Numerical Analysis of Transport Processes in Porous Layers

Jürgen Becker, Andreas Wiegmann

Math2Market GmbH

ModVal 11, Winterthur 2014

MATH 2 MARKET

Math2Market GmbH

- Founded September 21 2011 in Kaiserslautern.
- Spin-off of Fraunhofer Institute for Industrial Mathematics ITWM.
  Located in the Business and Innovation Center in Kaiserslautern.
- Business based on GeoDict software formerly developed by ITWM.
  Continued close cooperation with ITWM on algorithms.

GEO DICT

- GeoDict® exists since 2001,
  first sales in 2003, first sales for filtration (FilterDict® module) in 2005.
- The intellectual property rights to the GeoDict software belong to
  Math2Market GmbH since January 1, 2013.

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Outline

1. General approach: the virtual material lab
2. Import and analysis of CT data
3. Creating realistic 3D structure models
4. Determination of transport properties

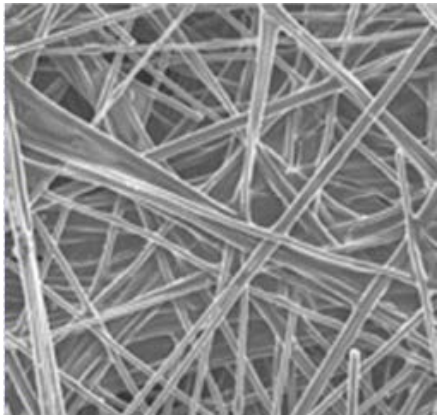
1. General Approach: The Virtual Material Lab

The Virtual Material Lab Approach:

The Virtual Material Lab Approach:

Experiment / Lab

Porous Material



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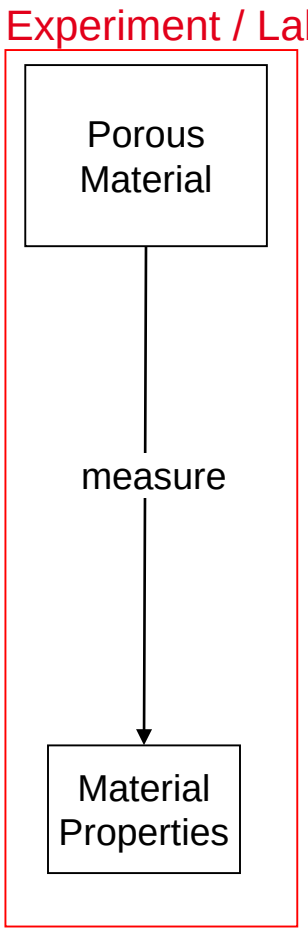

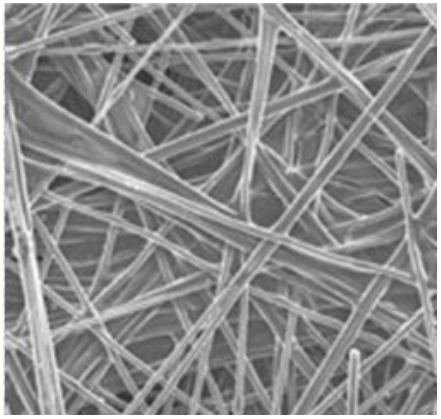

Properties are:
- pore size distribution
- effective diffusivity
- permeability
- stiffness
- …

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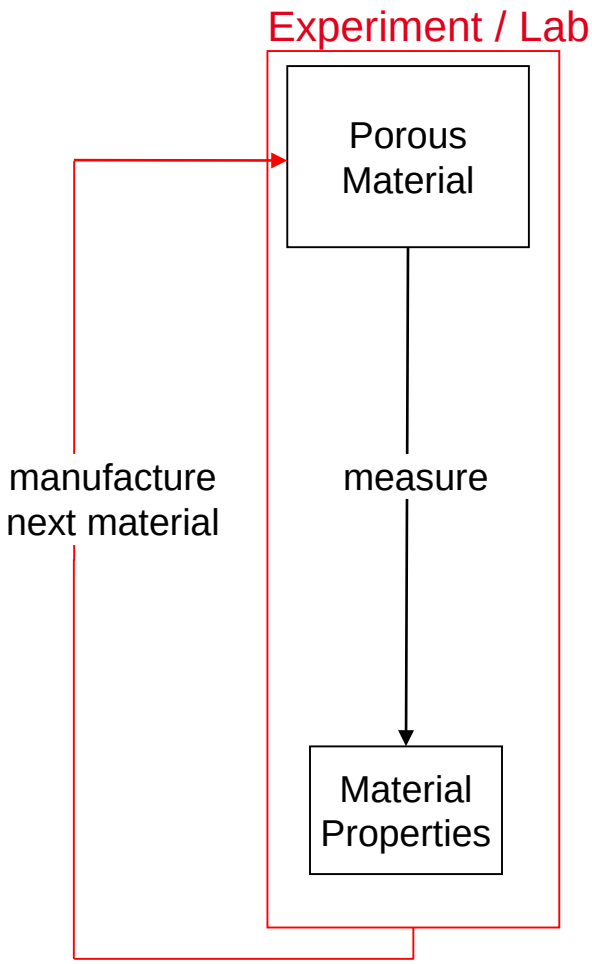

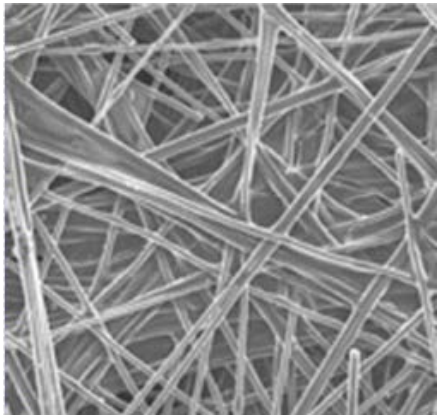

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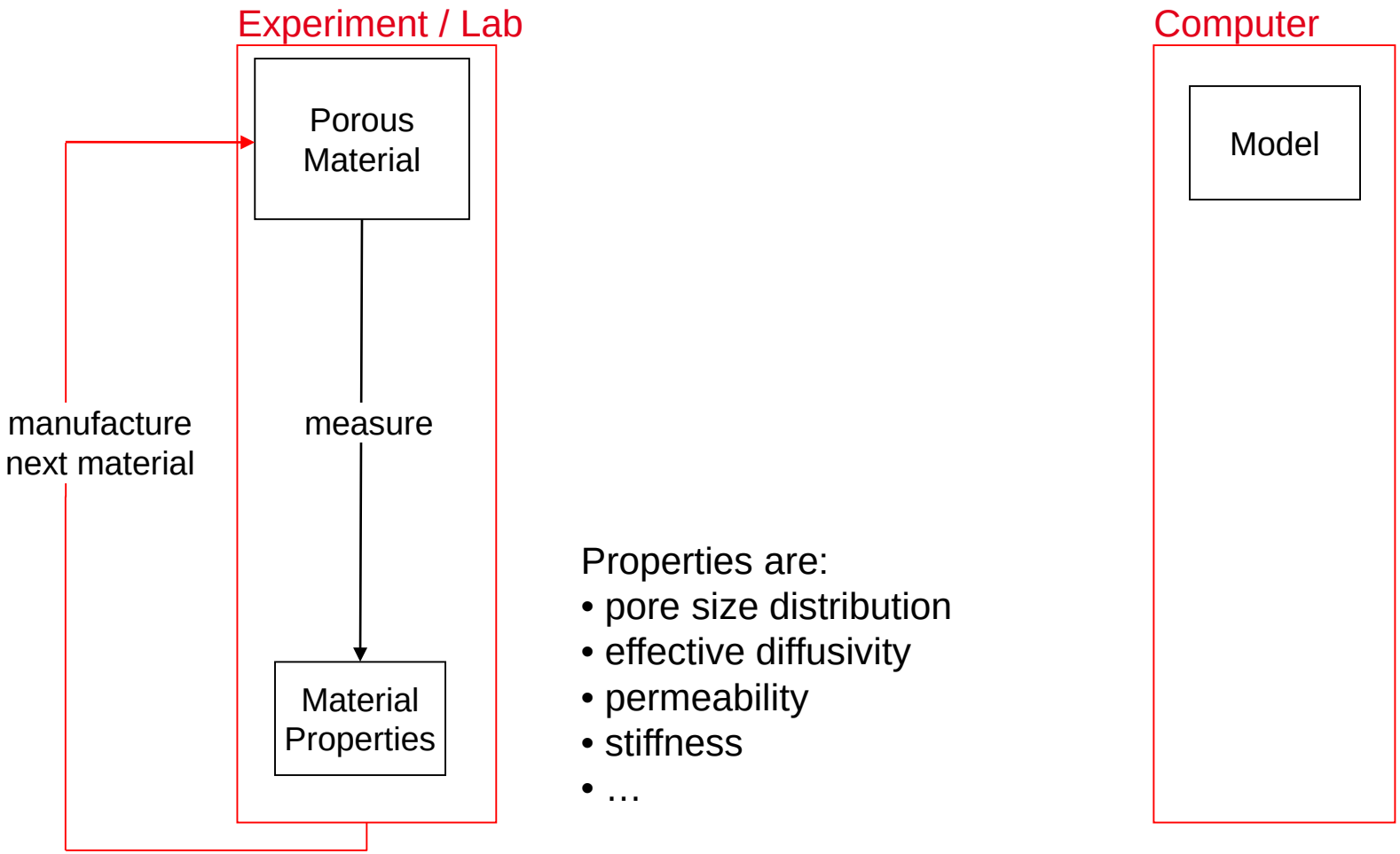

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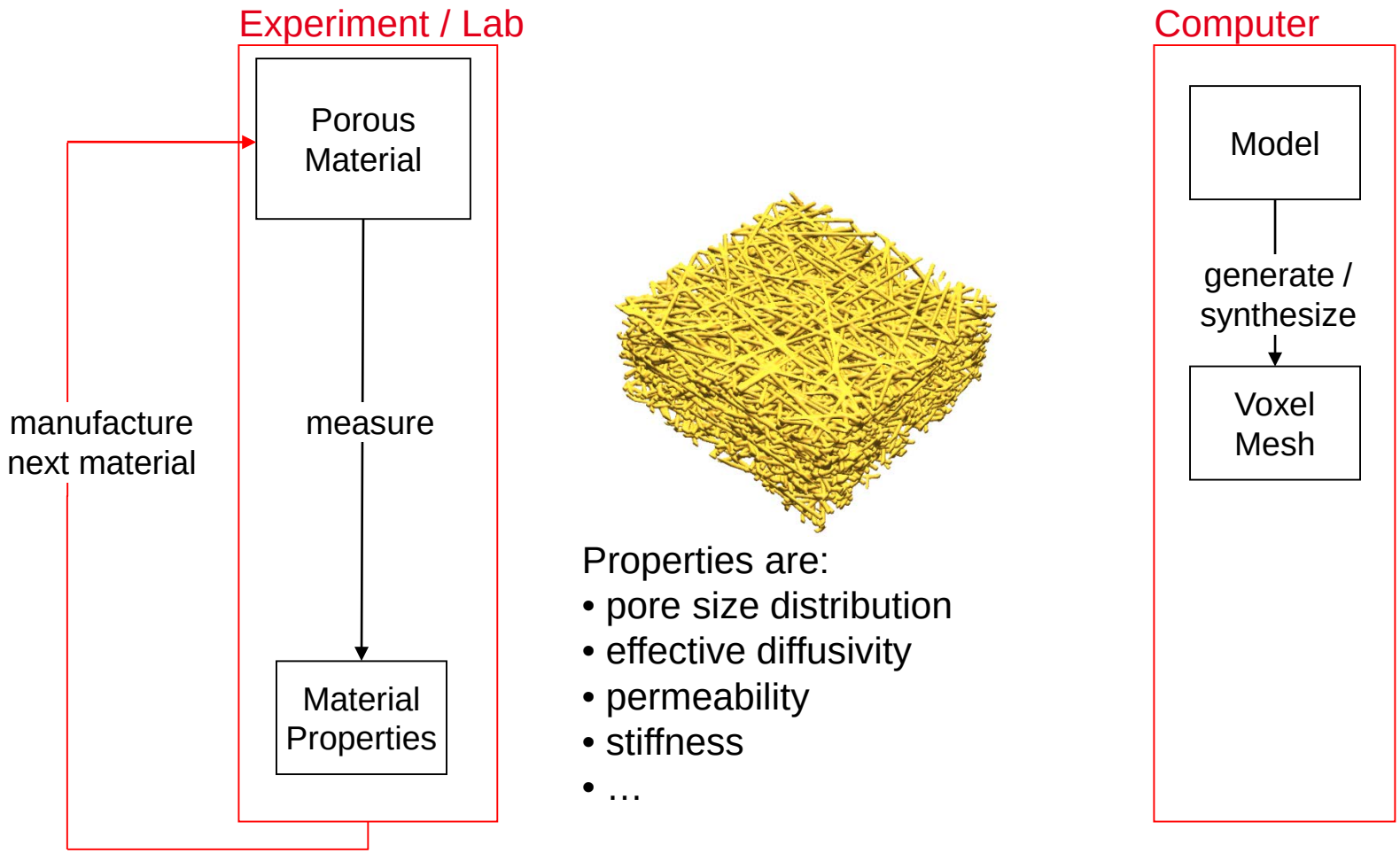


The Virtual Material Lab Approach:

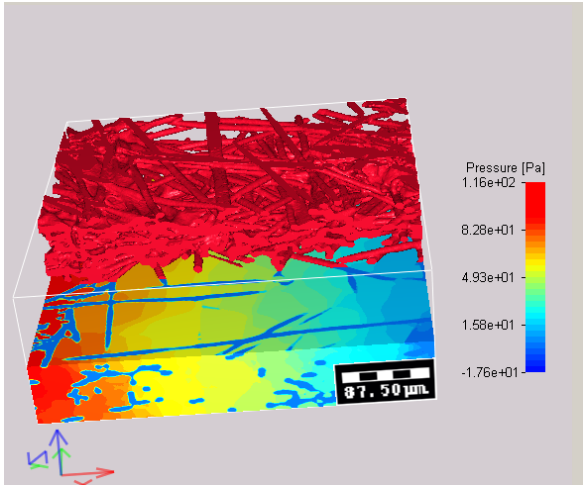
Experiment / Lab

Porous Material

measure

Material Properties

manufacture next material



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Computer

Model

generate / synthesize

Voxel Mesh

compute / analyze

Material Properties

MATH 2 MARKET

The Virtual Material Lab Approach:

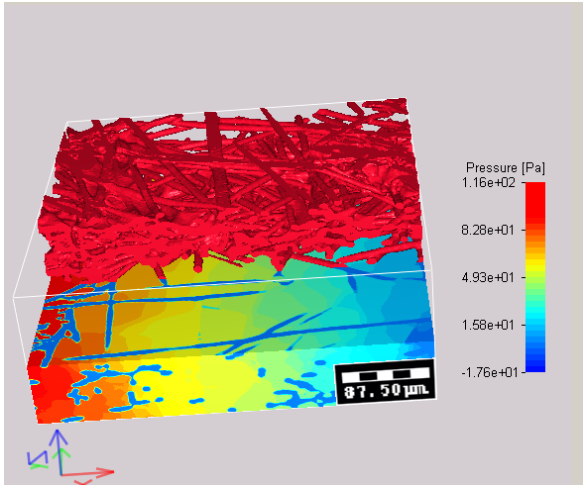
Experiment / Lab

Porous Material

measure

Material Properties

manufacture next material



Properties are:
- pore size distribution
- effective diffusivity
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Computer

Model

generate / synthesize

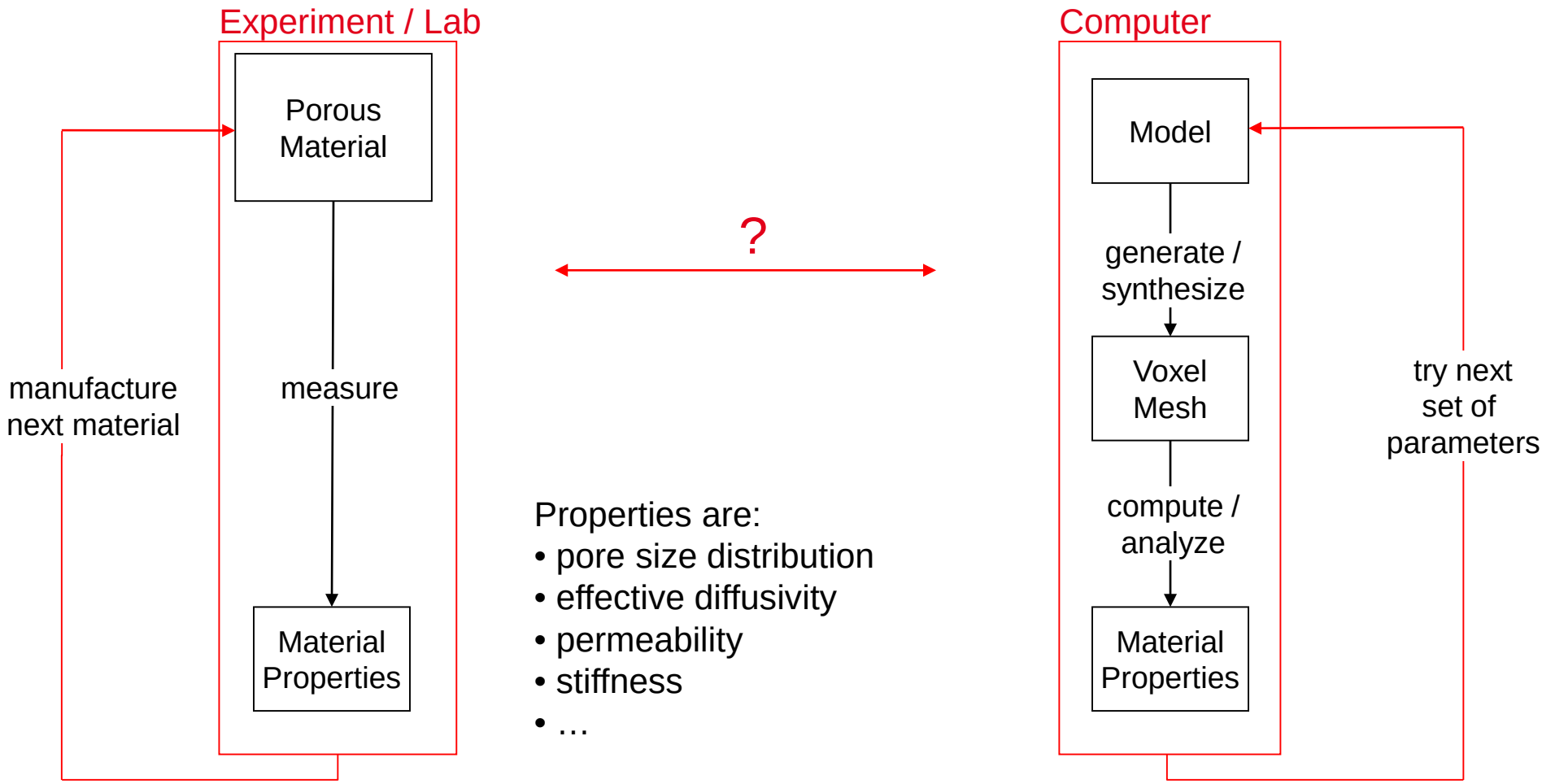
Voxel Mesh

compute / analyze

Material Properties

try next set of parameters

The Virtual Material Lab Approach:



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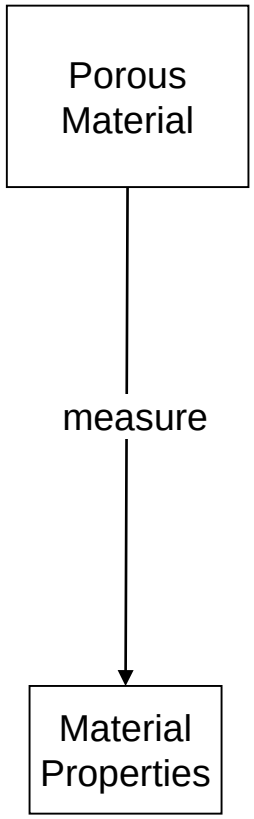
Validation - Step 1:
Analysis or Property Computations



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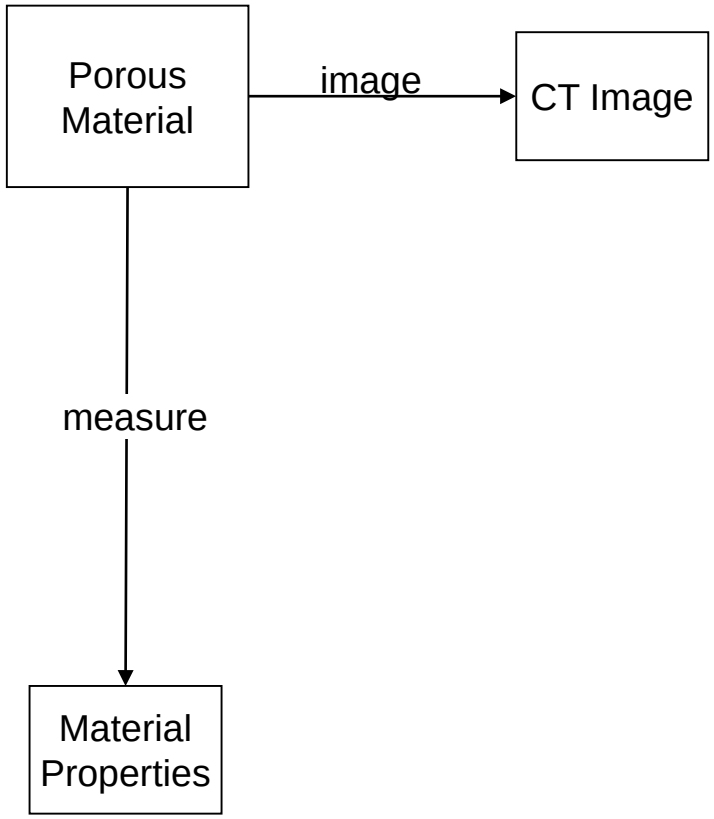

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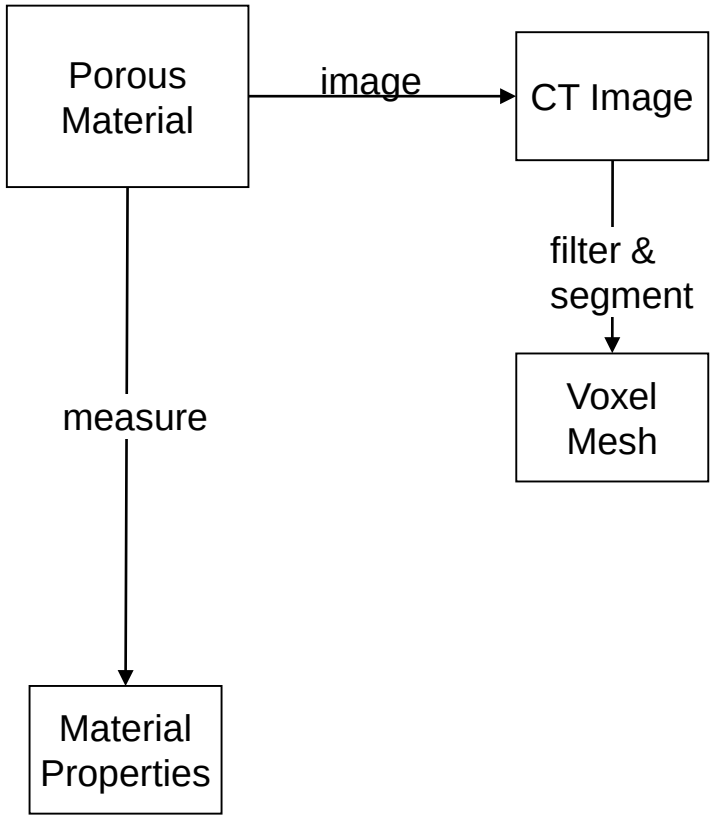

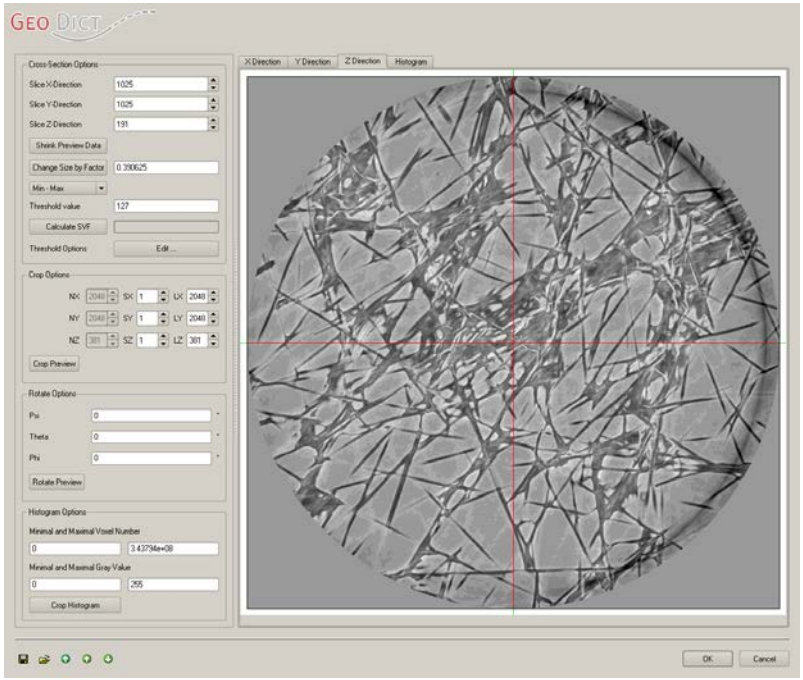

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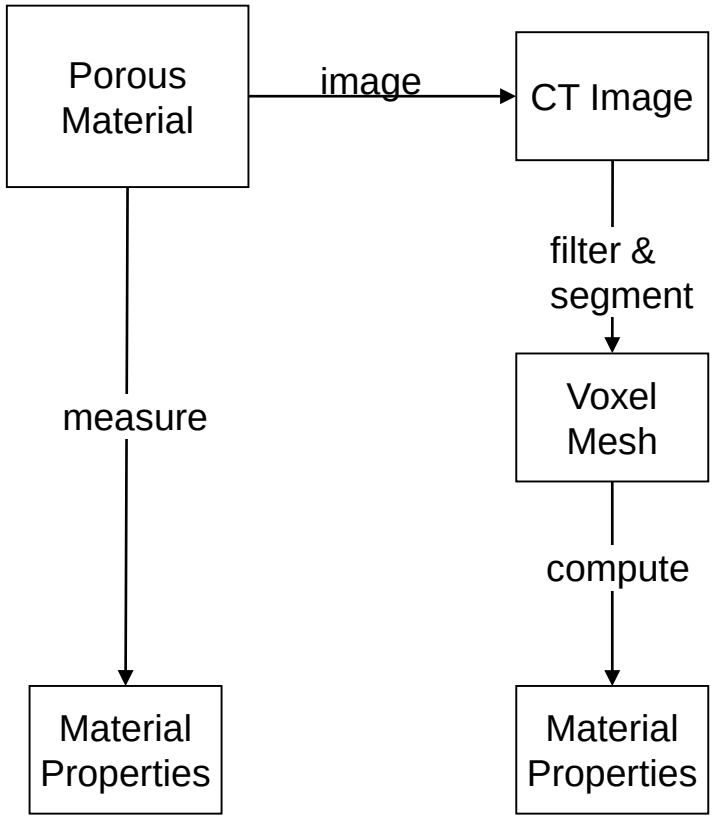

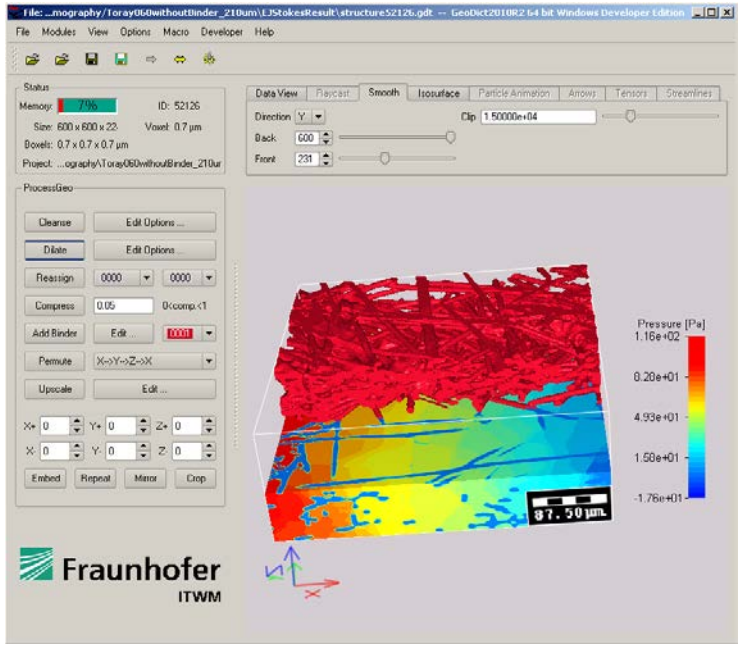

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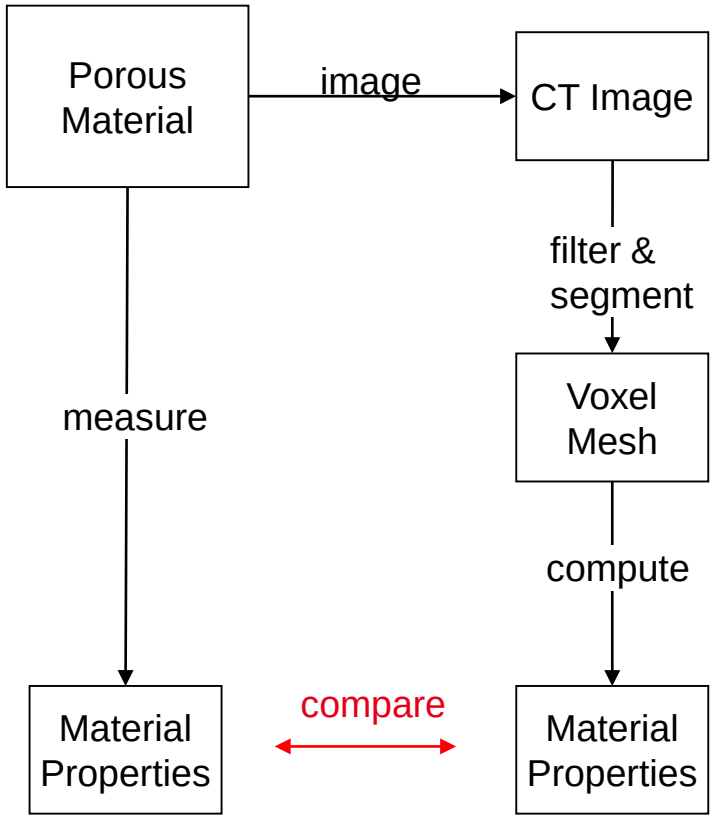
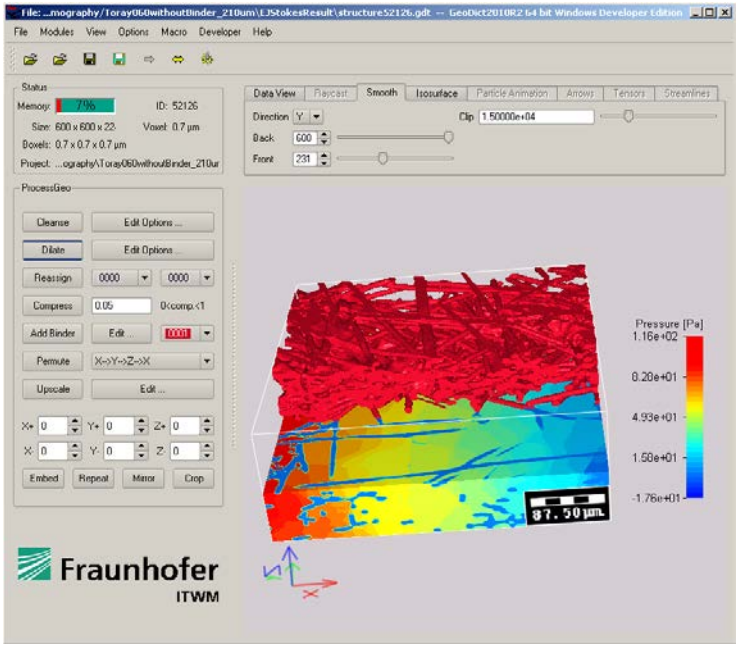
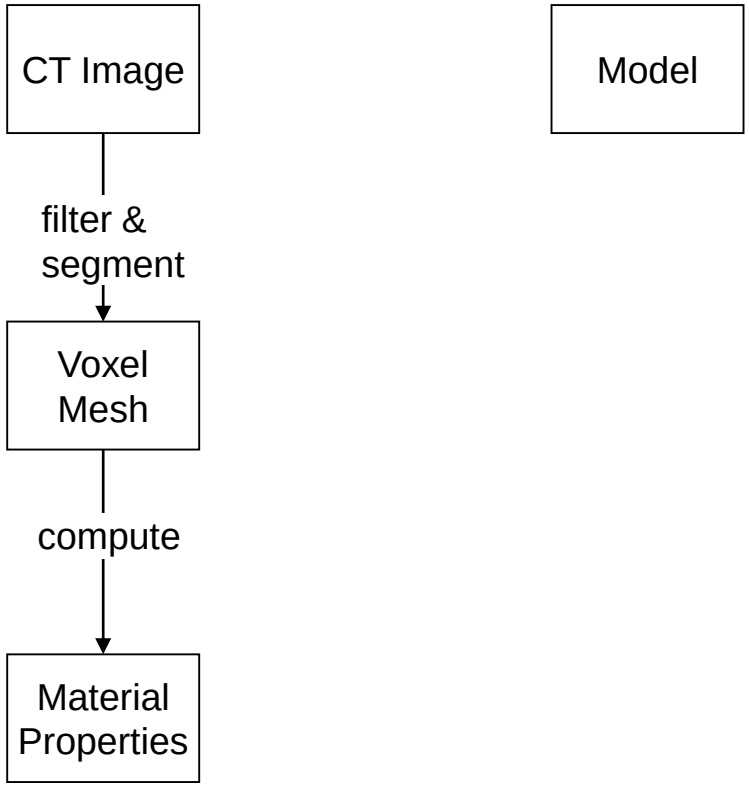




Validation - Step 2: Synthesis or Material Models



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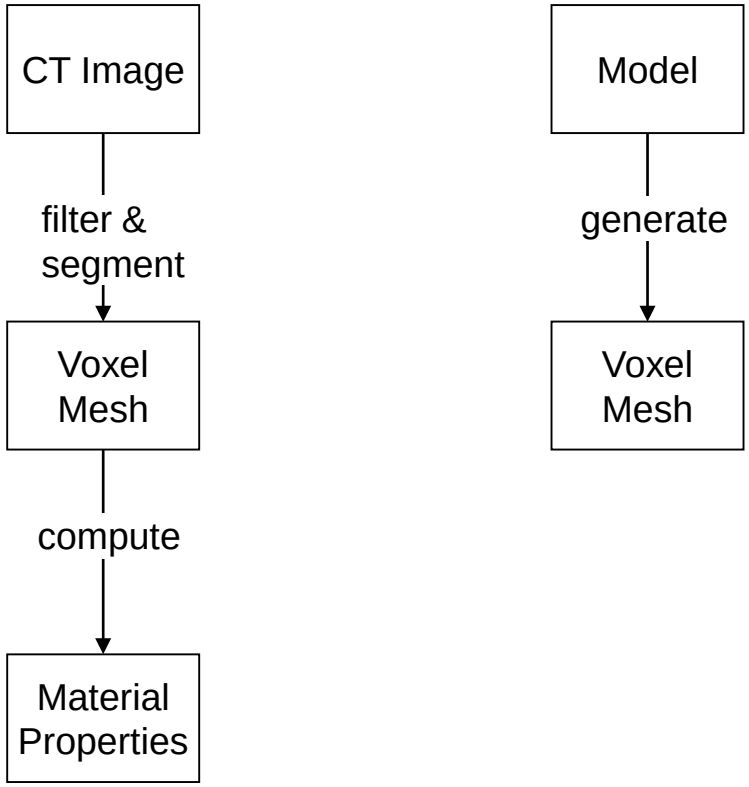

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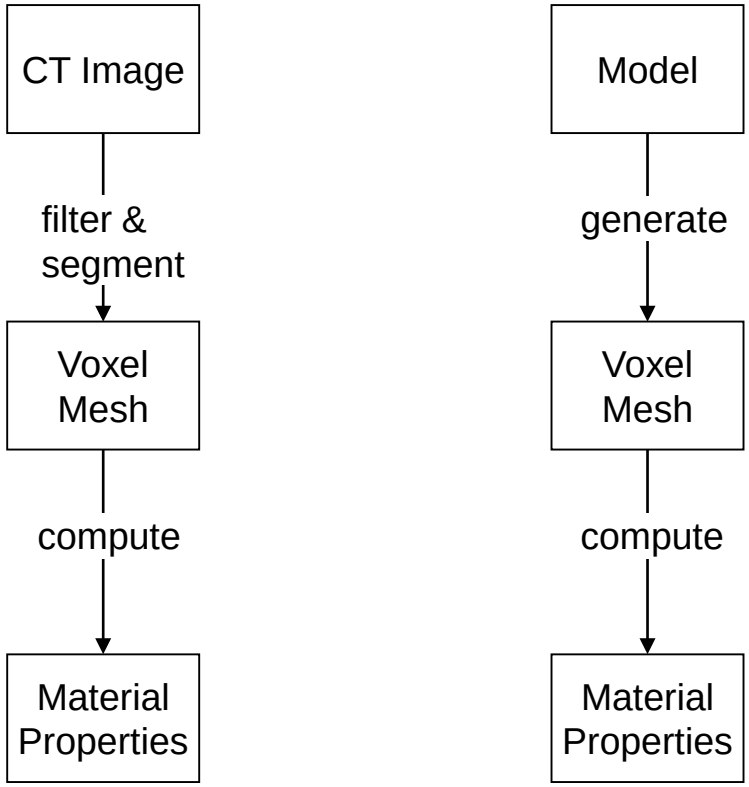

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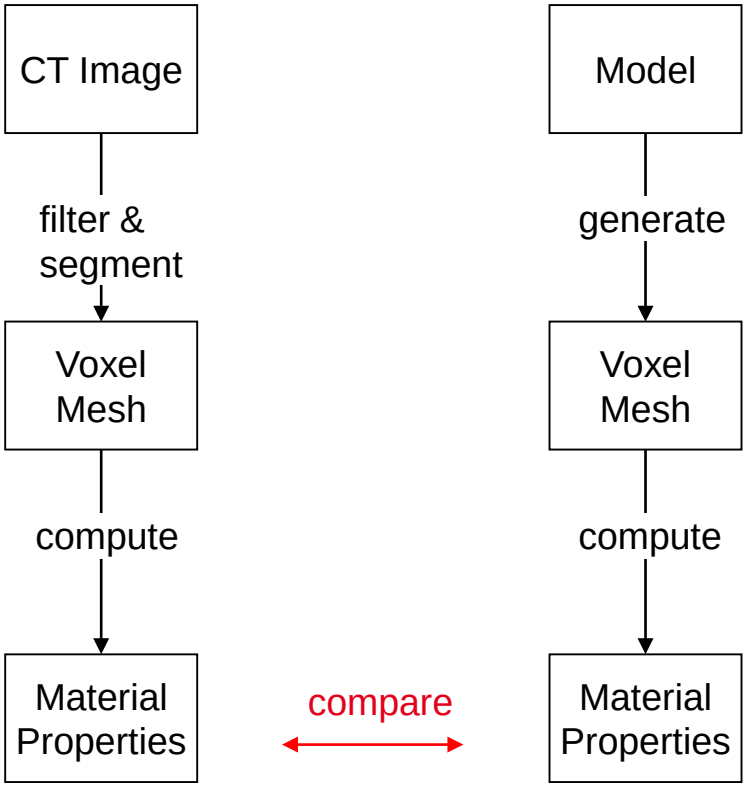

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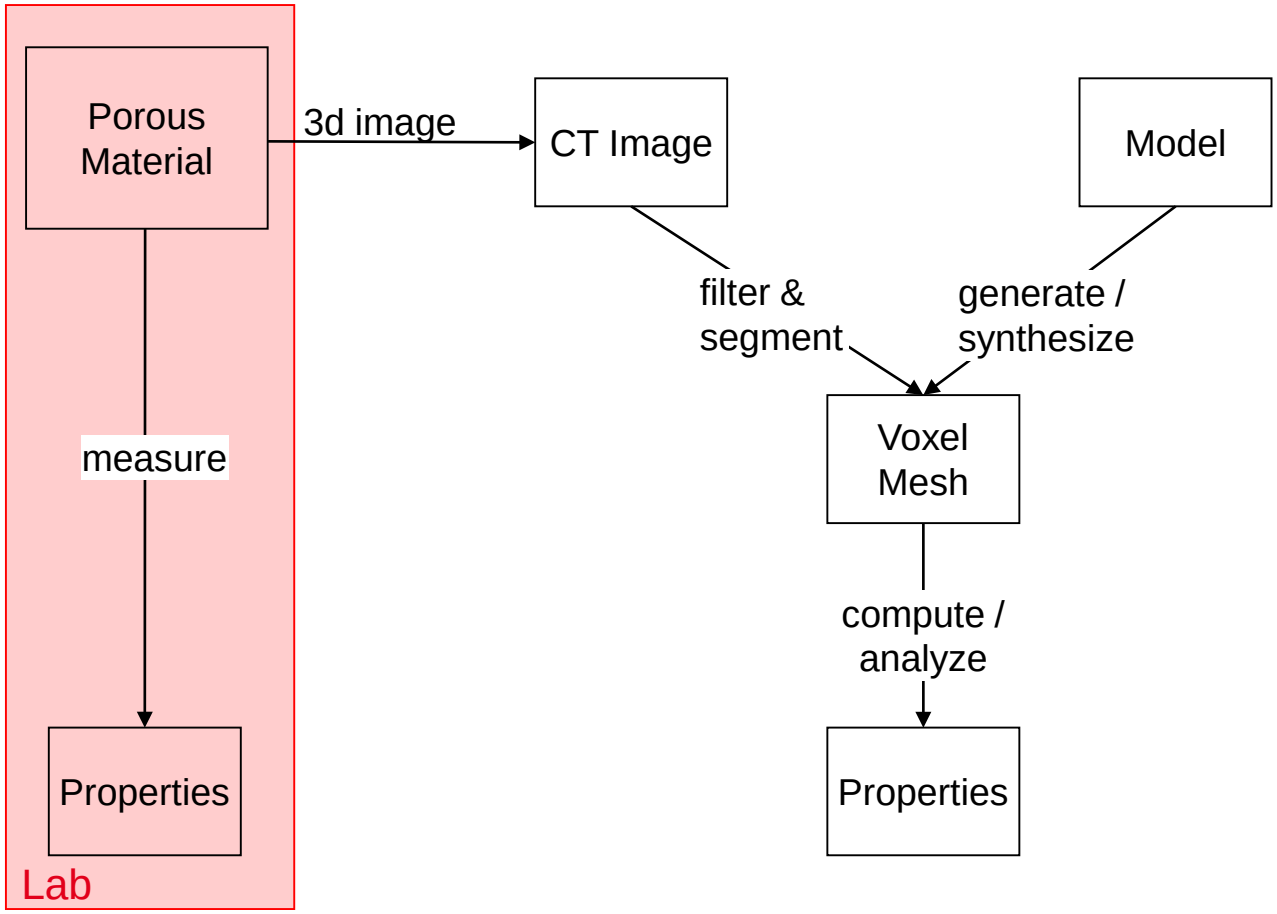

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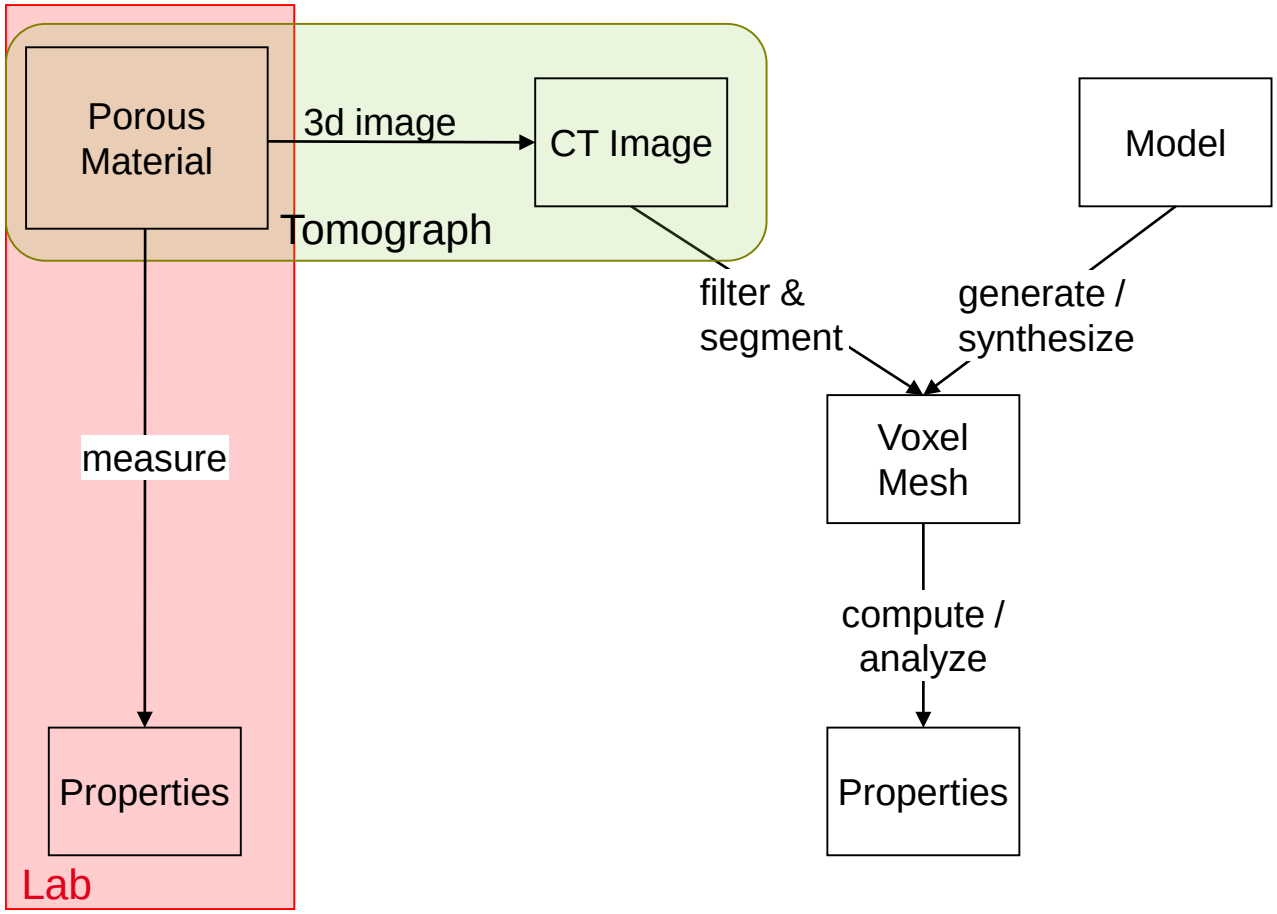

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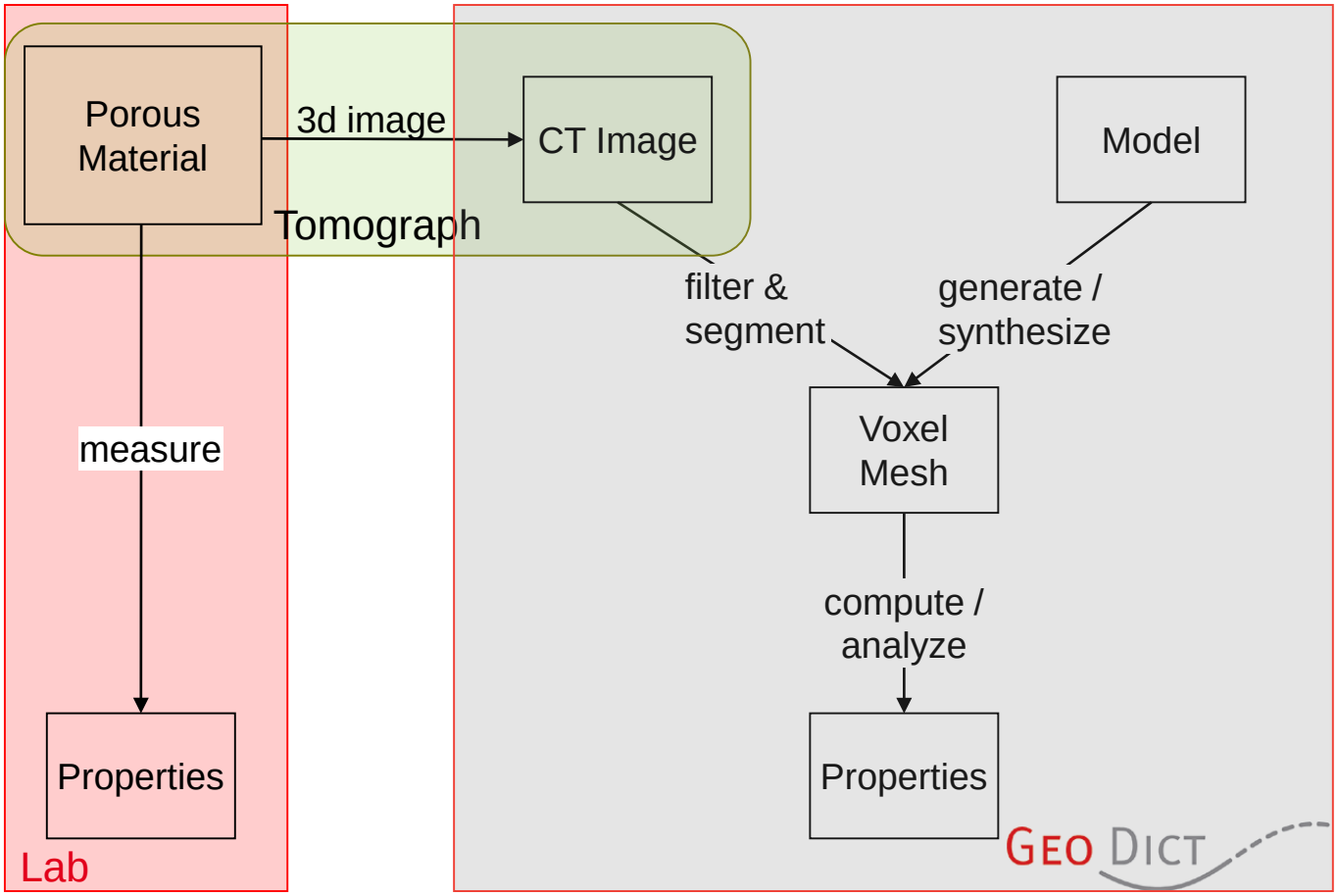
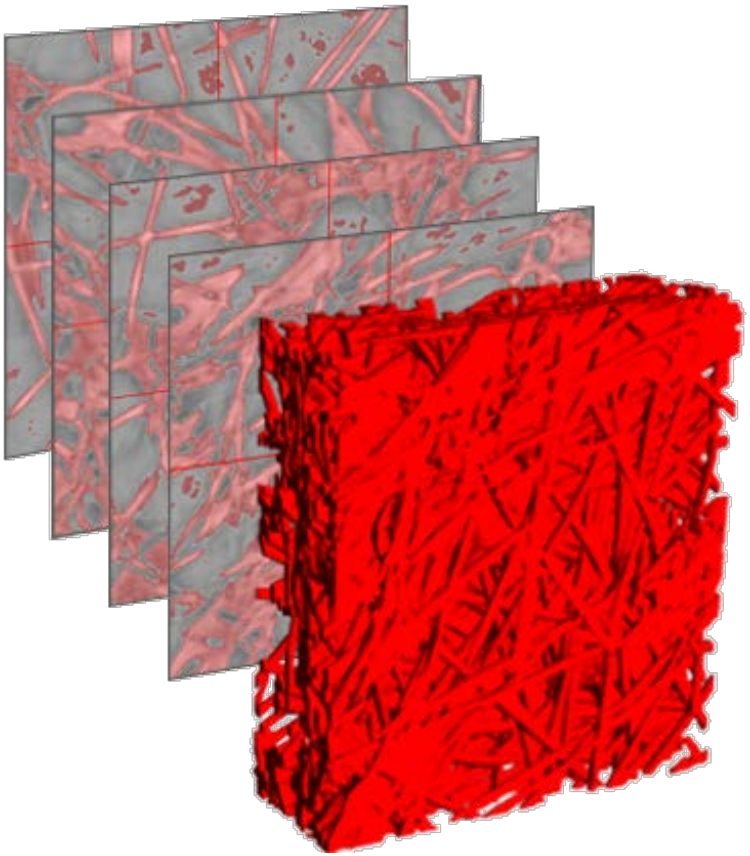
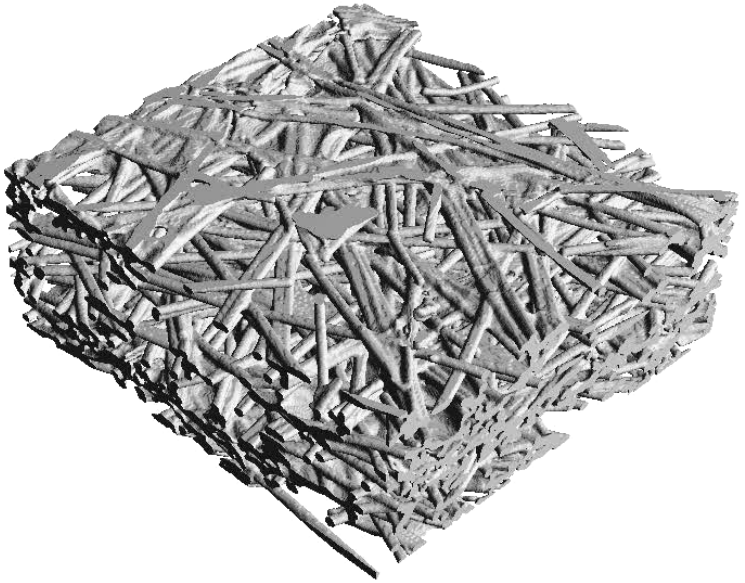


2. Import and Analysis of CT Images

Import of CT Data (GDL)

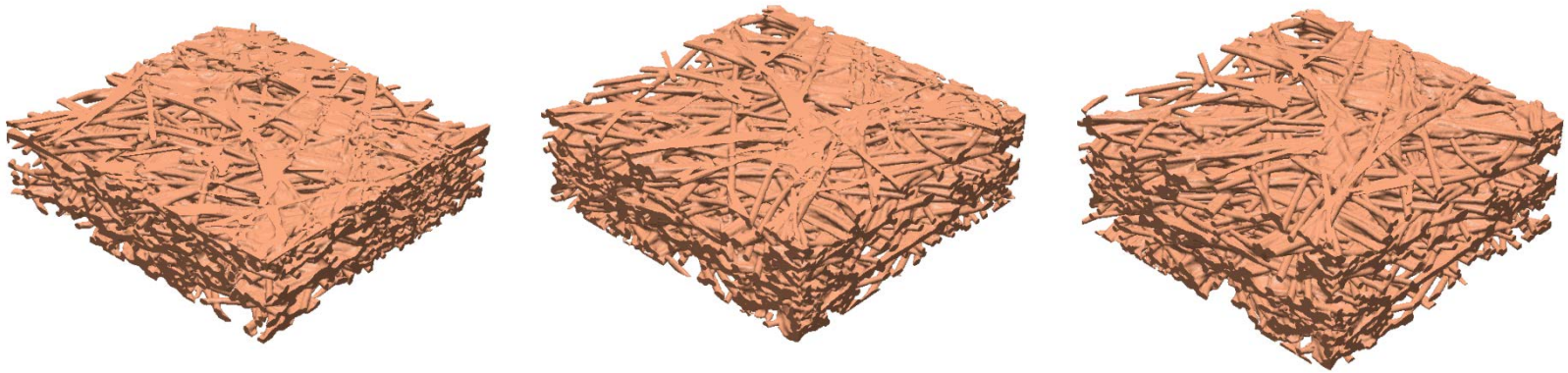




Transport Properties at Different Compression Levels

Data from Paul Scherrer Institute:

- Tomography images of Toray TGP H 060 at different compression levels
- Diffusivity, permeability and conductivity were measured at different compression levels experimentally



Becker, Flückiger, Reum, Büchi, Marone, Stampanoni, 2009, J. Electrochem. Soc. 156

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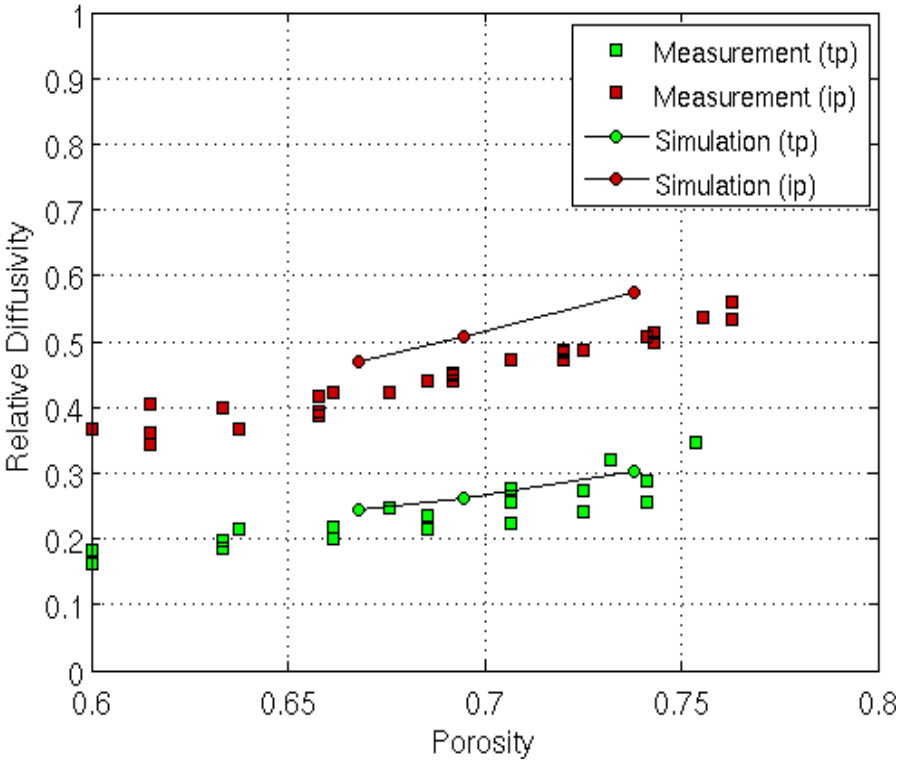

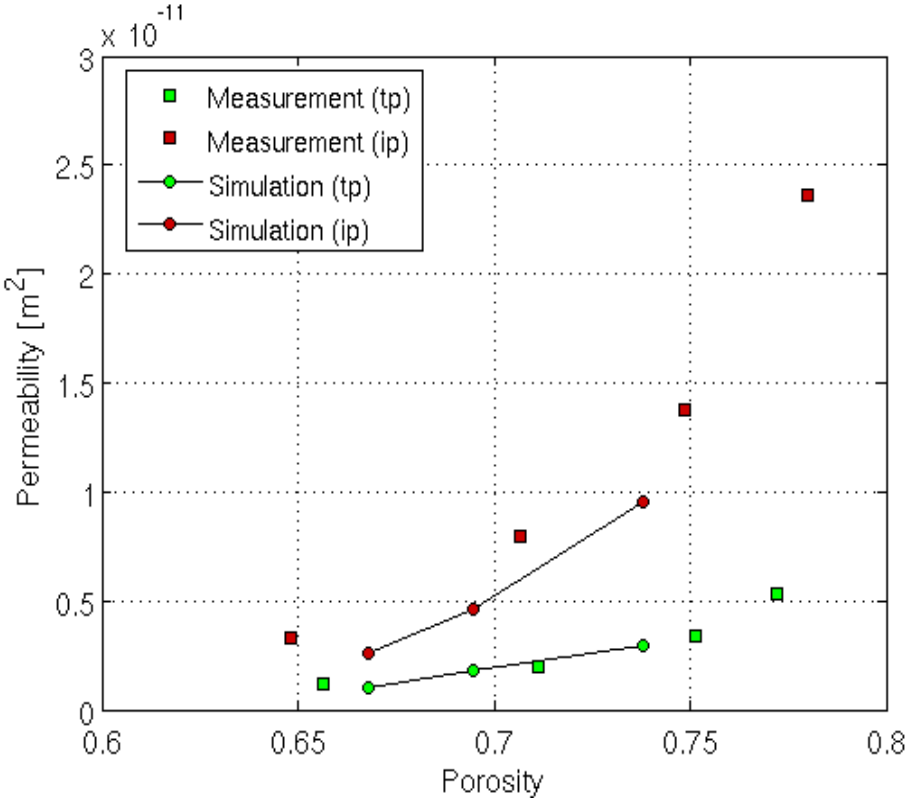

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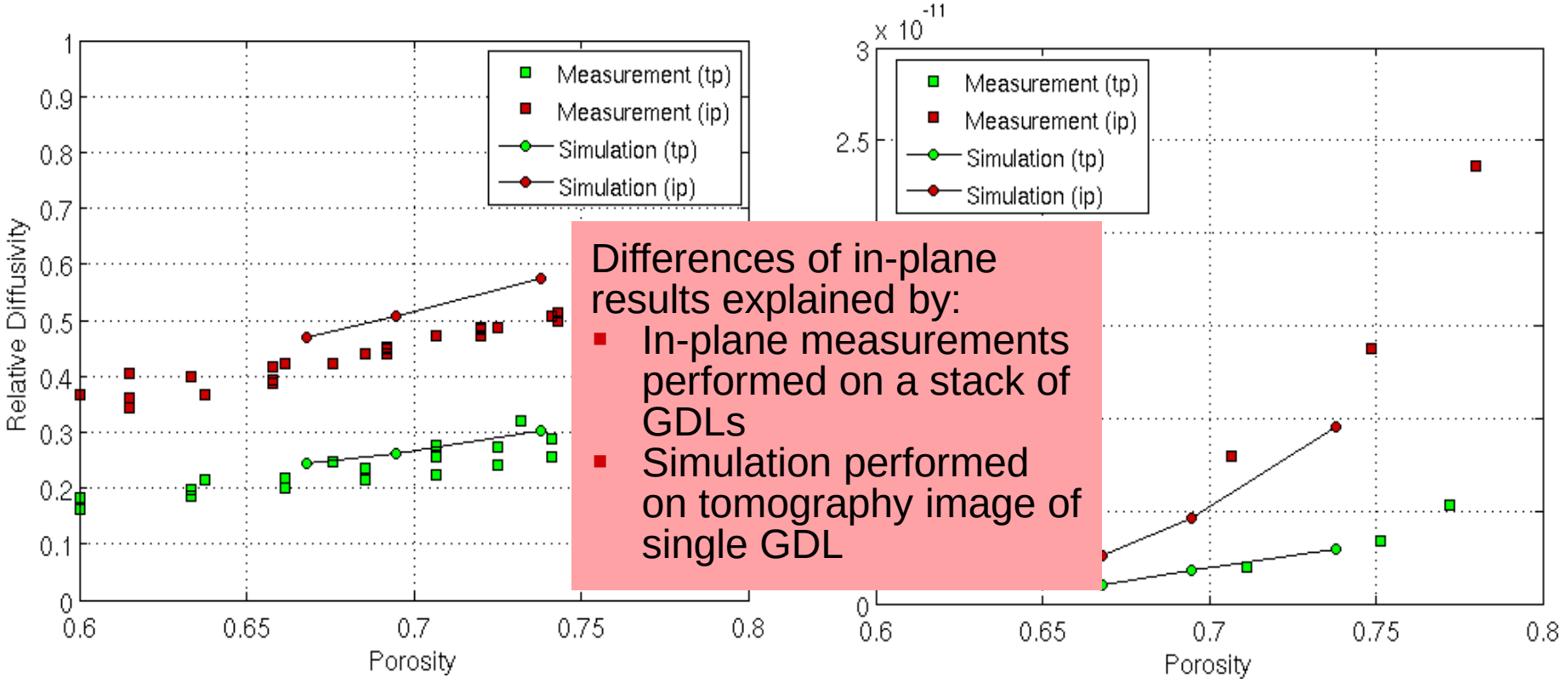


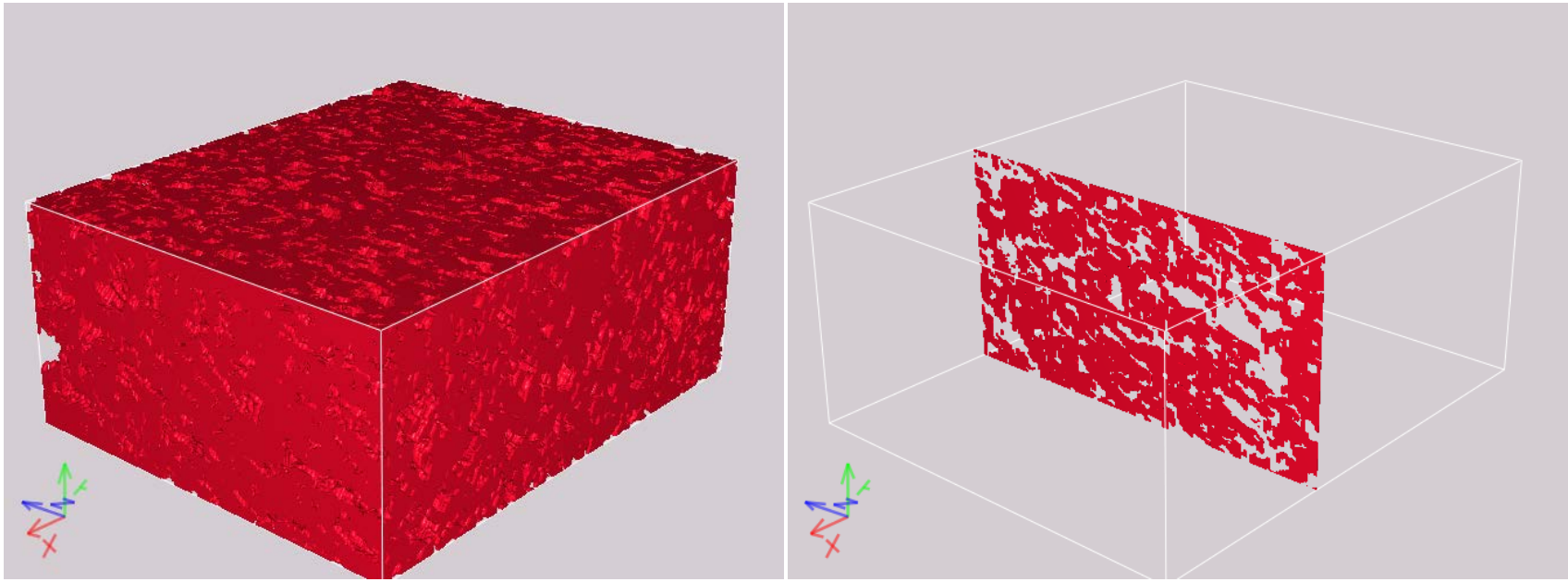
Differences of in-plane results explained by:

- In-plane measurements performed on a stack of GDLs
- Simulation performed on tomography image of single GDL

Becker, Flückiger, Reum, Büchi, Marone, Stampanoni, 2009, J. Electrochem. Soc. 156

FIBSEM Data of Catalyst Layer

- Pore Structure obtained from FIBSEM Data (IMTEK, Uni Freiburg)



T. Hutzenlaub, J. Becker, R. Zengerle und S. Thiele, J. Power Sources 227, pp 260-266, 2013.

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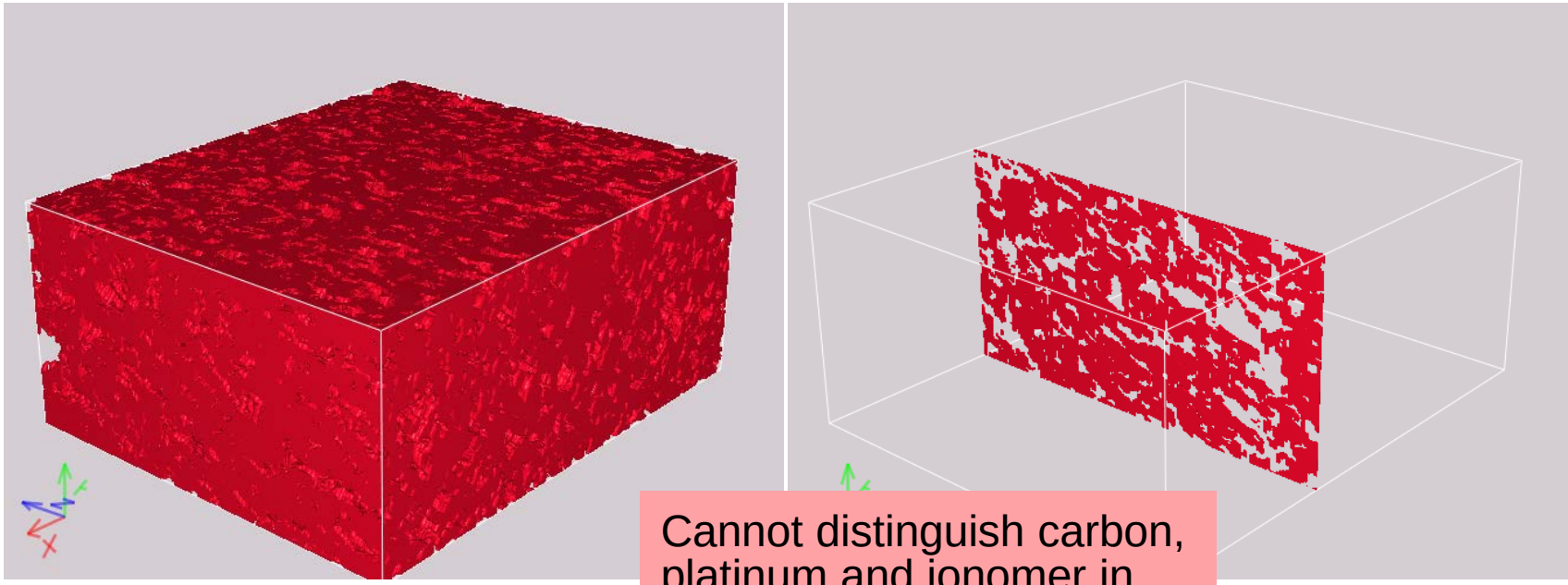

Cannot distinguish carbon, platinum and ionomer in image

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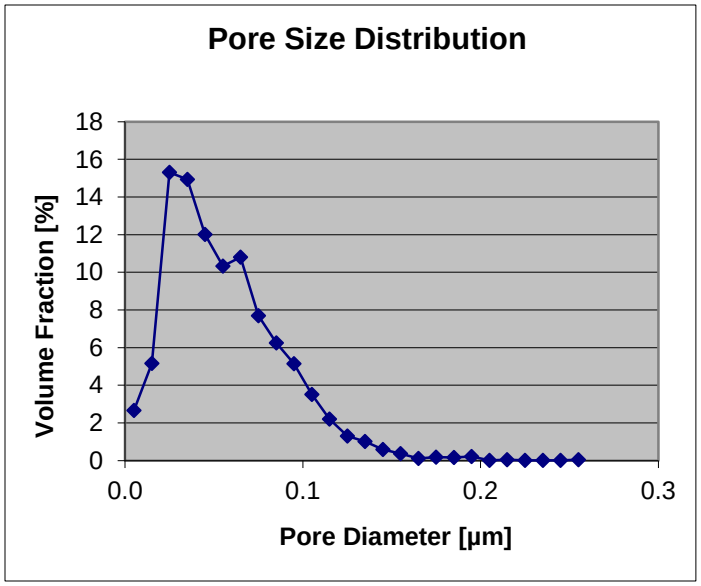
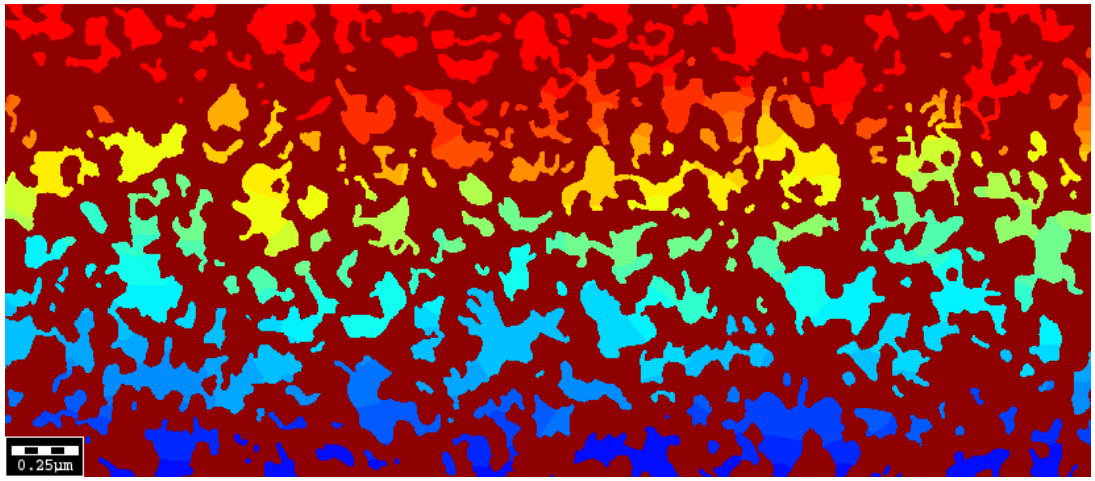




Concentration field from diffusion simulations

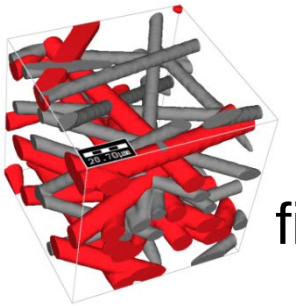
Determine:

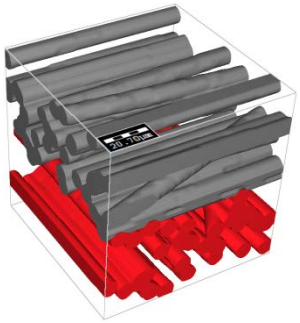
- Pore size distribution, diffusivity

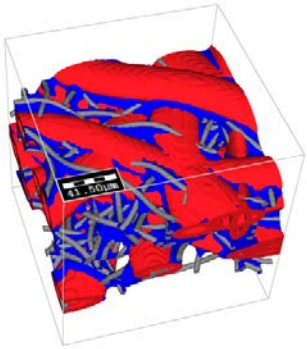
T. Hutzenlaub, J. Becker, R. Zengerle und S. Thiele, J. Power Sources 227, pp 260-266, 2013.

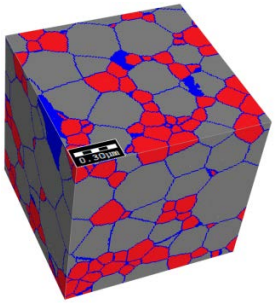
3. Structure Generation

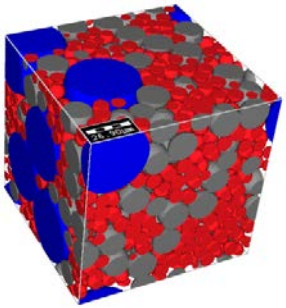
GeoDict Material Models

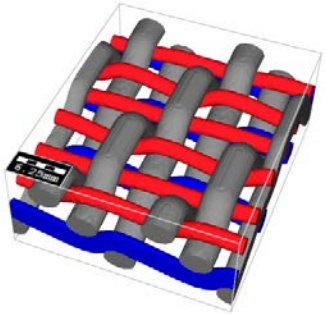


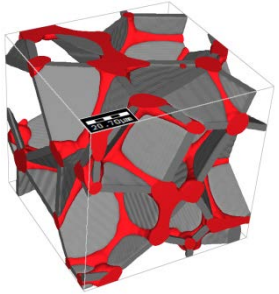


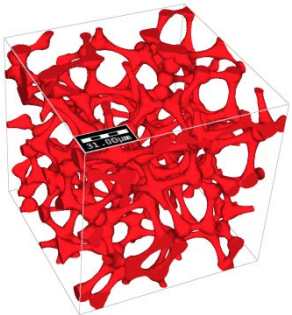












nonwovens

fiber reinforced composites

papers

ceramic materials

rocks

dense (sphere) packing

woven materials

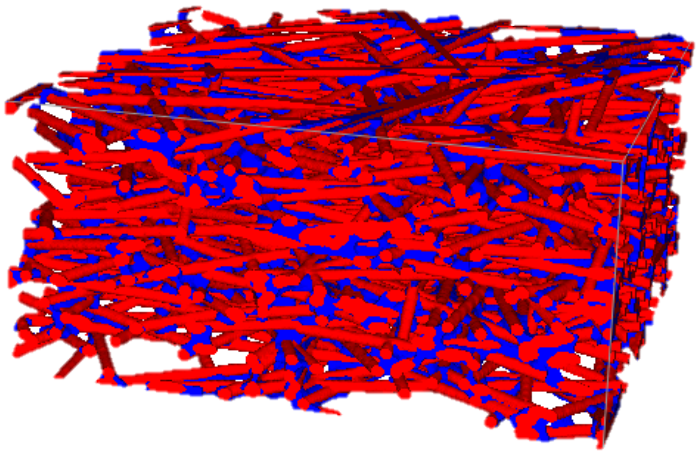
foams

sponges

regular materials

GeoDict Material Models

Gas Diffusion Layer



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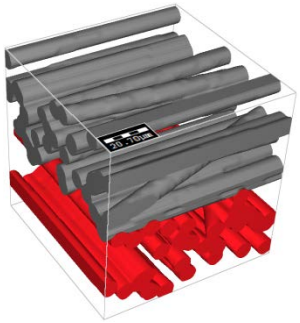
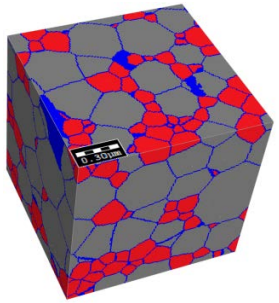
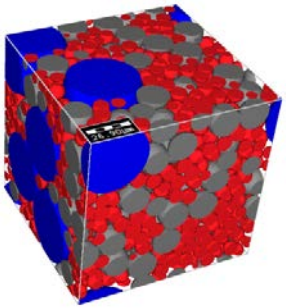
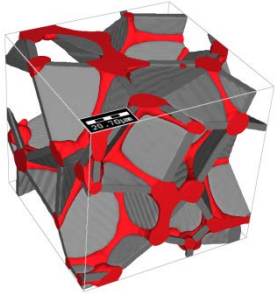
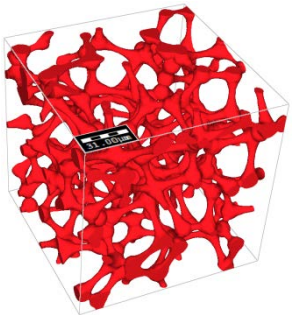
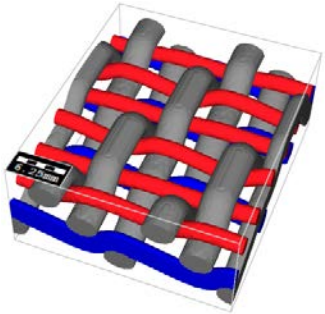






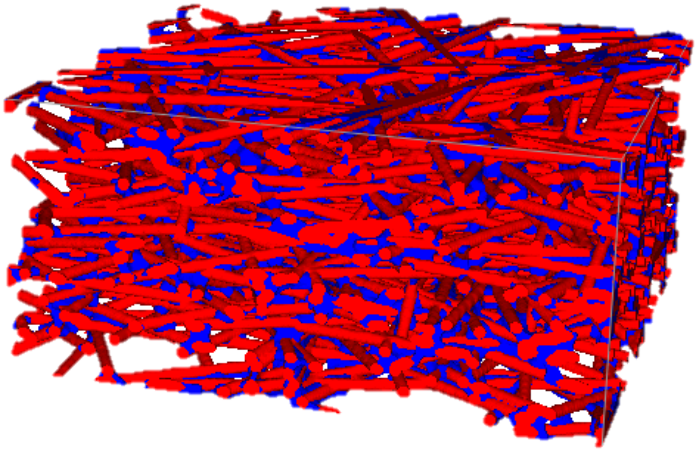




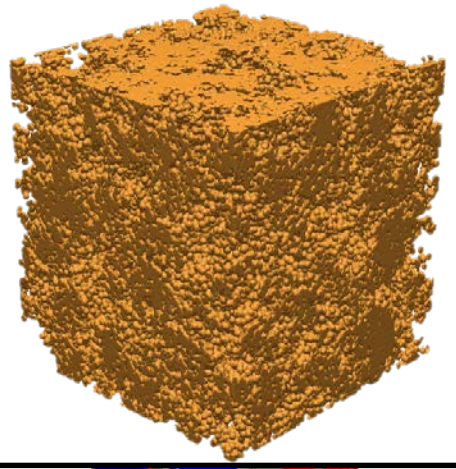


GeoDict Material Models

Gas Diffusion Layer



Microporous Layer



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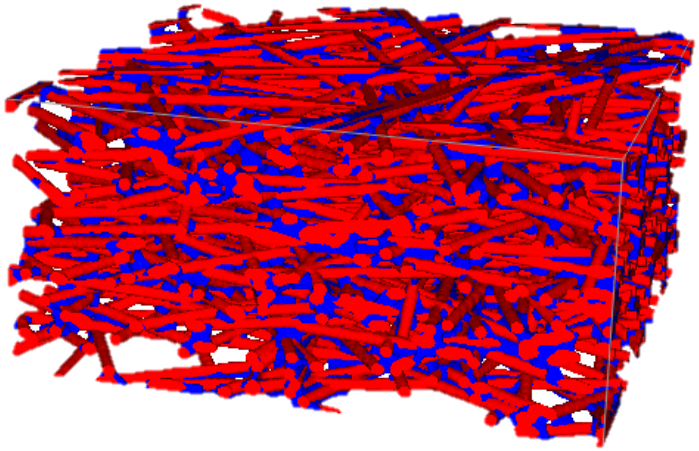
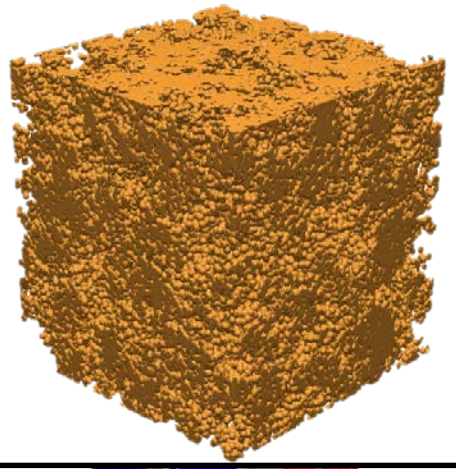
GeoDict Material Models

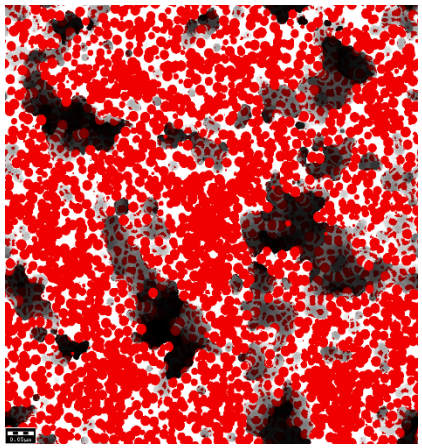
Gas Diffusion Layer



Microporous Layer



Catalyst Layer



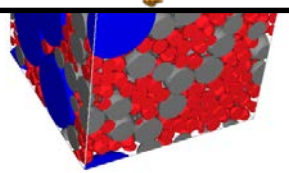
ere) packing

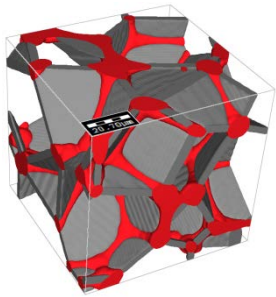
materials

ms

nges

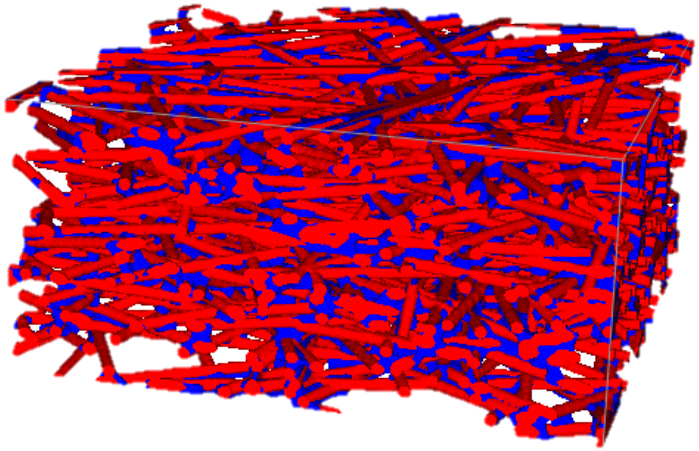
materials



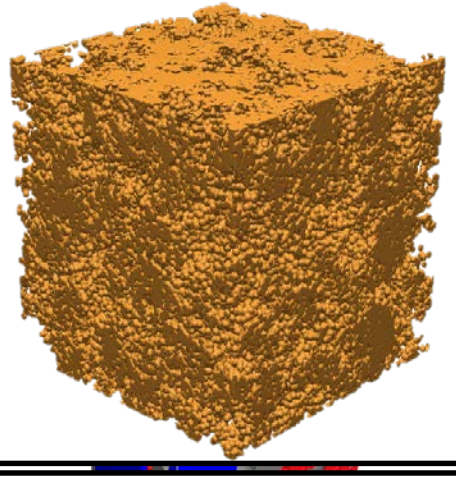


GeoDict Material Models

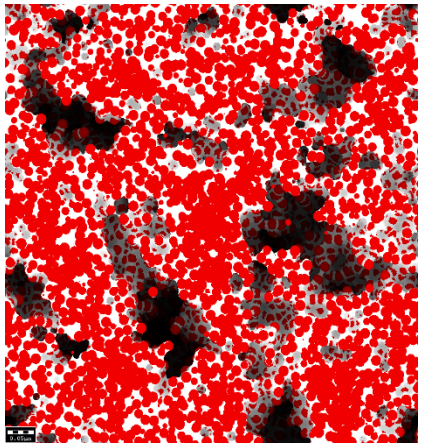
Gas Diffusion Layer



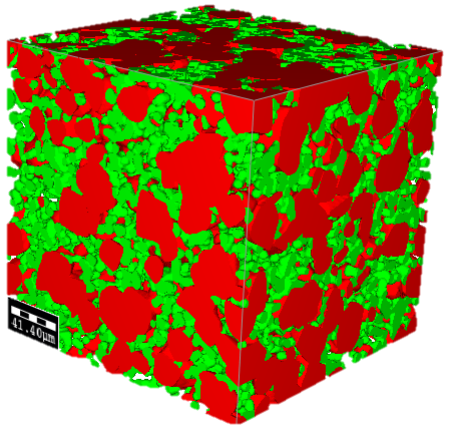
Microporous Layer



Catalyst Layer



LiO Battery Electrode



Gas Diffusion Layer Model

Created with a stochastic process

Input:
- Porosity
- Thickness
- Fiber diameter and length
- Fiber cross sectional shape
- Fiber orientation tensor

MATH 2 MARKET

Gas Diffusion Layer Model

Created with a stochastic process

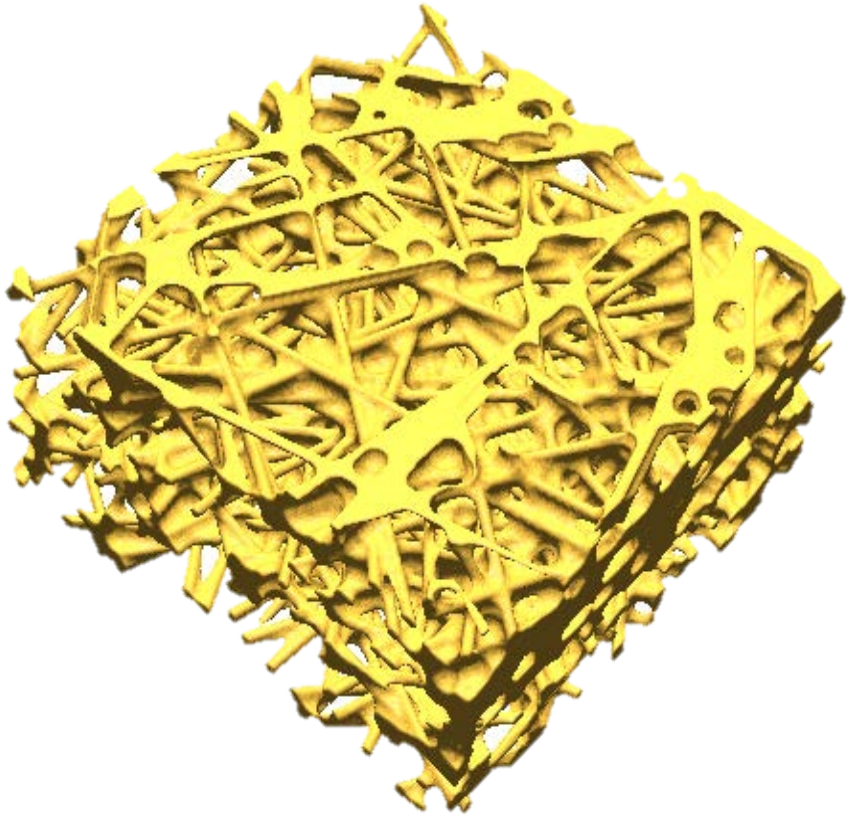
Input:
- Porosity
- Thickness
- Fiber diameter and length
- Fiber cross sectional shape
- Fiber orientation tensor
- (Fiber crimp)

MATH 2 MARKET

Gas Diffusion Layer Model

Created with a stochastic process

Input:
- Porosity
- Thickness
- Fiber diameter and length
- Fiber cross sectional shape
- Fiber orientation tensor
- (Fiber crimp)
- (Weight% binder)



MATH 2 MARKET

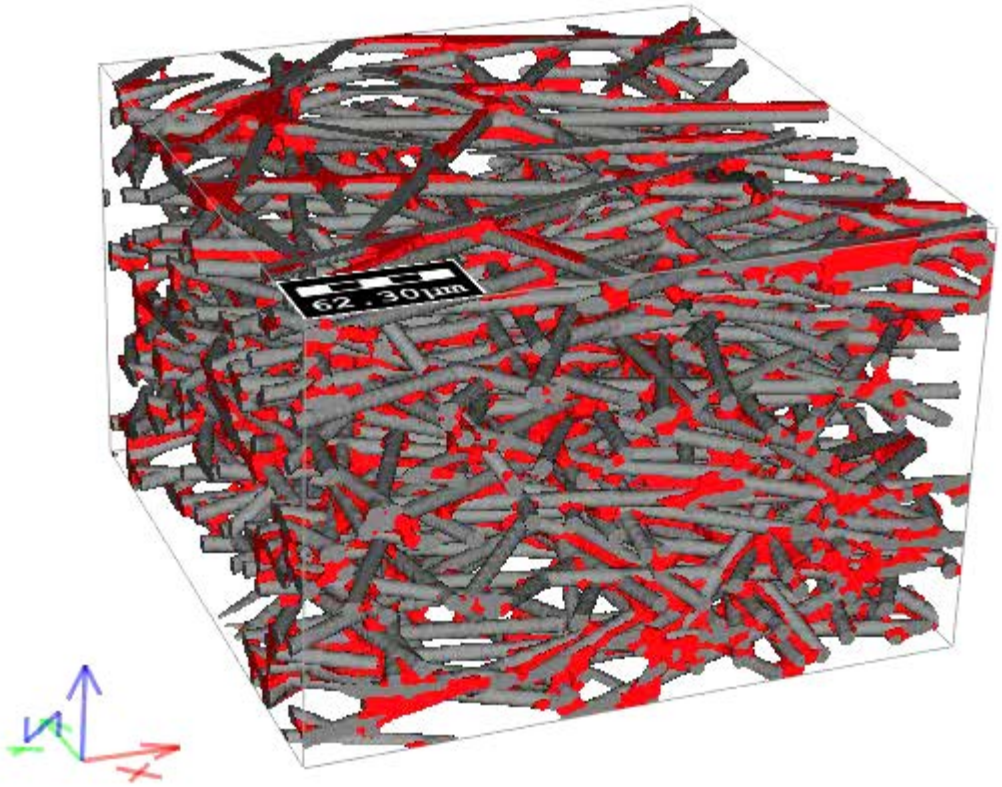
Compression of a GDL

Clamping pressure applied to GDL

FeelMath
Fraunhofer ITWM

- Transverse isotropic elastic modulus for fibers
- Isotropic elastic modulus for binder
- 30% compression

10 min on Laptop
13.5 mio grid points



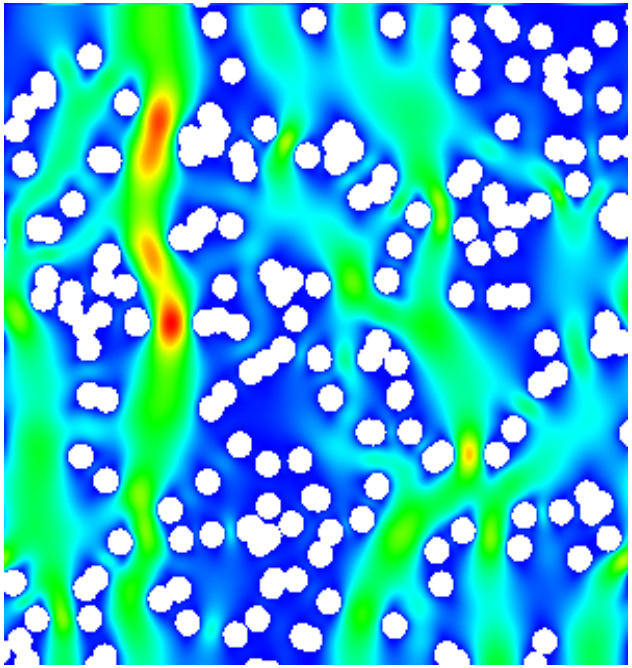
4. Determination of Transport Properties

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



Permeability

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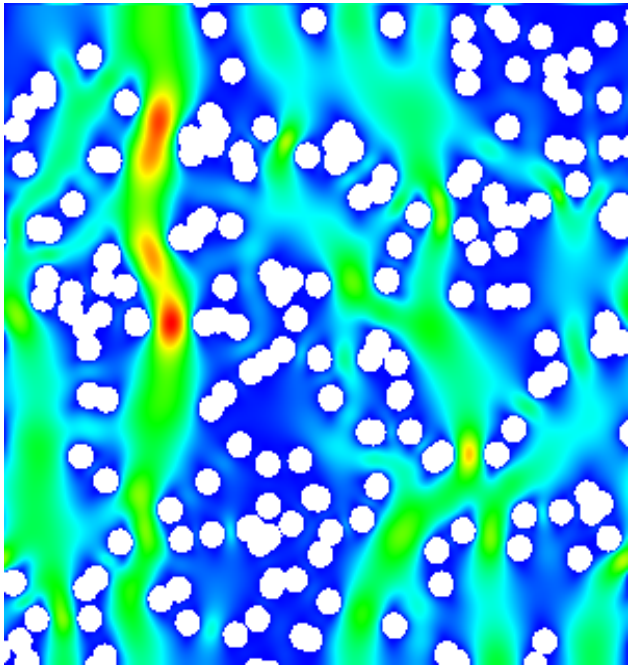


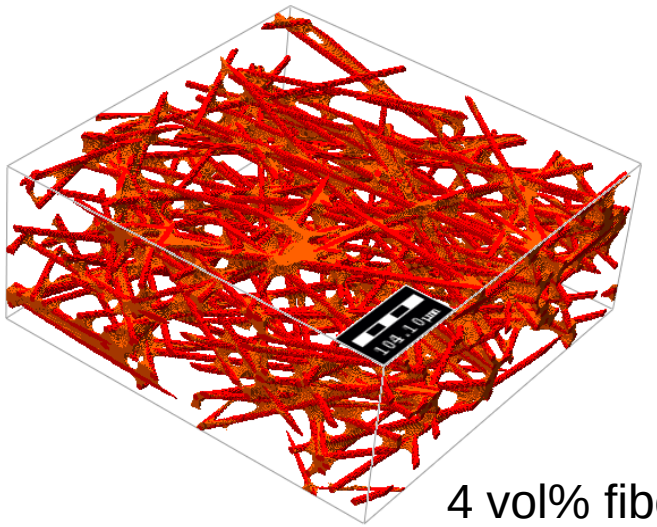
Microscopic description
(pore structure model)

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

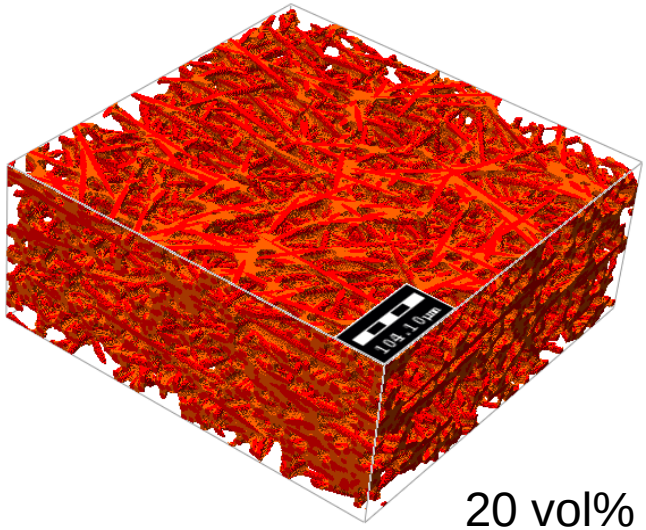
Boundary conditions: no-slip on fibre surface, pressure drop
κ can be determined from the solution!

Design Study: Effect of GDL Porosity

- 7 µm fiber diameter
- 40 wt% binder content

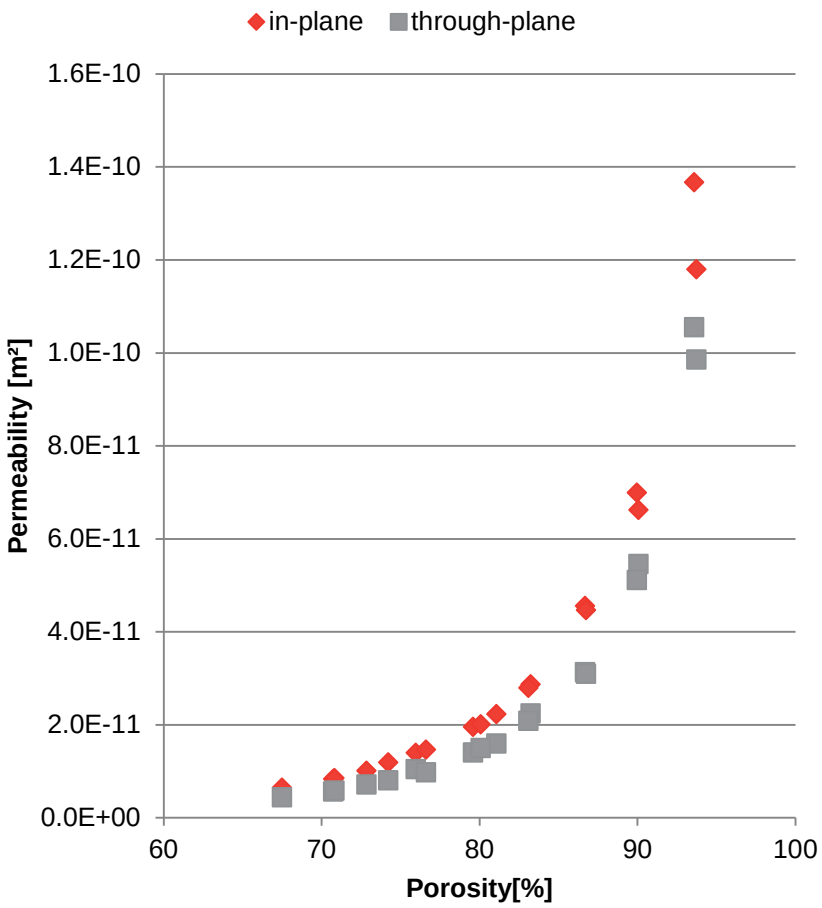


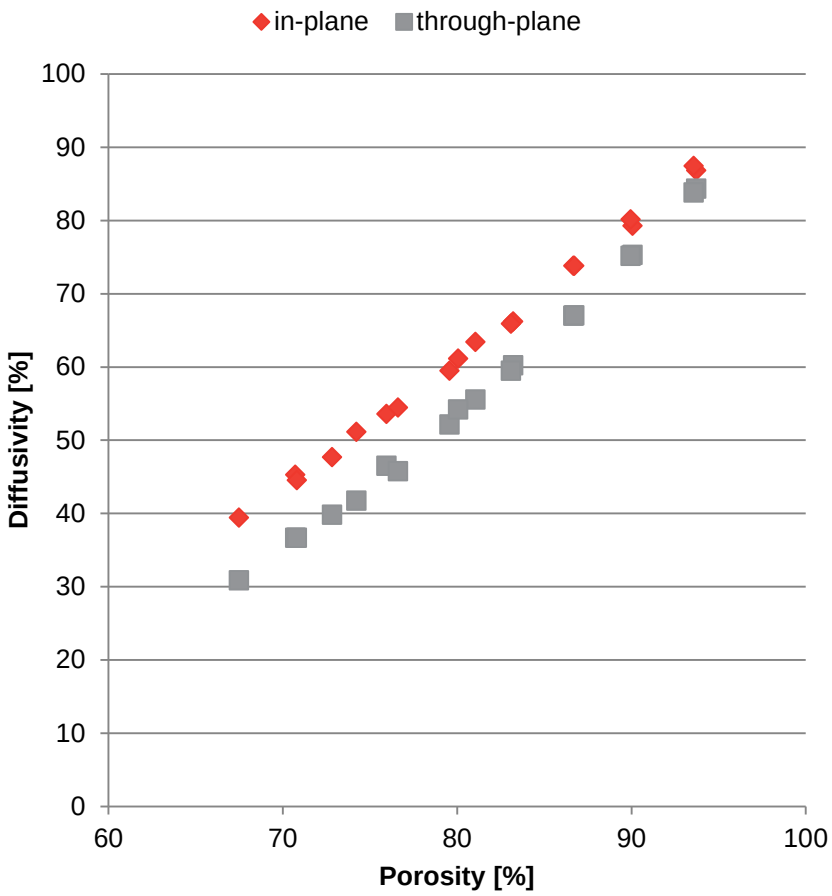
4 vol% fibers



20 vol% fibers

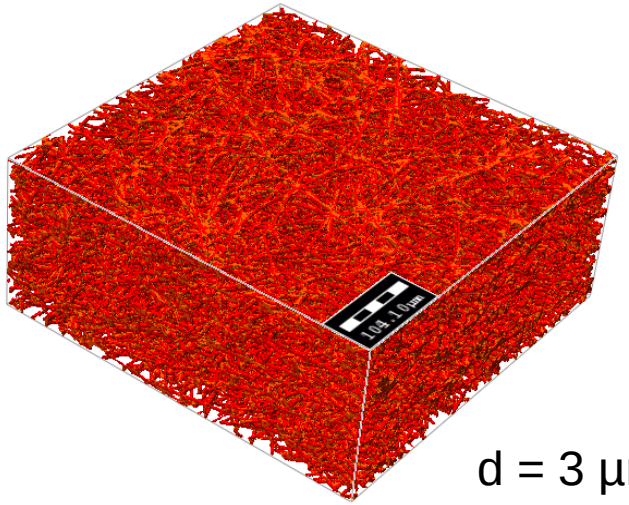
Permeability and Diffusivity



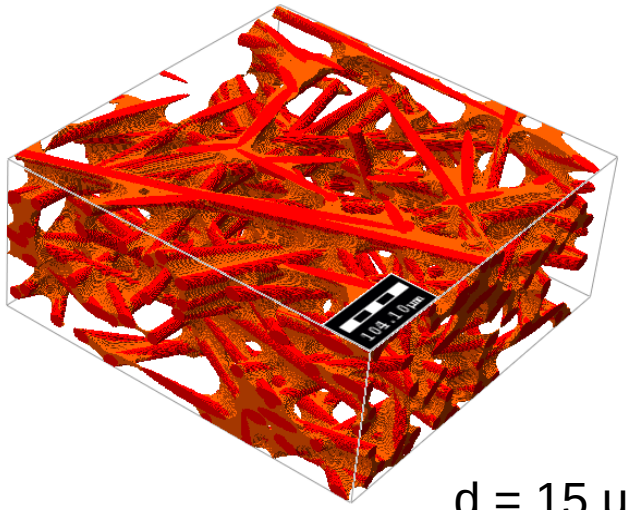


Design Study: Fiber Diameter

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

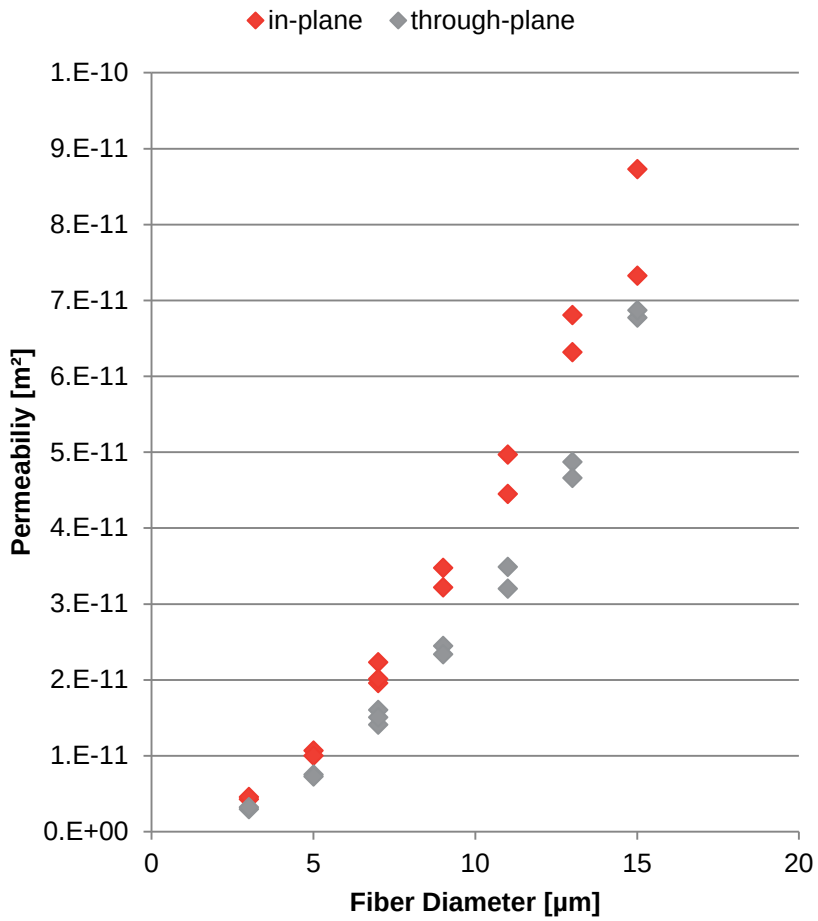


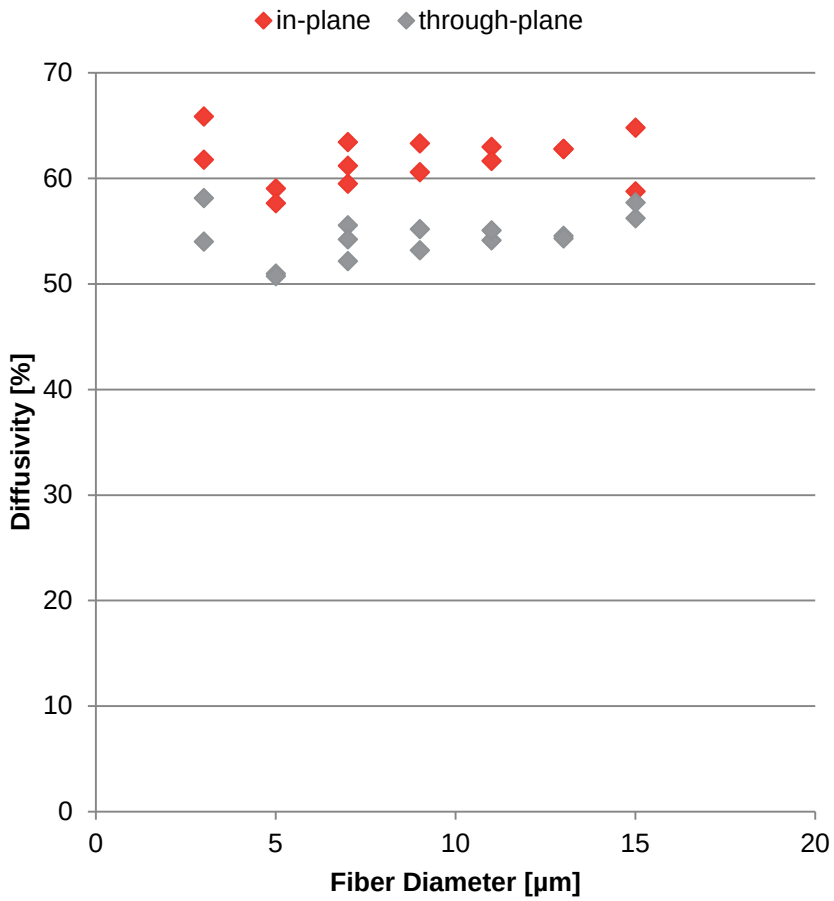
d = 3 µm



d = 15 µm

Permeability and Diffusivity





Thank You !

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