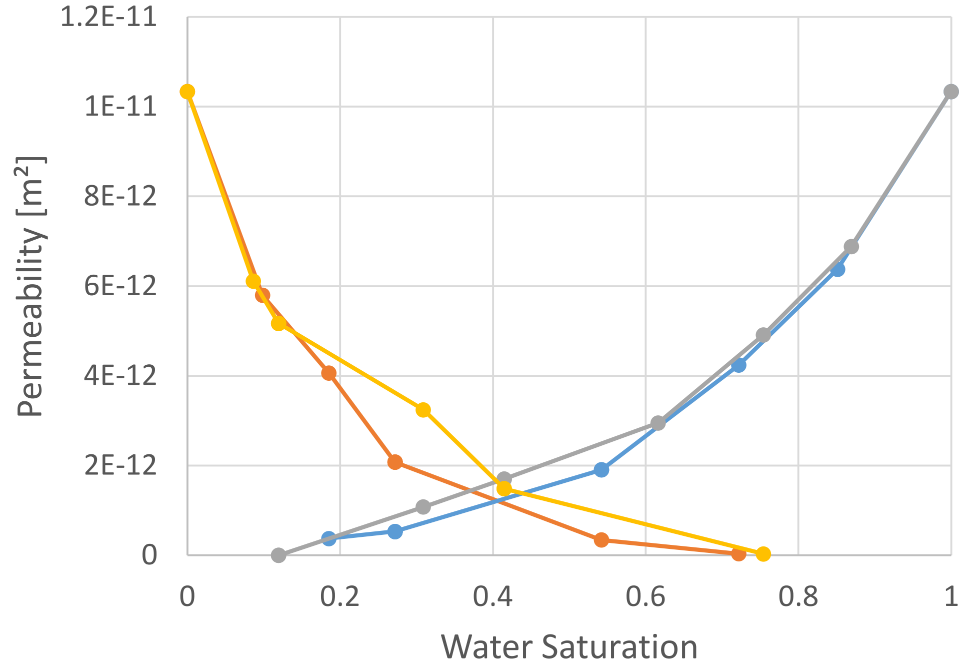
2.007e-11	-2.87729e-13	-4.85037e-13
-2.43395e-13	**2.10784e-11**	-5.02884e-14
-5.9795e-13	1.09459e-13	**1.56916e-11**

Effective diffusivity in %

63.2608	-0.395186	-0.643377
-0.364076	64.7705	-0.18344
-0.962924	-0.22963	58.9095

Tortuosity factors and Tortuosity

	Tortuosity Factor κ	Tortuosity τ
X Direction	1.27950494	1.13115
Y Direction	1.249680381	1.11789
Z Direction	1.37401316	1.17218

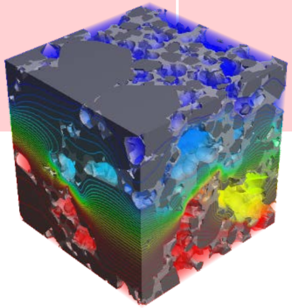


Macroscopic Material Parameters

Development of Materials

Development of Materials by Digital Material Design

Geometric parameters	Conduction parameters	Diffusion & flow parameters	Saturation parameters
▪ Porosity ▪ Pore size distribution ▪ Surface area ▪ Length of contact lines ▪ Tortuosity/Gurley value	▪ Thermal conductivity ▪ Thermal Flux ▪ Temperature distribution ▪ Electrical conductivity ▪ Electrical Flux ▪ Electrostatic potential distribution	▪ Permeability ▪ Diffusivity ▪ Particle concentration ▪ Path of single particle	▪ Cap. pressure curve for Drainage and Imbibition ▪ Saturation dependent permeability, diffusivity, conductivity



Macroscopic Material Parameters

Development of Materials

Development of Materials by Digital Material Design

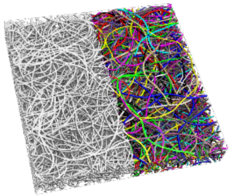
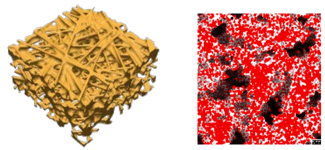
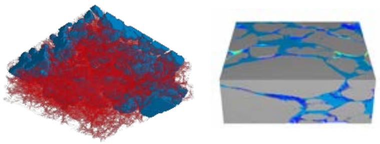


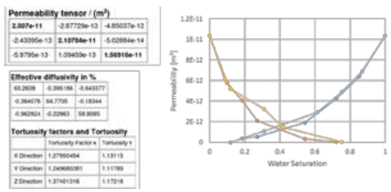
Image Analysis



Modelling Microstructures



Microstructure Simulation



Macroscopic Material Parameters

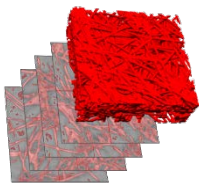
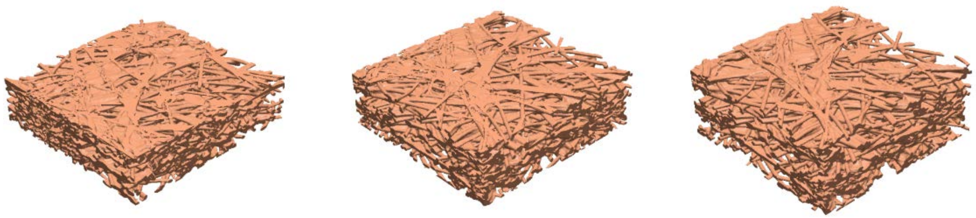


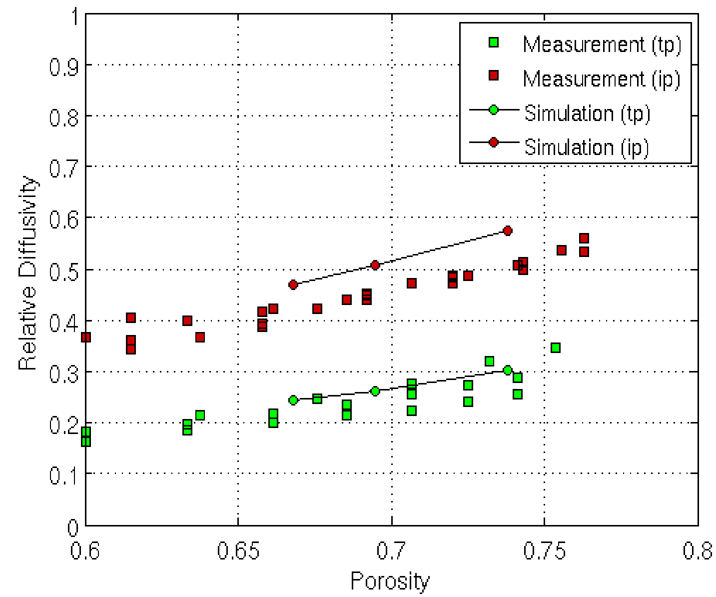
Image Acquisition

Development of Materials

Development of Materials by Digital Material Design

1. Made CT scans of Toray TGP H 060 at different compression levels
2. Measured diffusivity at different compression levels experimentally
3. Computed diffusivity on the CT scans

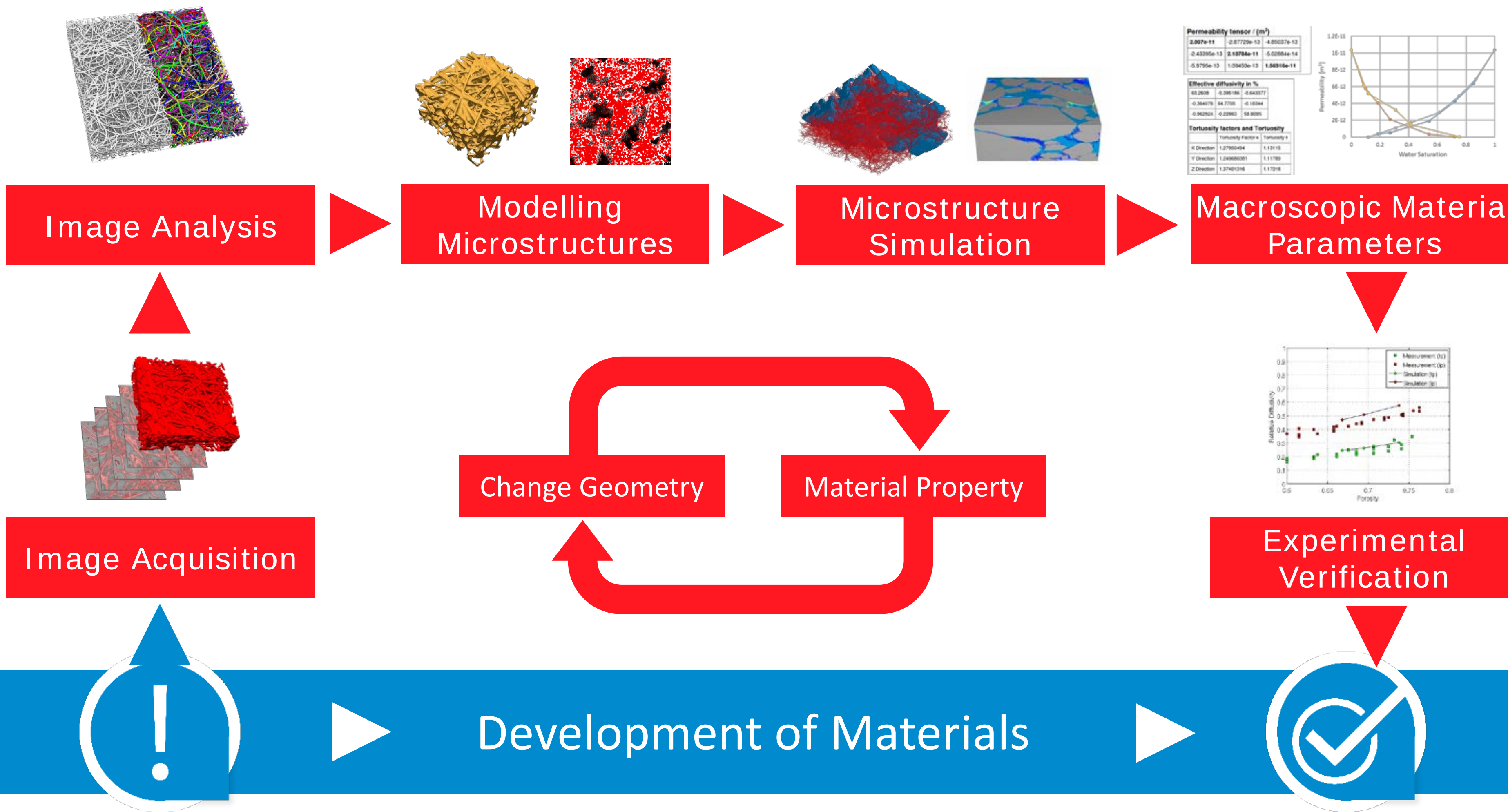




Experimental Verification

Development of Materials

Development of Materials by Digital Material Design



Case Study:
Determine relative permeability for a gas diffusion layer

… considering variable wettability

… and compression.

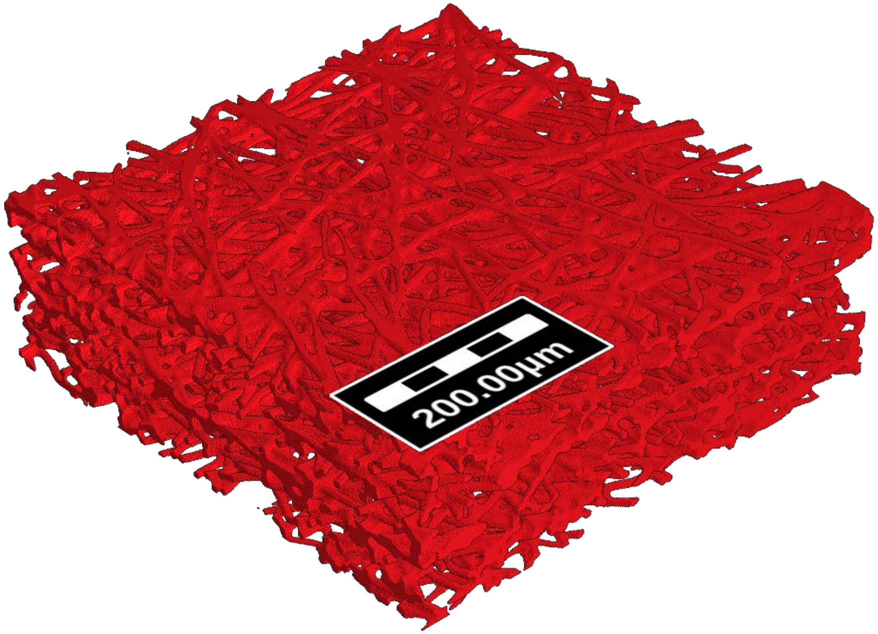
Gas Diffusion Layer Model

GDL:

- Carbon fibers, 7 µm diameter
- 20 wt% binder
- 200 µm thickness

Model

- 1 µm resolution
- Voxel grid
- 600x600x200 = 72 Mio. cells
- Stochastic process



Modelling of Clamping Pressure

Fibers: linear elastic, transverse isotropic

Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM

Runtime: 1h 17 min (8x)

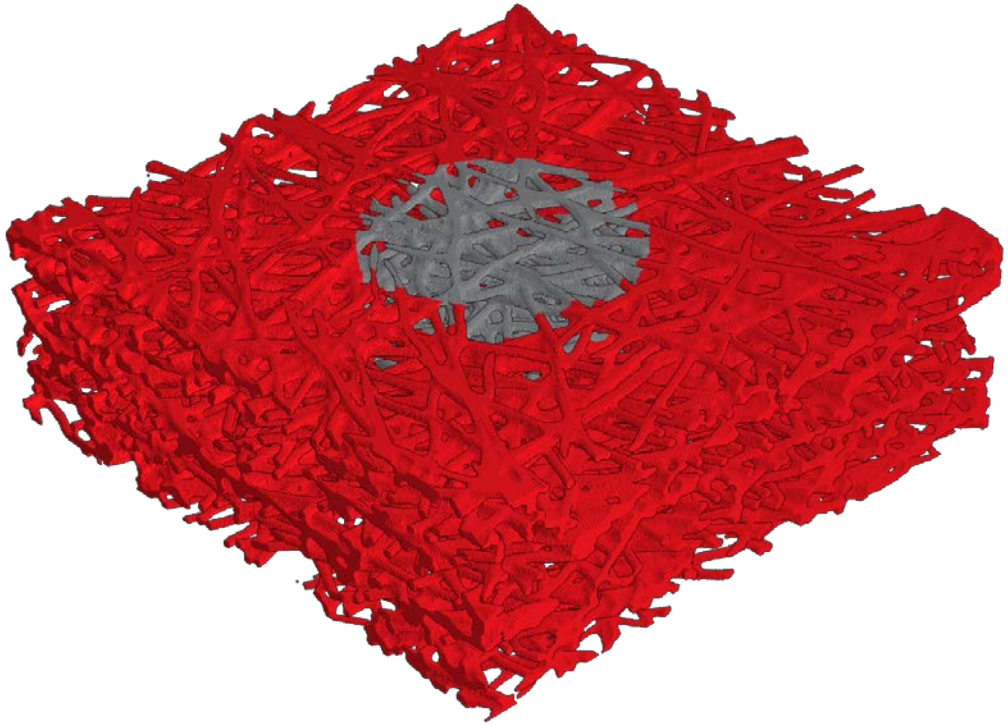
Compression	0	0.05	0.1	0.15	0.2	0.25

Introducing Variable Wettability

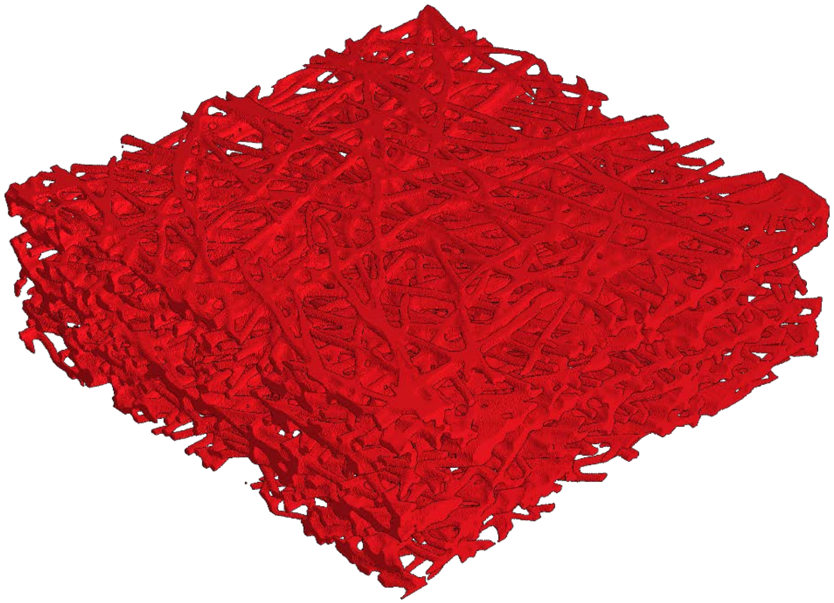
- Marked a cylinder as area with higher wettability

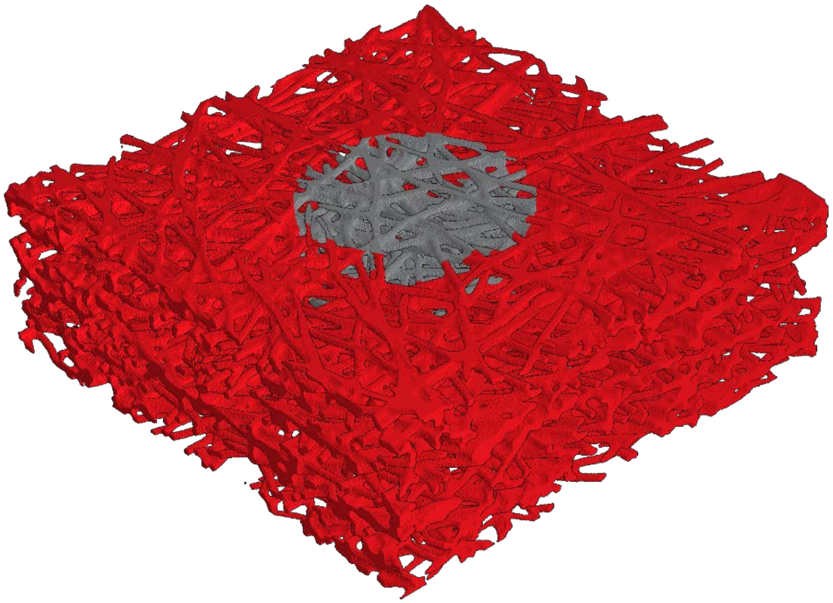
Other options:

- distinguish between binder and fibers
- mark individual fibers
- ...



Gas Diffusion Layer Models with Different Wettability





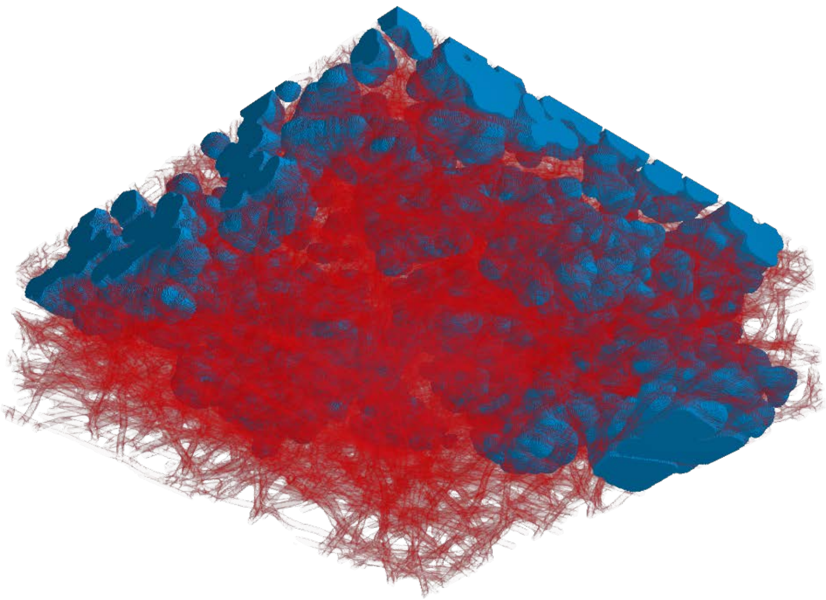
Constant Wettability

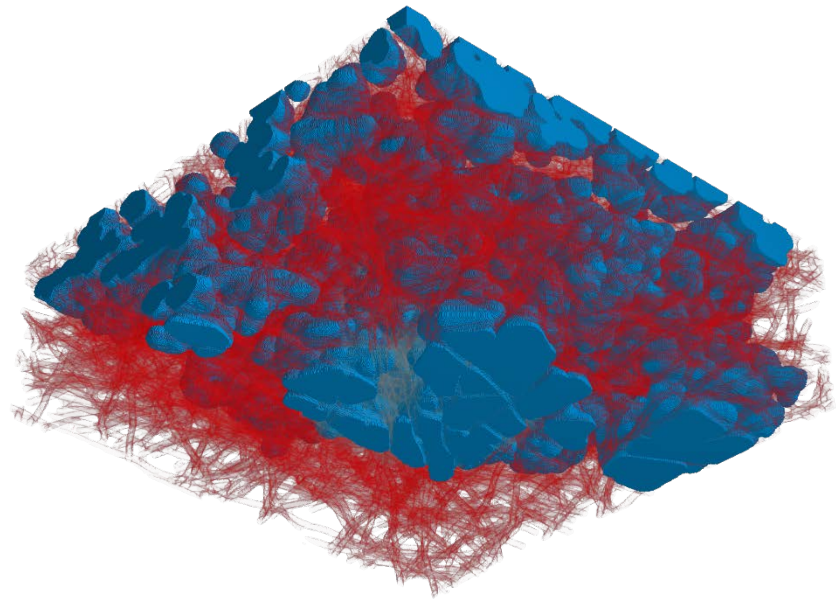
Variable Wettability

Water Entering into an Uncompressed GDL with Constant Wettability

Water Entering into an Uncompressed GDL with Variable Wettability

Comparison:
Saturation at Fixed Capillary Pressure





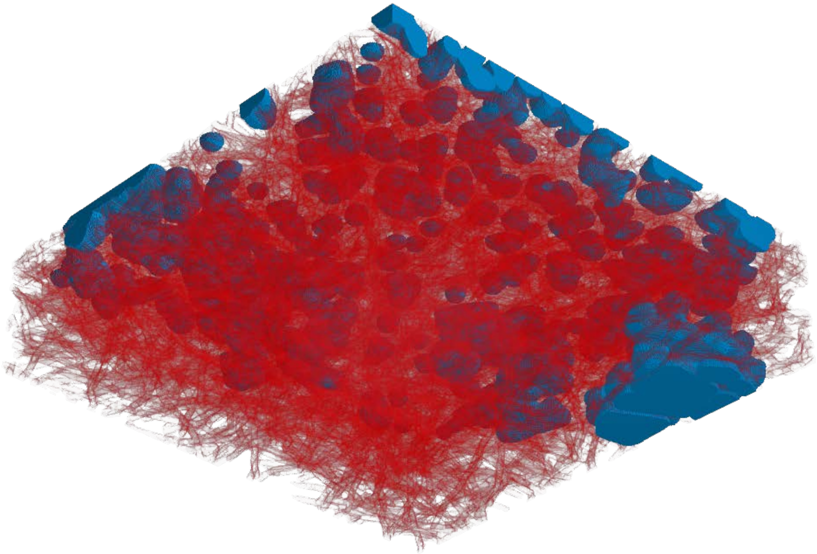
Constant Wettability

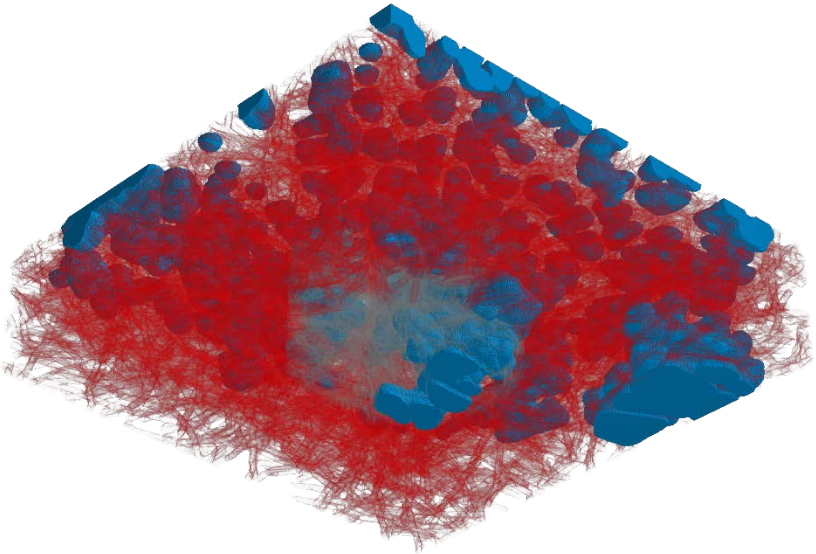
Variable Wettability

Water Entering into a Compressed GDL with Constant Wettability

Water Entering into a Compressed GDL with Variable Wettability

Comparison:
Saturation at Fixed Capillary Pressure

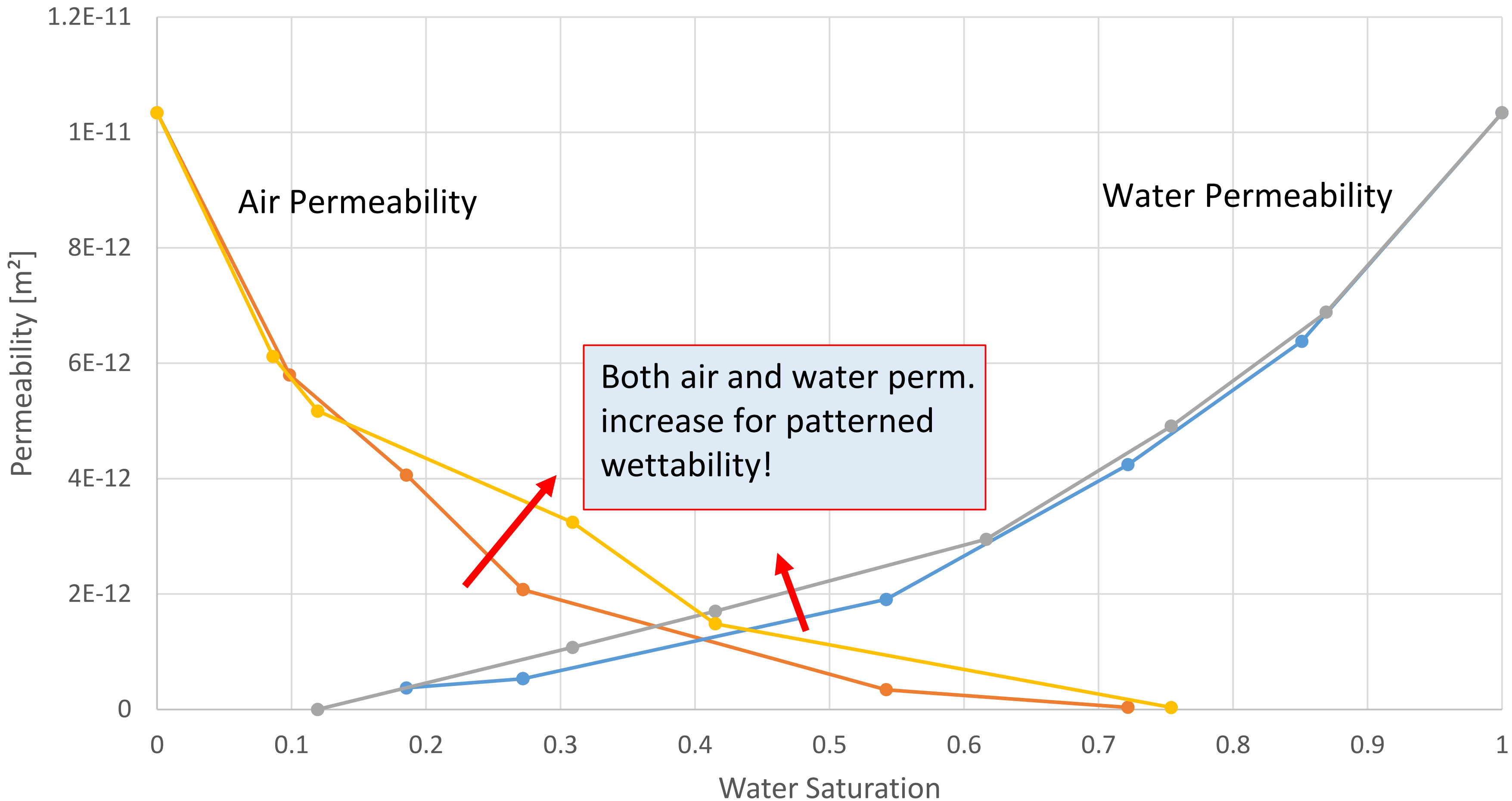




Constant Wettability

Variable Wettability

Simulated Relative Permeability (Uncompressed GDL)



Summary

The basic idea:
Microstructures define macroscopic properties!

- Model porous microstructure of transport layers and electrodes
- Simulate transport processes
- Simulate mechanical behavior
- Analyze geometry

GeoDict predicts macroscopic material properties based on the 3D microstructure and enables you to improve the materials.

Thank You!

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