Determination of Material Parameters of Gas Diffusion Layers by Combining Pore-Morphology Method and Single Phase Simulations

PEMSim Berlin, 18.-20.09.2006

Jürgen Becker, Oleg Iliev, Volker Schulz, Konrad Steiner,
Andreas Wiegmann

Fraunhofer ITWM, Kaiserslautern

Fraunhofer Institut
Techno- und
Wirtschaftsmathematik

Introduction

Starting Point:

- three dimensional model of GDL fibre/pore structure given
- origin of 3d model:
  - reconstructed from a 3d tomography image
  - virtually created model

Aim:

- determine saturation dependent effective material parameters:
  - capillary pressure $p_c(s)$
  - permeability K(s)
  - diffusivity coefficients D(s)
  - thermal conductivities $\beta(s)$

Idea:

- use *pore morphology method* to determine phase distributions
- use single phase simulations to determine material parameters

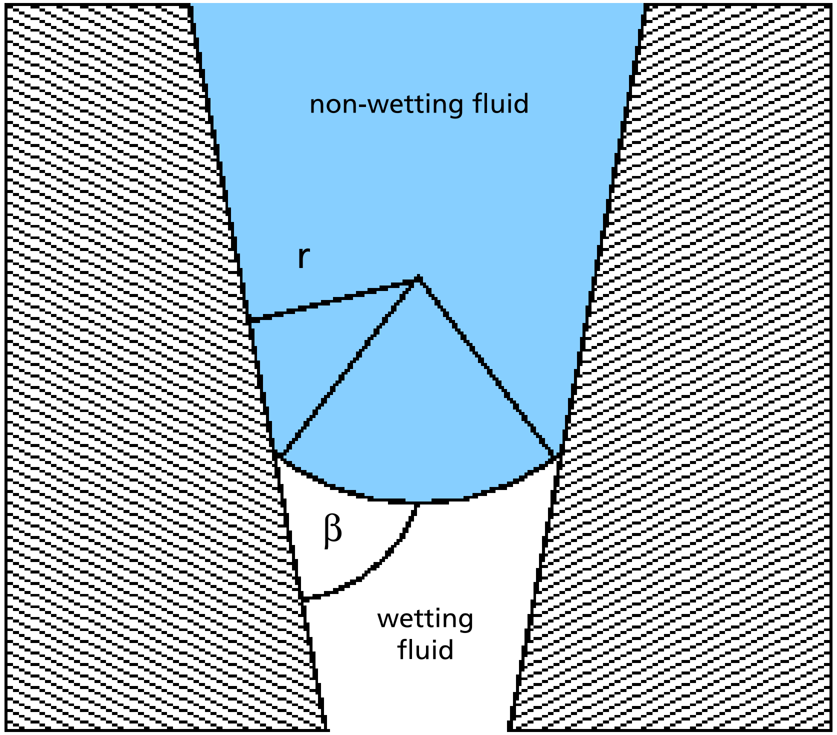
Pore Morphology Method

ingredient 1:

– Young – Laplace equation $p_c = \frac{2\sigma}{r} \cos\beta$

idea: a pore is filled with the NWP, if

$$p_c \geq \frac{2\sigma}{r} \cos\beta$$



Pore Morphology Method

ingredient 2:

– image analysis to determine pore sizes

X : pore space

B_r : structuring element (e.g. spheres of radius *r*)

morphological opening: $\mathcal{O}_{B_r}(X) = \bigcup_{B_r \subseteq X} B_r$

Opening = Dilation (Erosion)

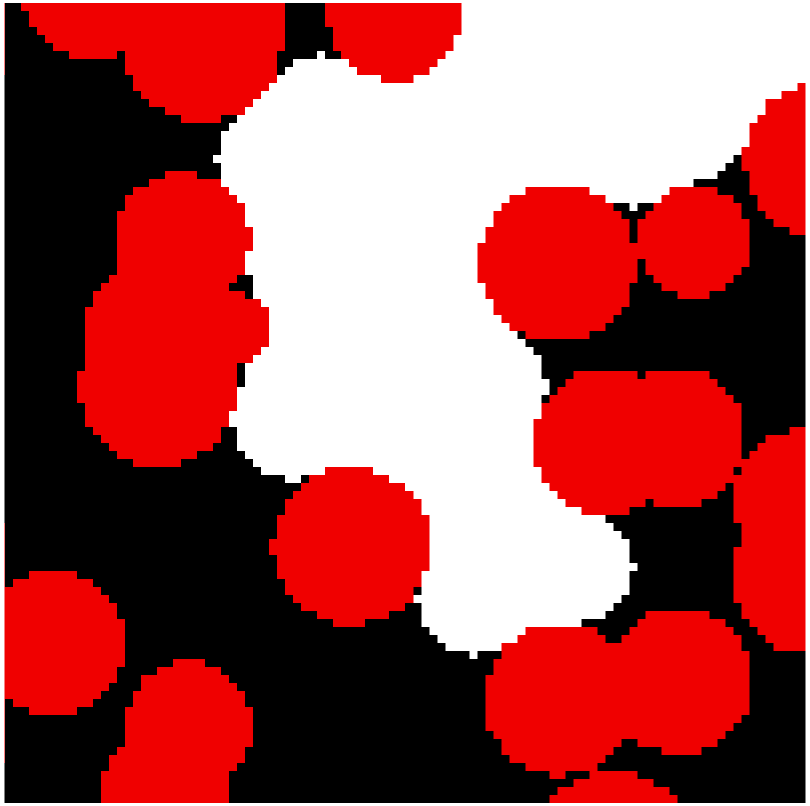
$$\begin{aligned} \mathcal{O}_{B_r}(X) &= \mathcal{D}_{B_r}(\mathcal{E}_{B_r}(X)), \\ \mathcal{E}_{B_r}(X) &= \{x | B_r(x) \subseteq X\} \\ \mathcal{D}_{B_r}(X) &= \{x | B_r(x) \cap X \neq \emptyset\} \end{aligned}$$

phase distribution: non-wetting phase $\mathcal{O}_{B_r}(X)$, wetting phase $X \setminus \mathcal{O}_{B_r}(X)$

Pore Morphology Method (Algorithm)

algorithm :

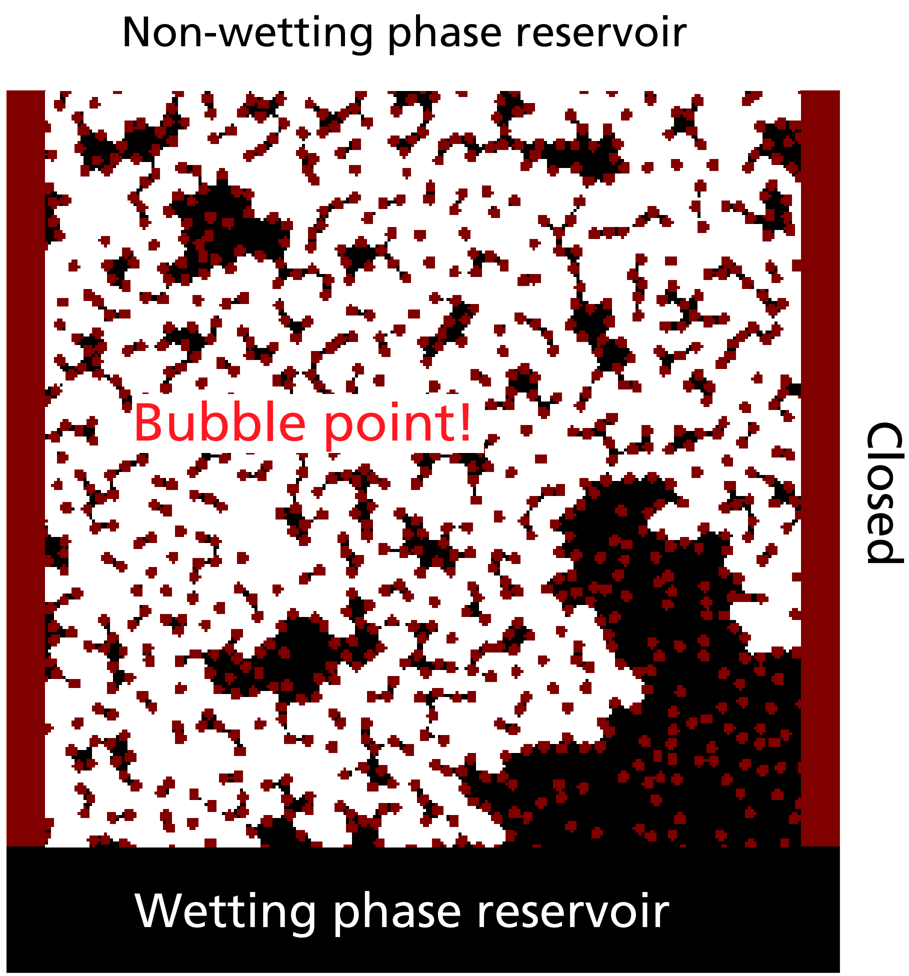
1. start configuration
2. erode pore space
3. eroded pore space has to be connected with non-wetting phase reservoir
4. dilate remaining pore space
5. final result



Pore Morphology Method (Drainage)

• starting point: pore space completely filled with wetting fluid

• determine pore space occupied by non-wetting fluid for increasing pressure (decreasing pore radius)

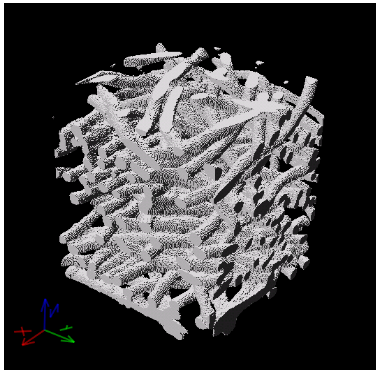


Fraunhofer Institut Techno- und Wirtschaftsmathematik

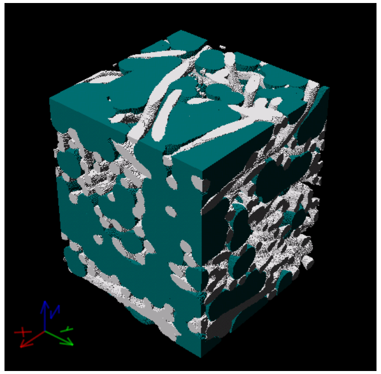
Pore Morphology Method (3D)

"drainage": only pores connected to the NWP reservoir are filled with the NWP

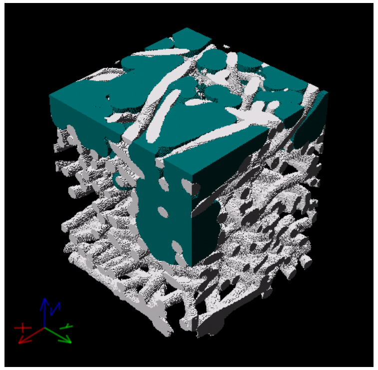
"imbibition" (or repeated drainage+imbibition) : all pores large enough are filled with the NWP



porous media



"imbibition"



"drainage (top)"

Assumptions:

- interface between wetting phase and non-wetting phase is assumed to be spherical (or a superposition of spheres)
- no residual wetting phase
- contact angles other than 0 are reflected only by the "factor" cos β in the Young-Laplace equation

Fraunhofer Institut Techno- und Wirtschaftsmathematik

Using the Pore Morphology Method to Determine Saturation Dependent Material Parameters

general approach:

first step:

- use pore morphology method to determine phase distributions for varying capillary pressures

for each cap. pressure:

- phase distribution is assumed to be stationary
- solve single-phase microscopic equations in the corresponding phase space
- determine macroscopic material parameters via upscaling

Using the Pore Morphology Method to Determine Saturation Dependent Material Parameters

capillary pressure curve $p_c(s)$:

first step:

- use pore morphology method to determine phase distributions for varying capillary pressures

saturation levels already determined

Using the Pore Morphology Method to Determine Saturation Dependent Material Parameters

permeability (wetting phase):

first step:

– use pore morphology method to determine phase distributions for varying capillary pressures

for each cap. pressure:

– phase distribution is assumed to be stationary

– solve Stokes equation $-\eta\Delta u + \nabla p = 0$ in the space occupied by the WP

– determine average velocity from the results and calculate permeability *K(s)* using Darcy's law

Using the Pore Morphology Method to Determine Saturation Dependent Material Parameters

permeability (non-wetting phase):

first step:

- use pore morphology method to determine phase distributions for varying capillary pressures

for each cap. pressure:

- phase distribution is assumed to be stationary
- solve Stokes equation $-\eta \Delta u + \nabla p = 0$ in the space occupied by the NWP
- determine average velocity from the results and calculate permeability *K(s)* using Darcy's law

Using the Pore Morphology Method to Determine Saturation Dependent Material Parameters

diffusivity:

first step:

– use pore morphology method to determine phase distributions for varying capillary pressures

for each cap. pressure:

– phase distribution is assumed to be stationary

– solve Laplace equation $-\Delta c = 0$ in the space occupied by the WP.

– determine macroscopic diffusivity coefficients *D(s)* via upscaling

Using the Pore Morphology Method to Determine Saturation Dependent Material Parameters

thermal conductivities:

first step:

– use pore morphology method to determine phase distributions for varying capillary pressures

for each cap. pressure:

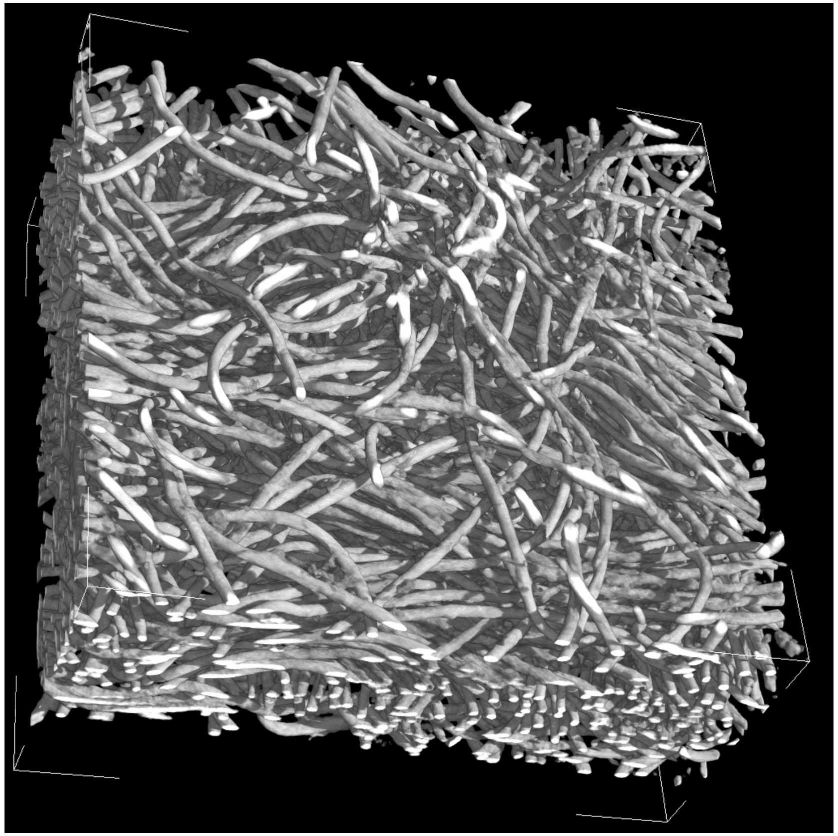
– phase distribution is assumed to be stationary

– solve heat transport equation $-\nabla(\tilde{\beta}\nabla u) = 0$ in the complete space, with discontinuous coefficient $\tilde{\beta}$ (differs for gas, water and fibres).

– determine macroscopic heat transport coefficient $\beta(s)$ via upscaling

Example: 3D tomography image of a Gas Diffusion Layer

- material:
  - carbon fibres of diameter ~ 7 µm
  - hydrophobic PTFE coating
  - porosity 78%
  - layer thickness ~ 200 µm
- 3D data
  - synchrotron tomography by ANKA GmbH (Karlsruhe)
  - picture shows area of size 717x717 µm
  - resolution: 0.7 µm/voxel



Fraunhofer Institut Techno- und Wirtschaftsmathematik

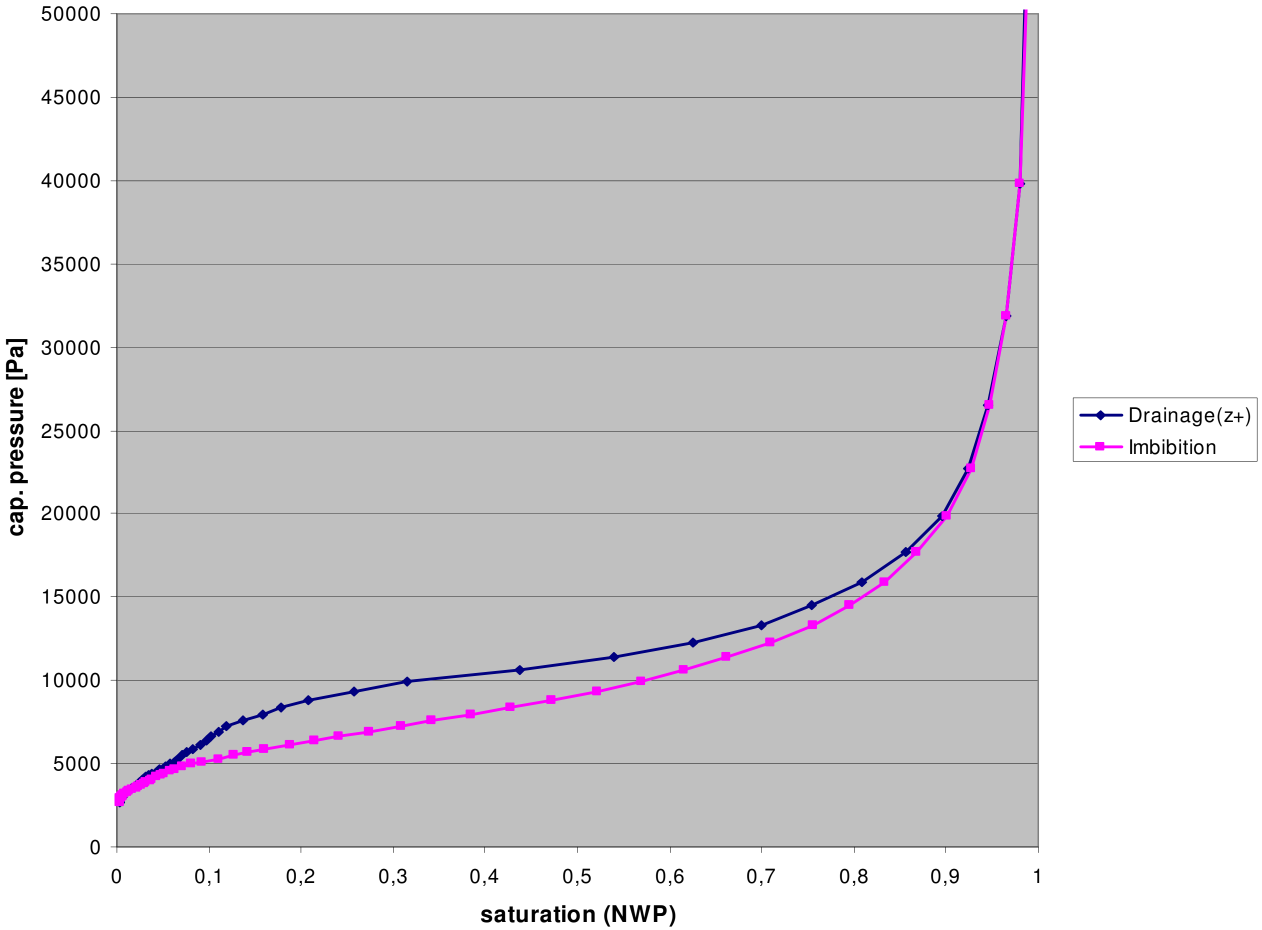
GDL: Capillary Pressure – Saturation

used parameter:

- contact angle: 140°

results:

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



Fraunhofer Institut Techno- und Wirtschaftsmathematik

GDL: Thermal Conductivity (Results)

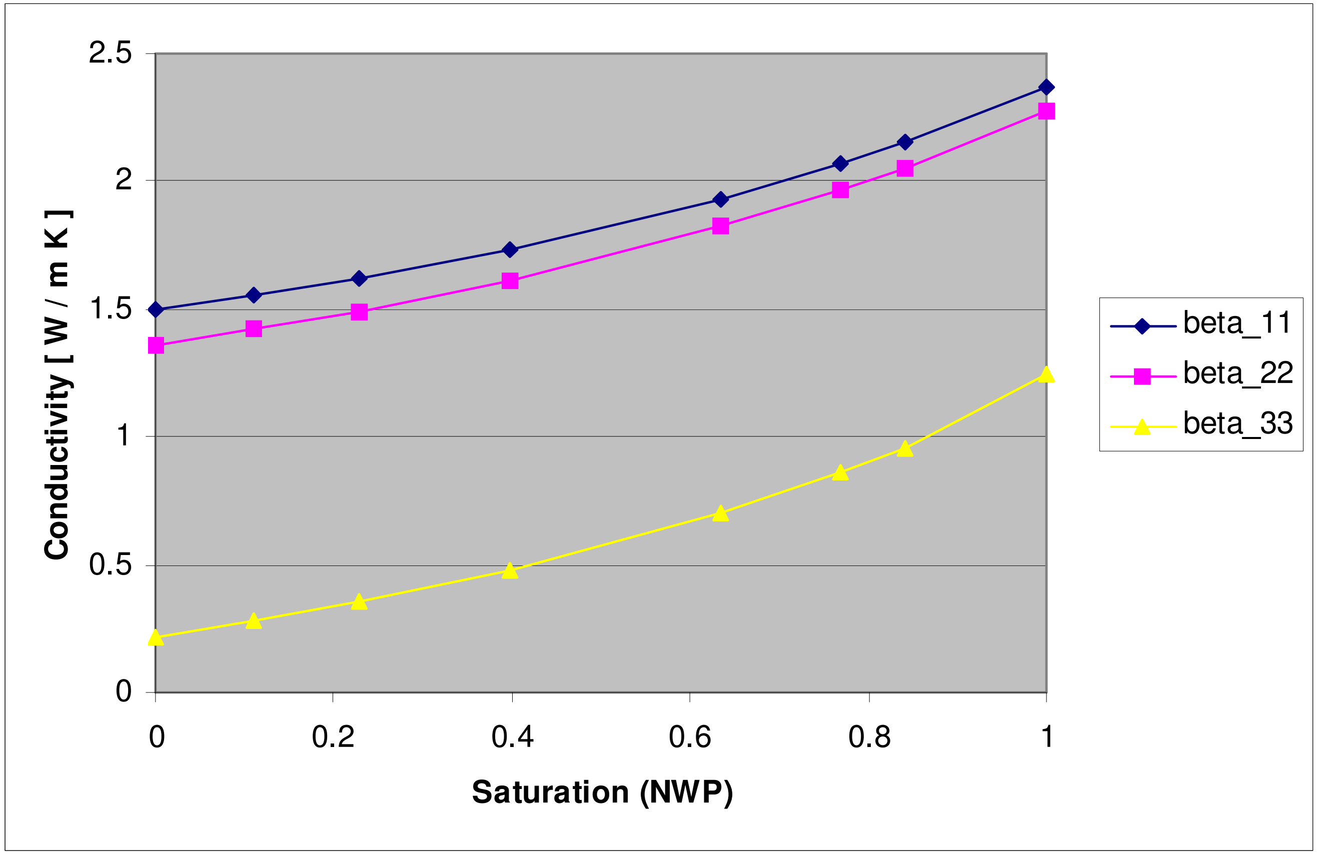
• averaged results over 3 cut-outs with 256 x 256 x 300 voxels

parameters used:

– water :0.606 W/Km

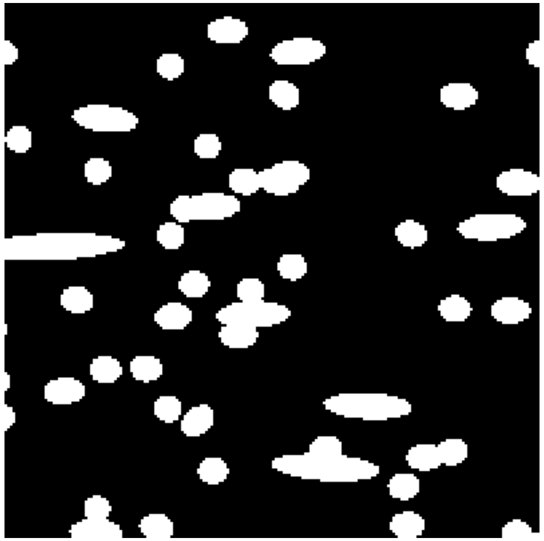
– air: 0.0262 W/Km

– fibres: 17 W/Km

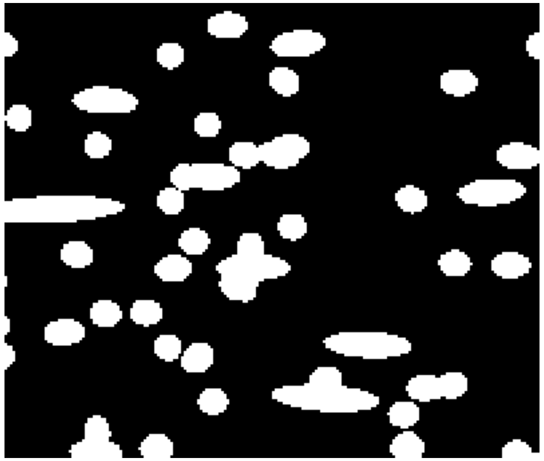


Fraunhofer Institut Techno- und Wirtschaftsmathematik

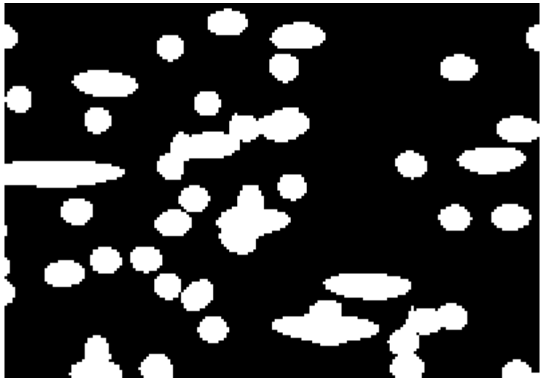
A Reduced Model for Compression



uncompressed

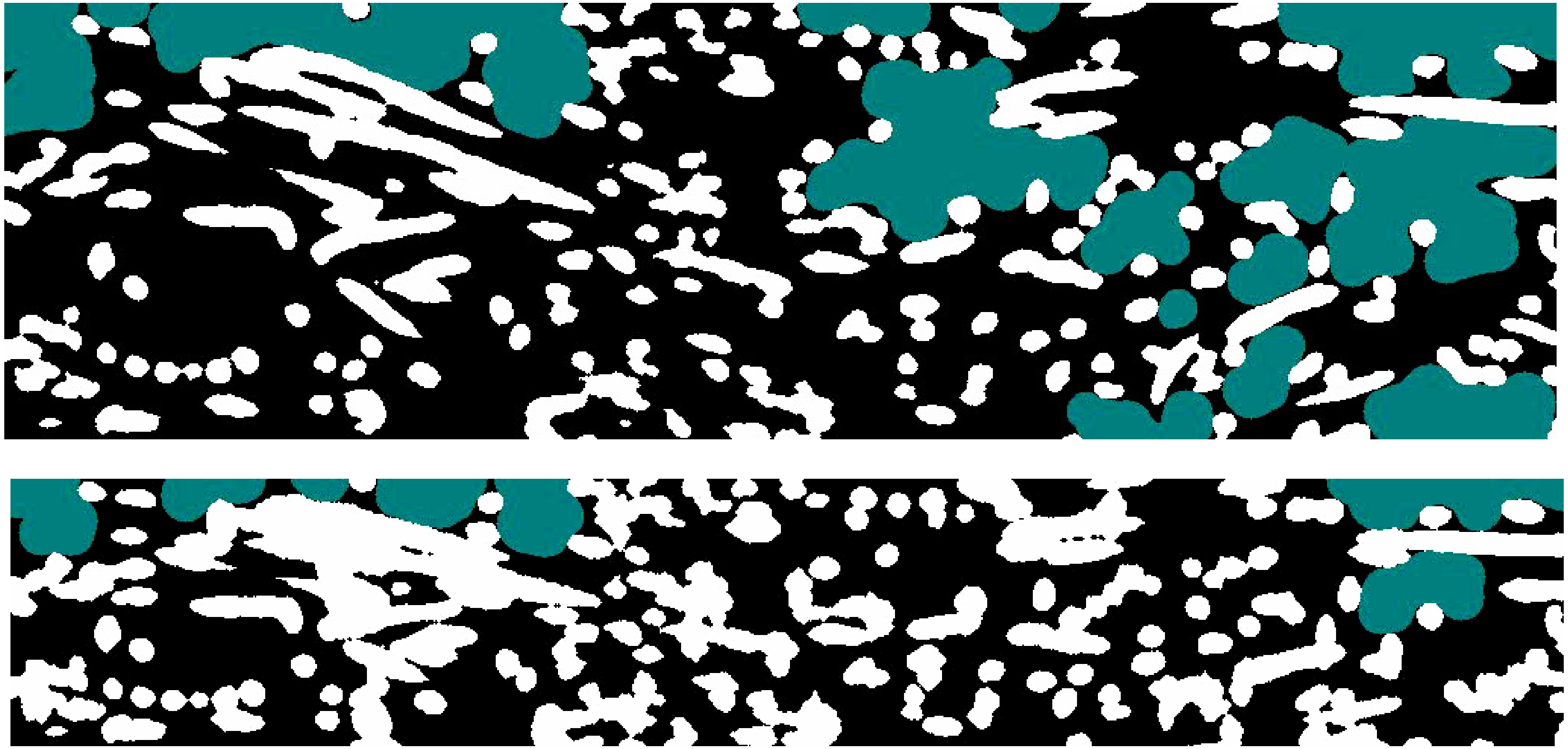


15% compression



30% compression

GDL: Water Distribution (uncompressed and 40% compressed)

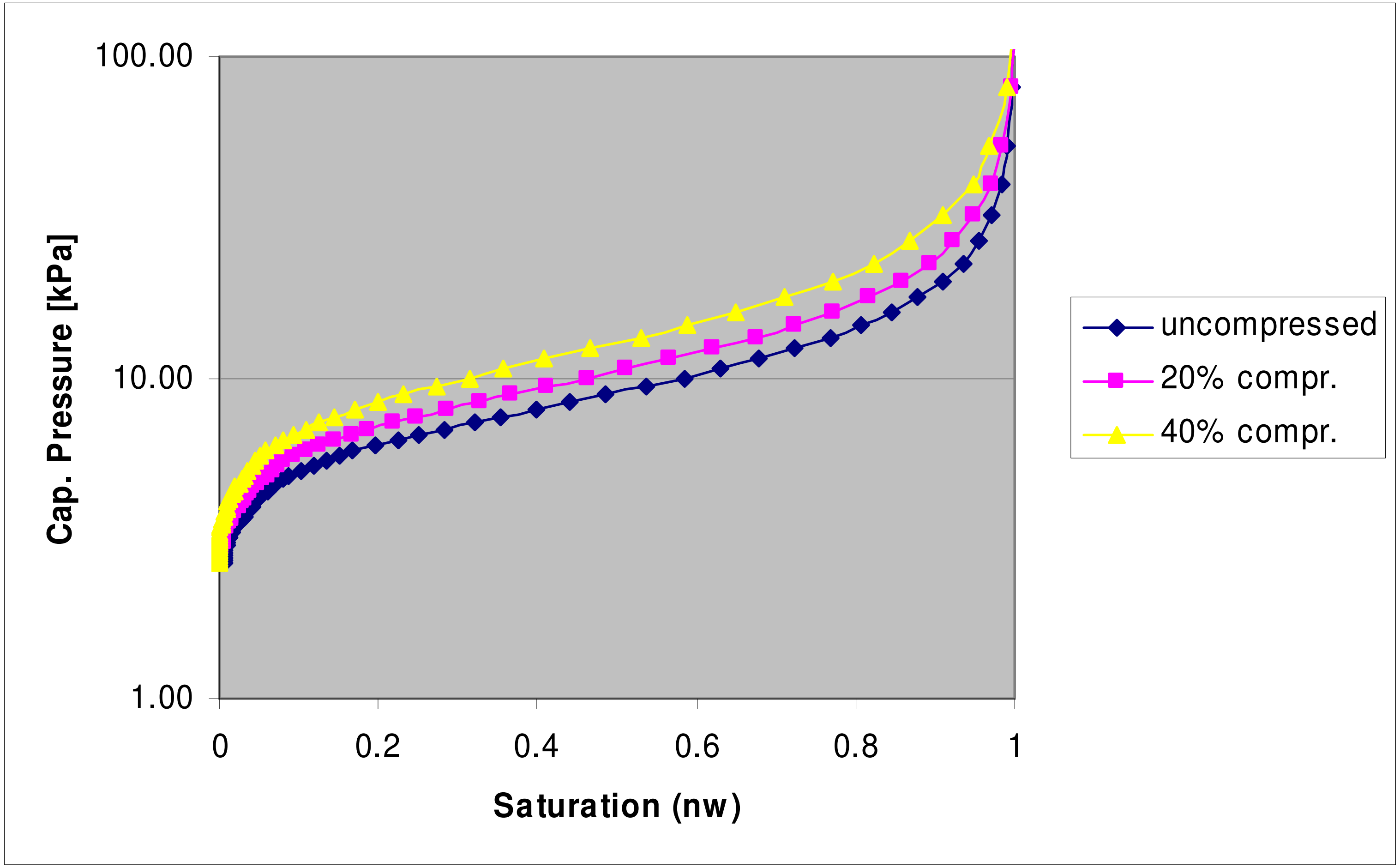


pc= 10.6 kPa

(r=10.5 μm)

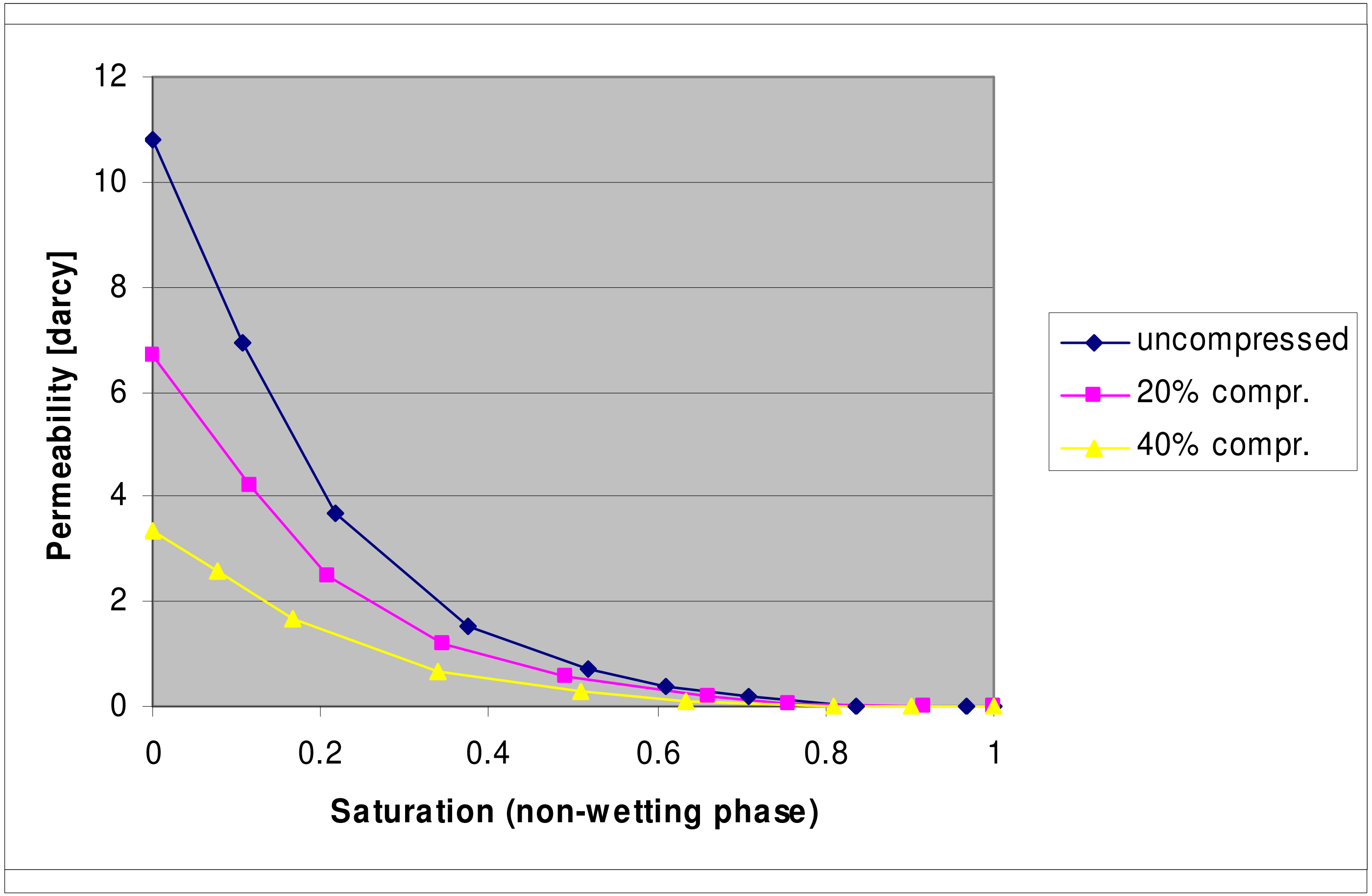
Fraunhofer Institut Techno- und Wirtschaftsmathematik

Capillary Pressure Curve



- Imbibition
- 1024x1024x300

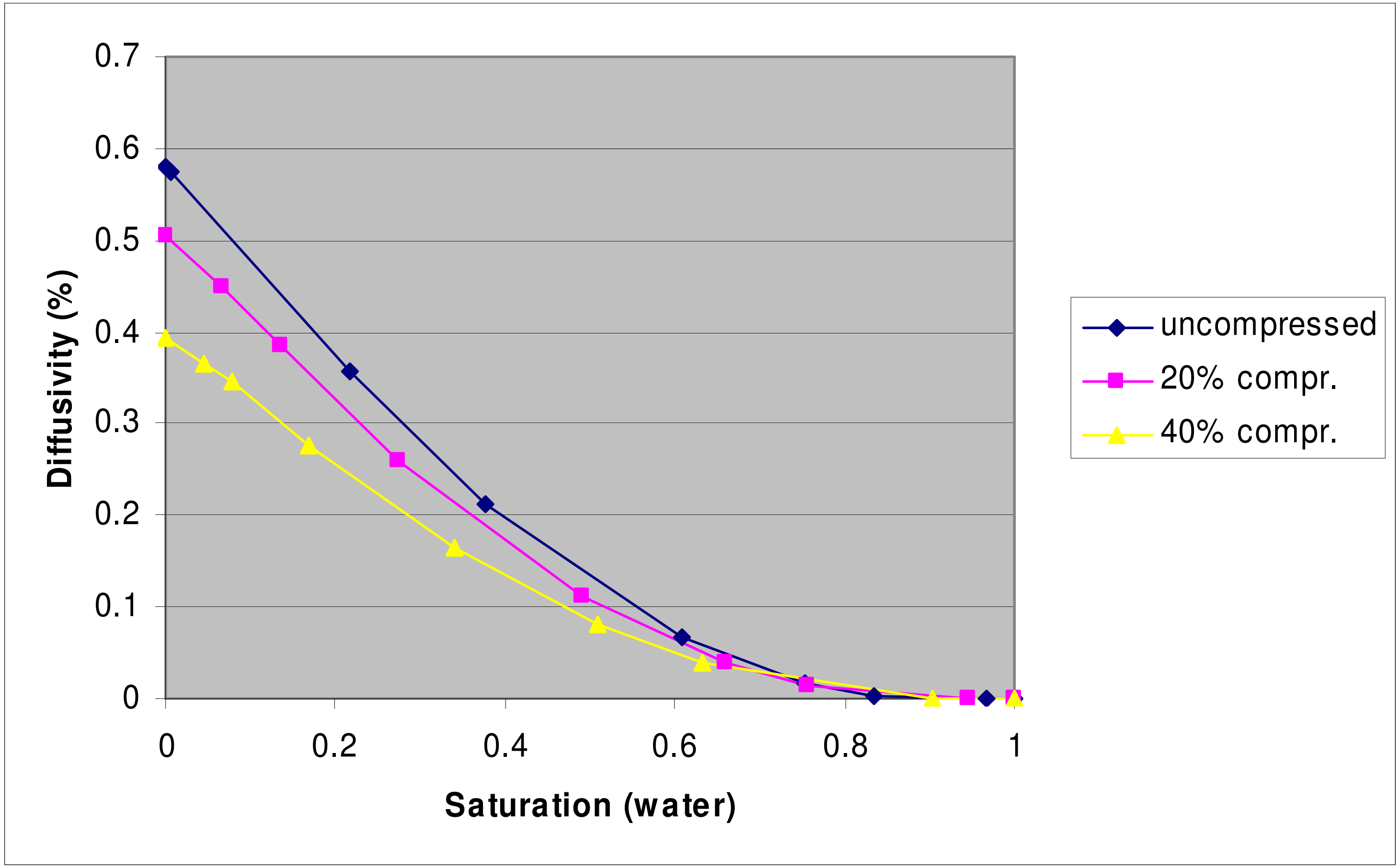
Permeability



- through-plane
- 512x512x300
- imbibition

Fraunhofer Institut Techno- und Wirtschaftsmathematik

Diffusivity



- through-plane
- 512x512x300
- imbibition

Fraunhofer Institut Techno- und Wirtschaftsmathematik

Summary

- starting point:
  - synchrotron tomography image
  - virtually generated fibre structure

- calculated effective material parameters:
  - pore size distribution
  - bubble point
  - capillary pressure – saturation relation
  - (relative) gas diffusivity tensor
  - (relative) permeability (wetting and non-wetting phase)
  - (relative) thermal conductivities

- results can be used in macroscopic CFD simulations