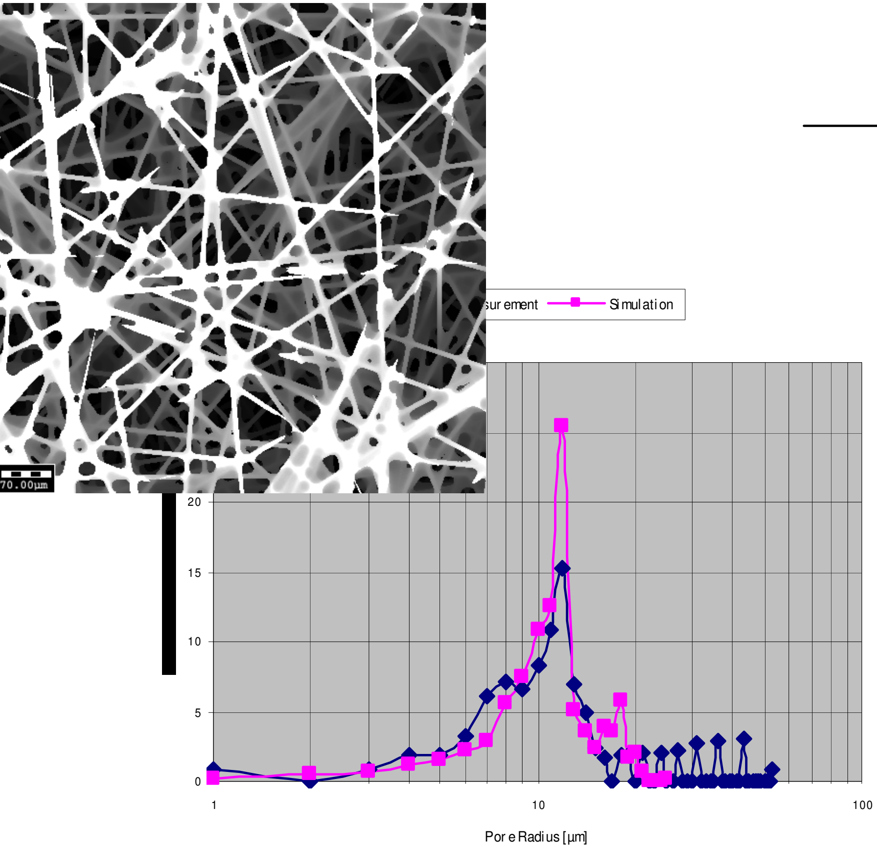
Virtual Characterization of the Pore Structure of Nonwoven



Andreas Wiegmann & Jürgen Becker

INTC 2007 Atlanta

September 26th, 2007

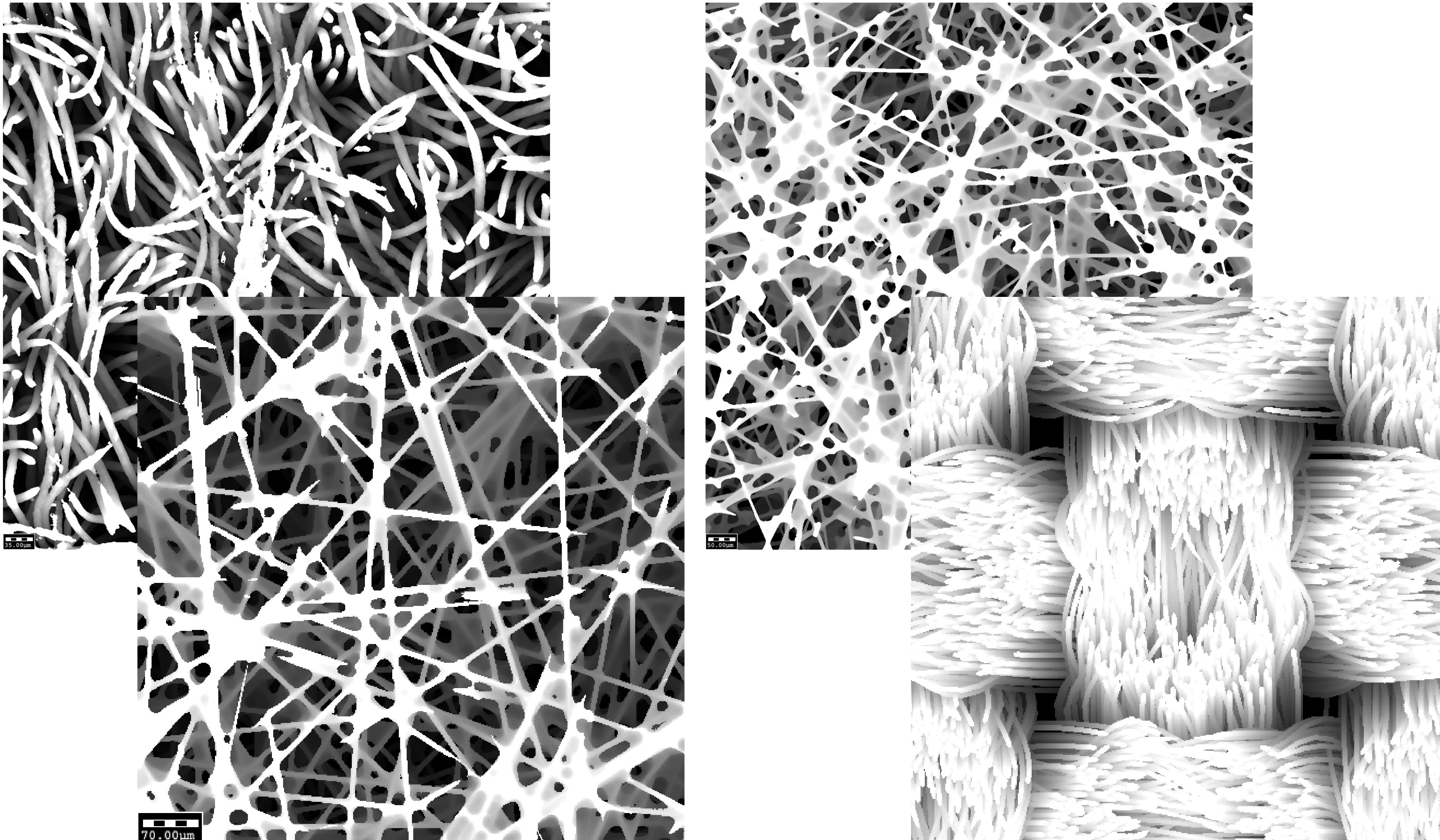
Fraunhofer Institut Techno- und Wirtschaftsmathematik
ITWM

Aim: Derive new characterizations for pore size distributions of nonwoven

1. Start from valid 3d nonwoven model
2. Relate model parameters to pore size measures
3. Capture trends in analytic formulas
4. Make obsolete need for 3d models and virtual pore size analysis

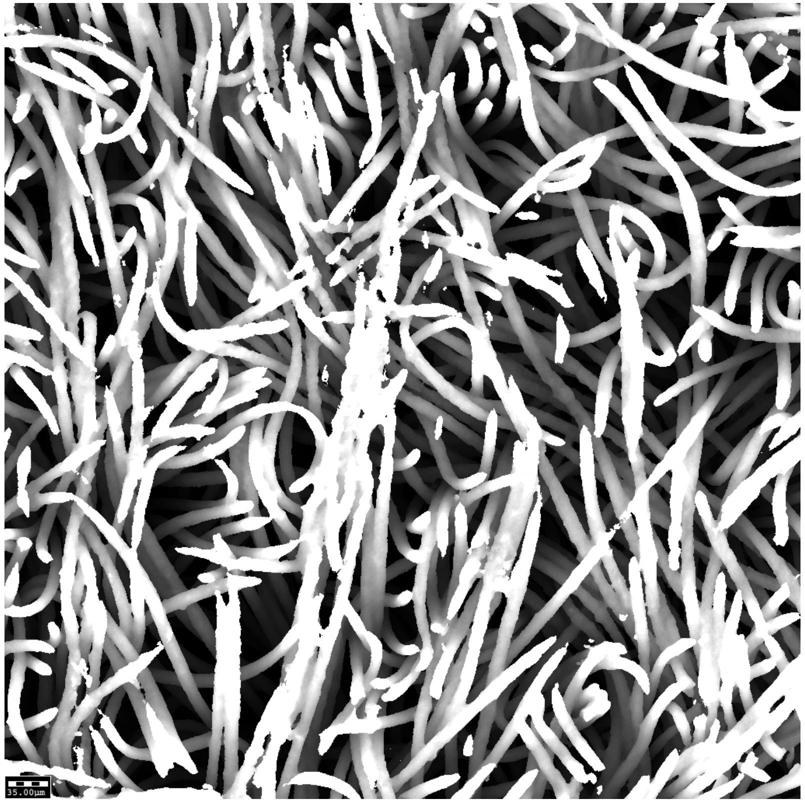
1. Virtual Textile Generation
   - Generation method
   - Input parameters
   - Model validation
2. Virtual Pore size Measures
   - Mercury intrusion Porometry (MIP)
   - Liquid extrusion Porometry
   - Bubble Point determination
   - Information extraction: D10, D50, D90
3. Analytic Formulas
   - Need for REV and multiple realizations
   - Automation
   - Examples: porosity and fiber diameter
   - Ansatz functions and fit parameters

1. Virtual Textile Generation



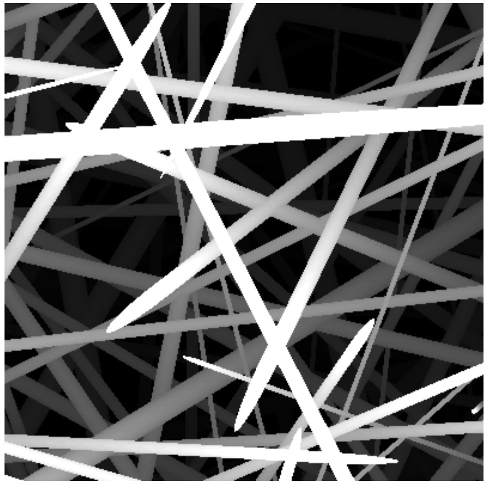
1. Option a): import 3d image of existing media

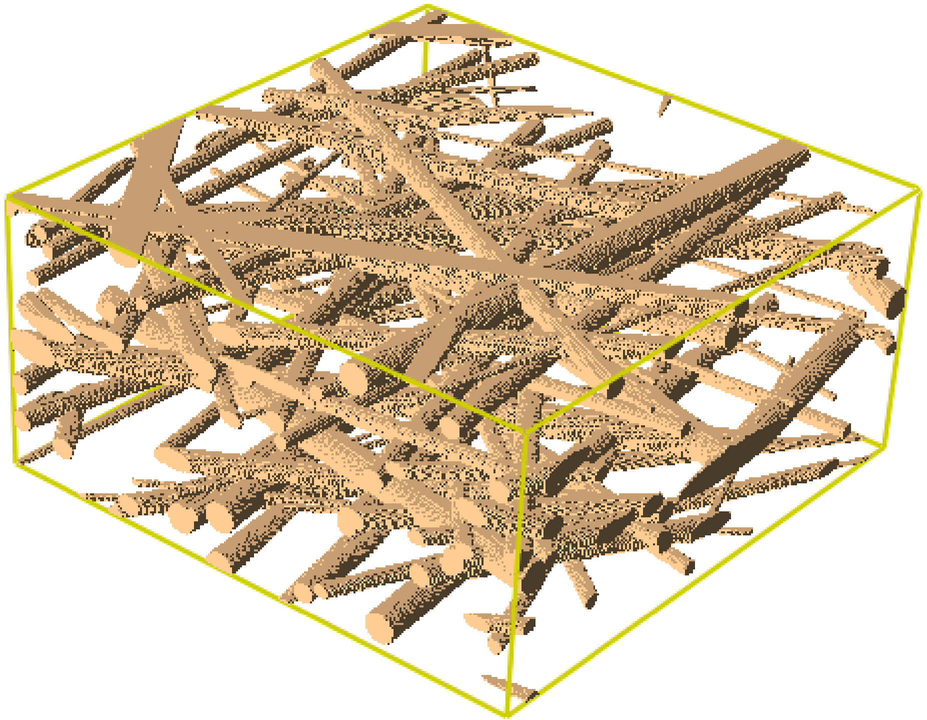
- Input: 3d gray-valued image obtained by DVI, tomography or similar 3d imaging method
- Options:
  - choice of threshold
  - filtering
  - edge smoothing



1. Option b): Virtually Generated Nonwoven: Input Parameters

- Porosity
- Fiber orientation distribution (anisotropy)
- Fiber diameter (distribution)
- Fiber cross sectional shape
- Fiber length (distribution)





In the "overlapping" model

Fibers are placed at random positions with appropriately randomized orientation and without consideration of each other

It is a surprise that such a simple model works!

1. Remarks on model sensitivity

Permeability (flow resistivity) prediction is not sensitive to fiber touch / overlap!

Permeability (flow resistivity) prediction is not sensitive to fiber crimp!

This is not always the case:

Thermal & electrical conductivity is sensitive to fiber touch / overlap!

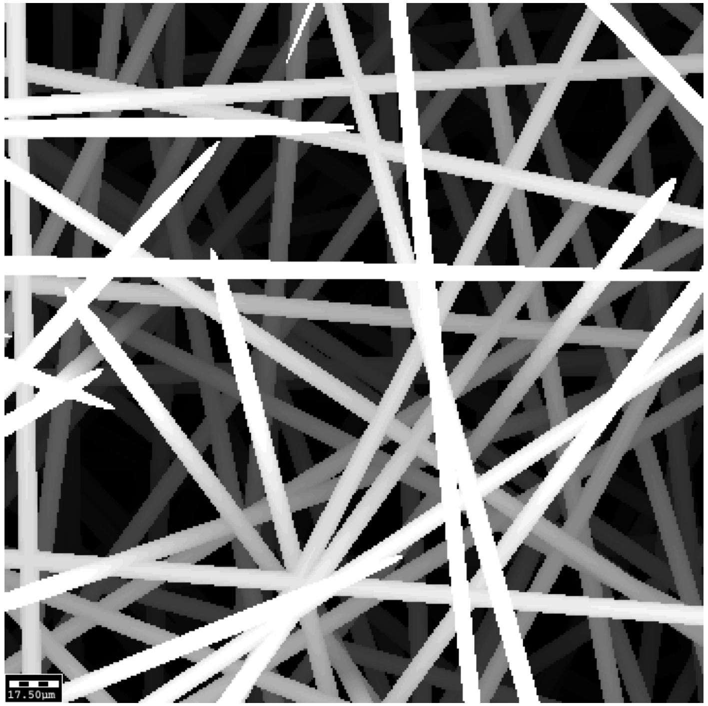
Explanation:

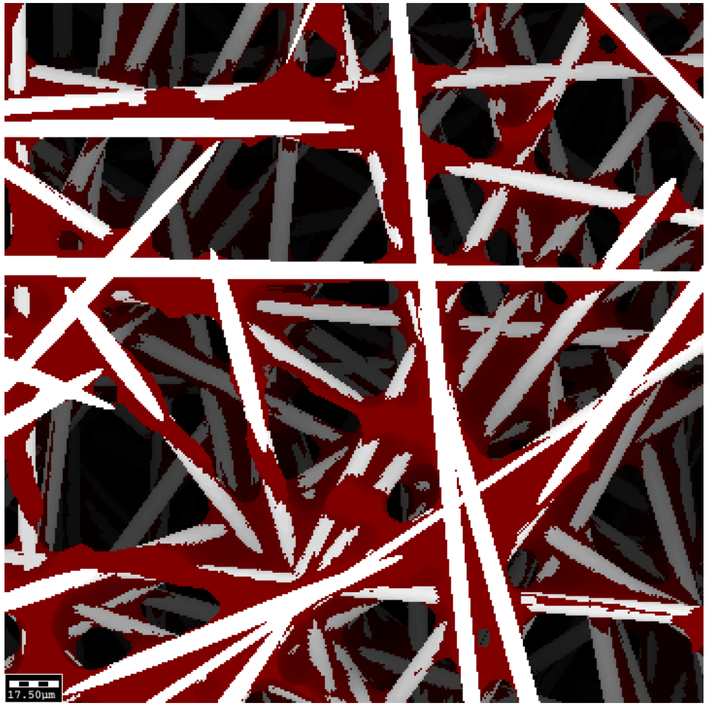
For fluid flow, the connectivity of pore space is crucial

For thermal and electrical conduction, the connectivity of the fibers is crucial!

1. Adding Binder

Assumption: the binder acts like a mobile wetting fluid and occupies the small pores





1. Comparison of Simulations and Experiments (Fuel Cell gas diffusion layer)

compare TEM visualization of model with TEM of original media

absolute permeability (through-plane):

– measurement: Toray 090 carbon paper (*Gostick et al, 2005*): 8.3 darcy
– simulation: virtually created Toray 090: 7.4 darcy
– simulation (tomography data): 11.7 darcy

bubble point:

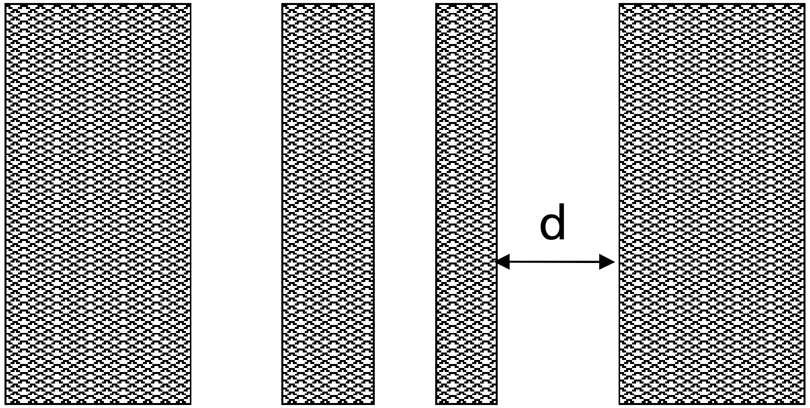
– measurement: Toray paper with 20% Teflon (*Benziger et al, 2005*): 7.1 kPa
– simulation (tomography data, contact angle 40°): 8.8 kPa

saturation at the bubble point:

– measurement: Toray paper with 20% Teflon (*Benziger et al, 2005*): 20 %
– simulation (tomography data): 20.8 %

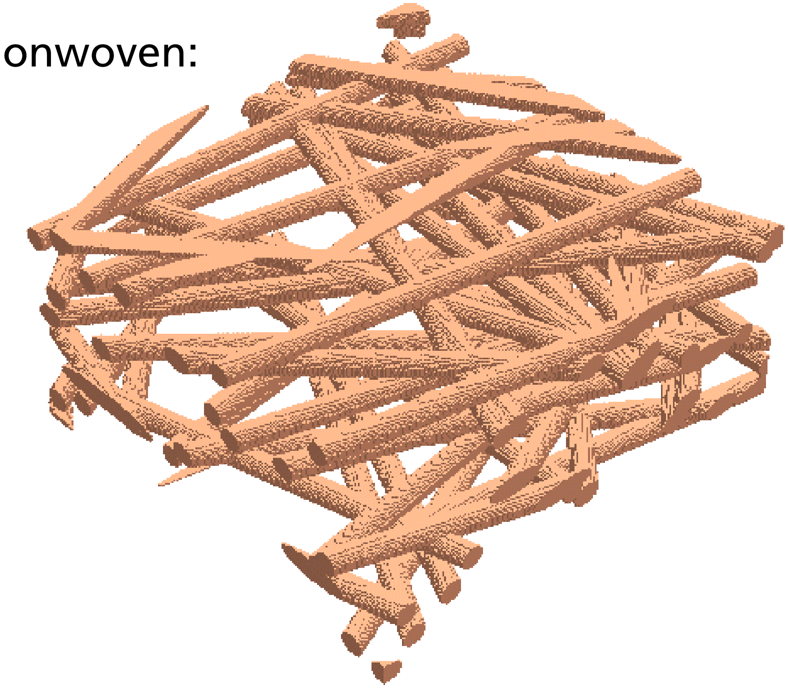
2. Pore Size Distribution

simple geometry:



Pore sizes well defined and easy to measure

nonwoven:



How to define a pore size ?

What is measured?

2. Defining Pore Sizes - Geometric Approach

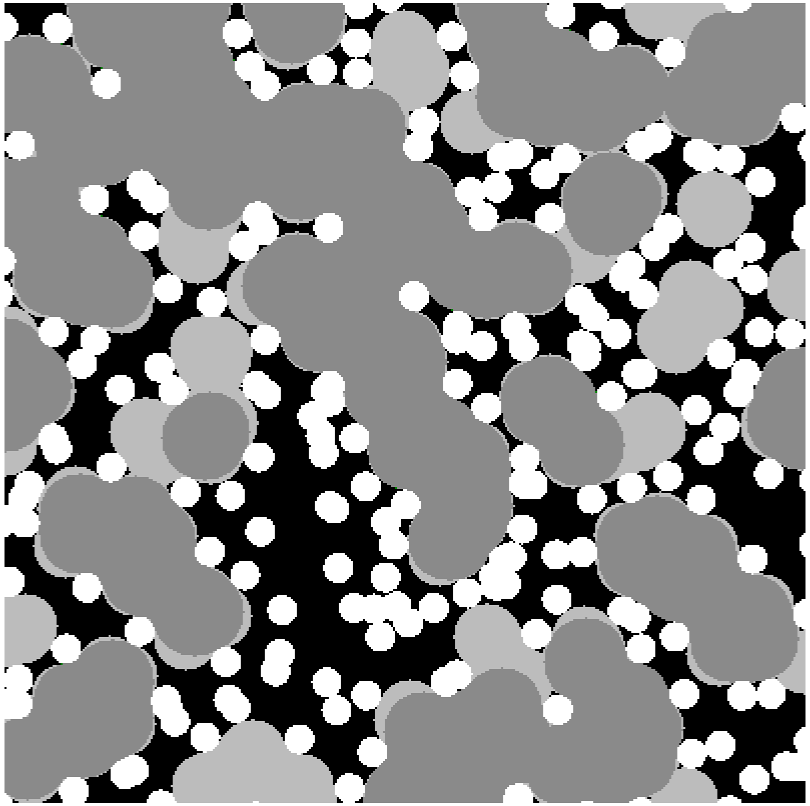
Pore space : *X*

Opening of radius *r* :

$$O_r(X) = \bigcup_{B_{r,x} \subset X} B_{r,x}$$

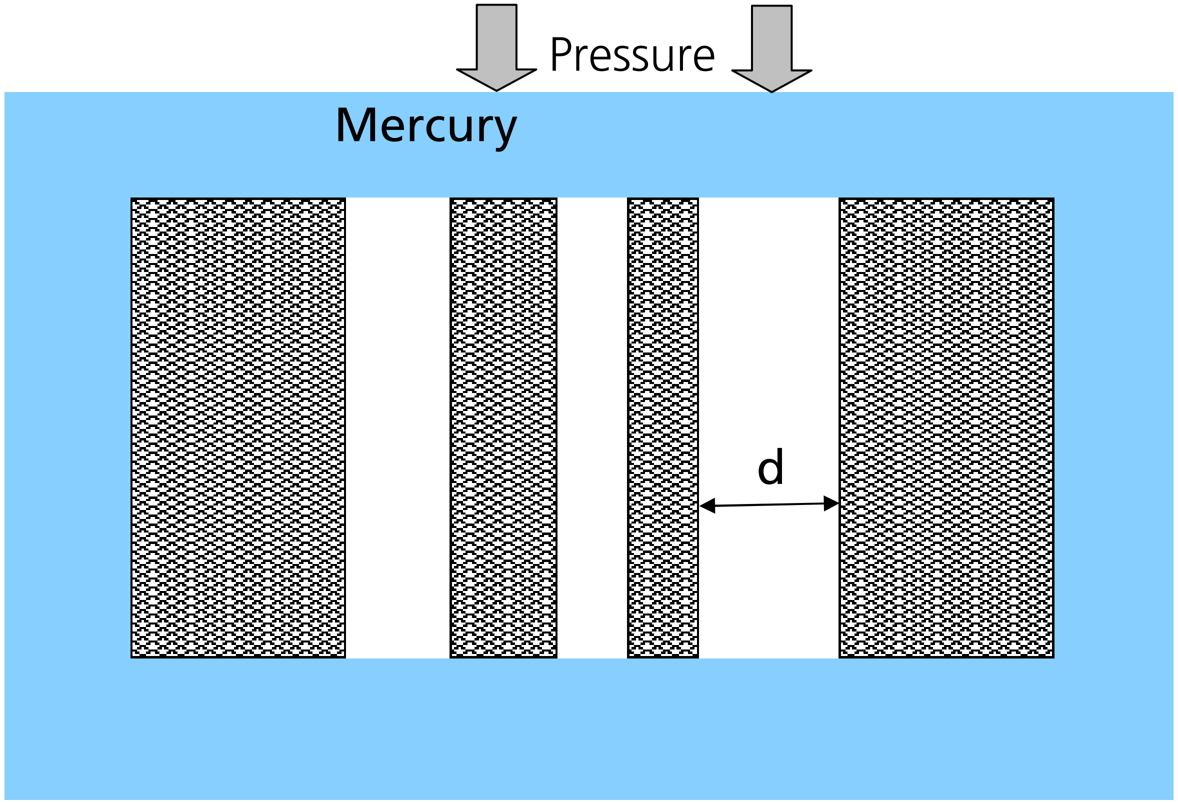
Volume of pores with radius $r_1 \leq r \leq r_2$:

$$O_{r_1}(X) - O_{r_2}(X)$$



dark grey: $r \geq 20$
light grey: $16 \leq r < 20$

2. Mercury Intrusion Porosimetry



- mercury (non-wetting) fills the pores, if pressure becomes large enough:

$$p = \frac{4\gamma}{d} \cos\theta$$

- volume of intruding mercury gives pore size distribution

2. Mercury Intrusion via Pore Morphology Method

algorithm :

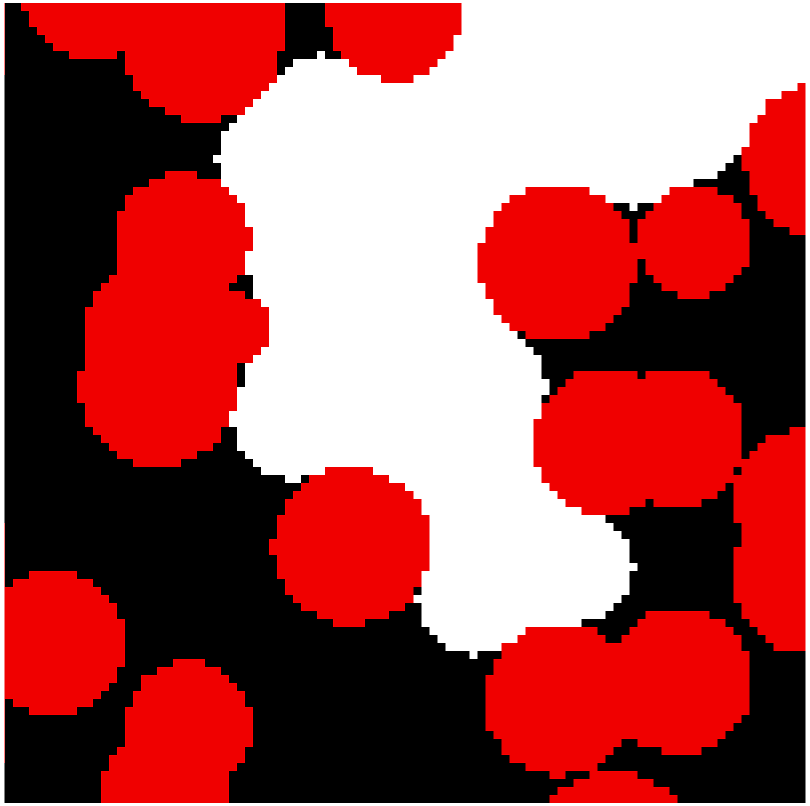
1. start configuration

2. erode pore space

3. eroded pore space has to be connected with non-wetting phase reservoir

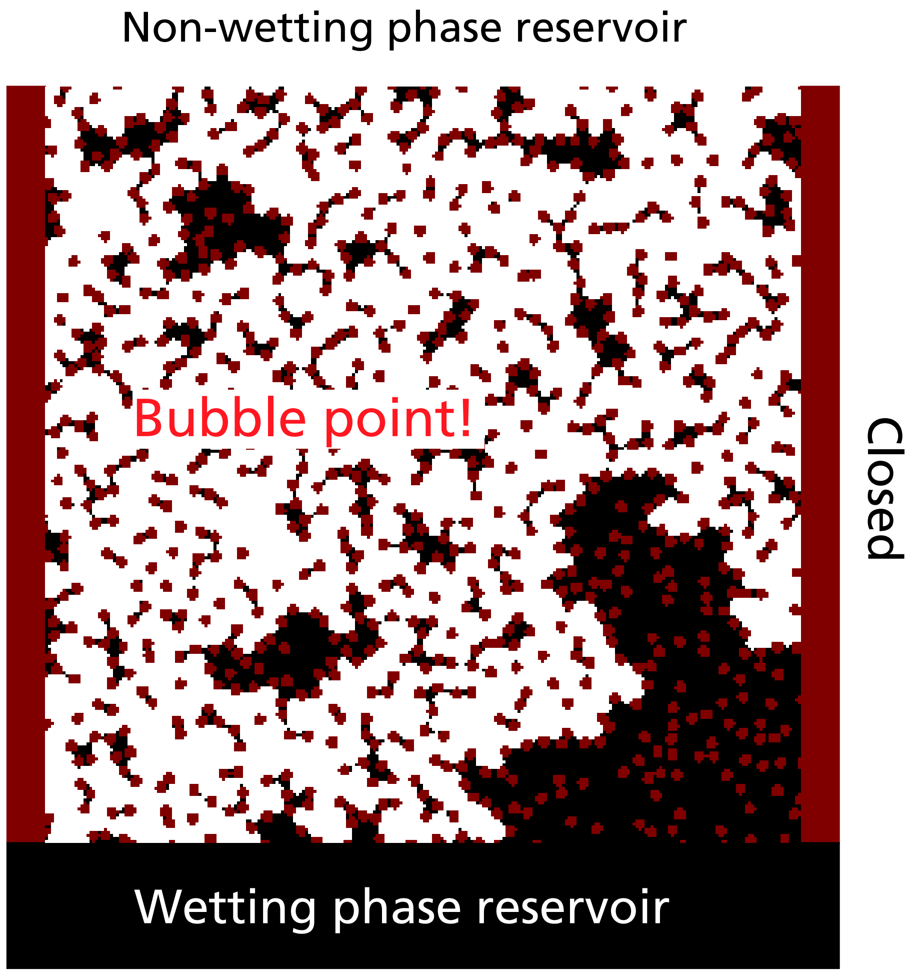
4. dilate remaining pore space

5. final result

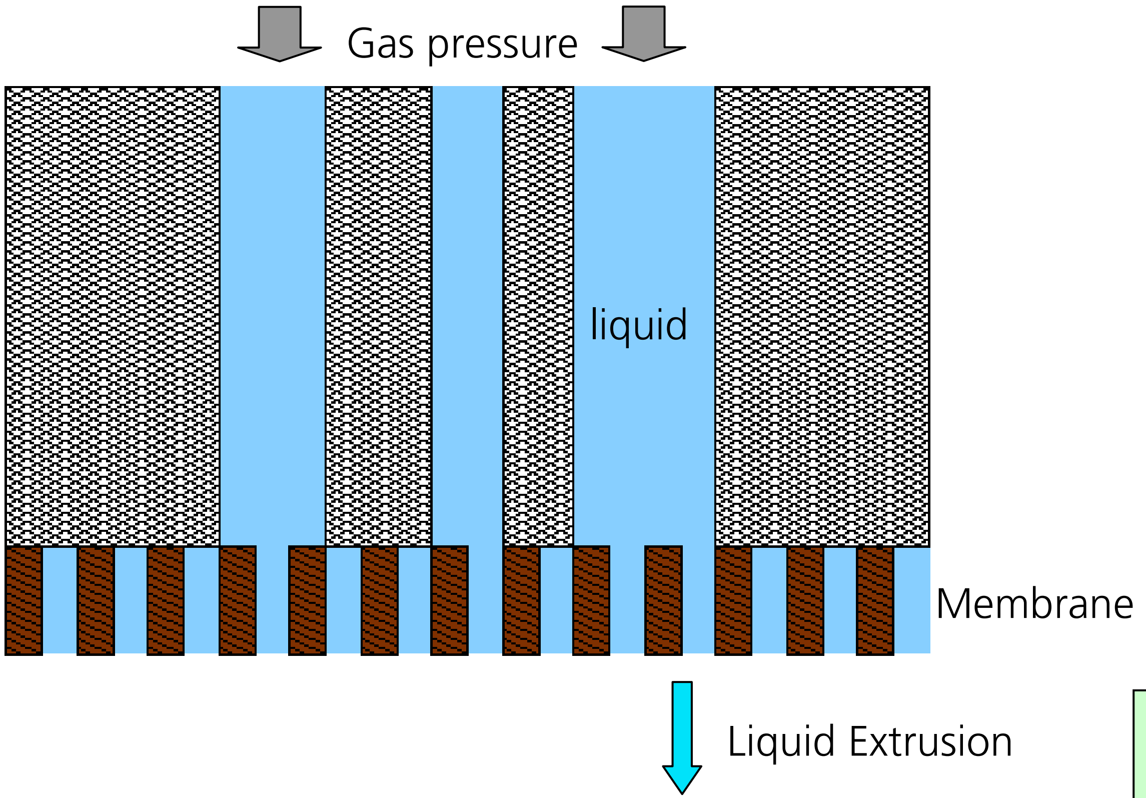


2. Bubble point via Pore Morphology Method: mercury "connects"

- starting point: pore space completely filled with wetting fluid
- determine pore space occupied by non-wetting fluid for increasing pressure (decreasing pore radius)



2. Liquid Extrusion Porosimetry



- sample and membrane initially filled with wetting liquid.
- air is pressed into the pores and fills pores with large enough diameter:

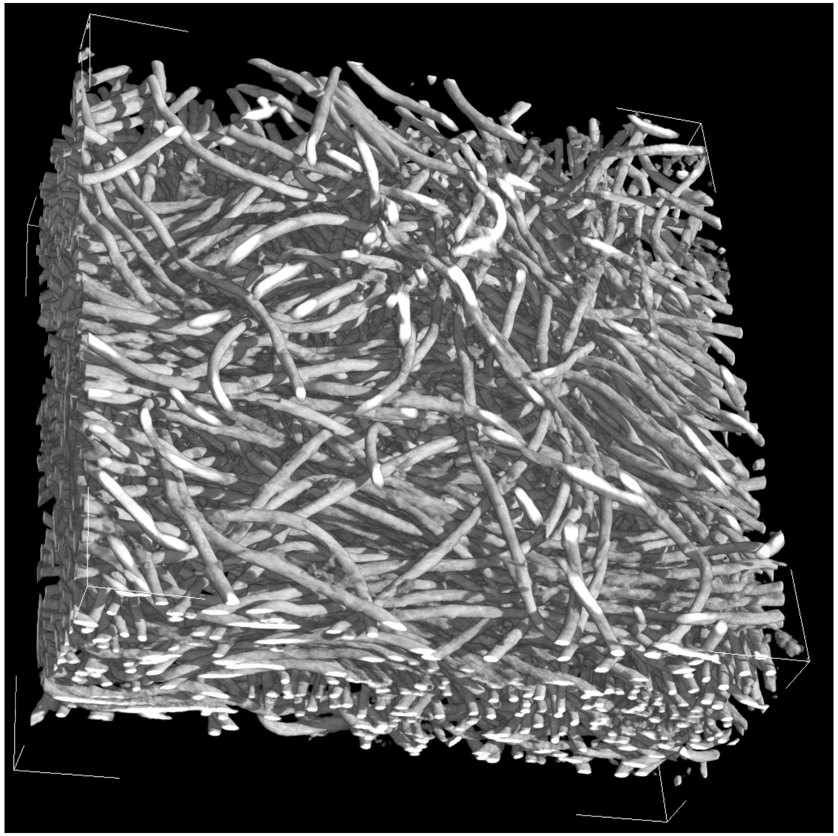
$$p = \frac{4\gamma}{d} \cos\theta$$

- volume of extruded liquid is used to calculate pore size distribution

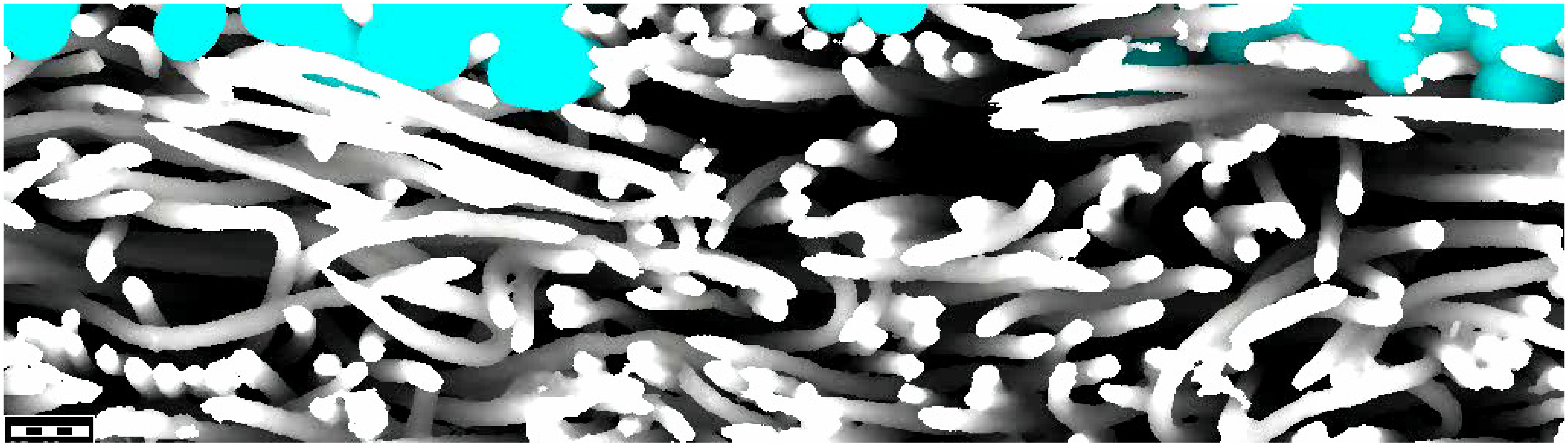
Simulation can use methods developed for MIP (but other reservoir position)

2. Example: GDL Model Obtained by Synchrotron Tomography

- 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



2. Simulated mercury Distribution at Bubble Point in tomography



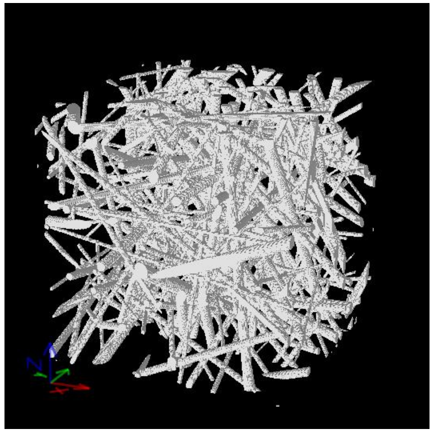
2. Comparison of Measurement and Simulation

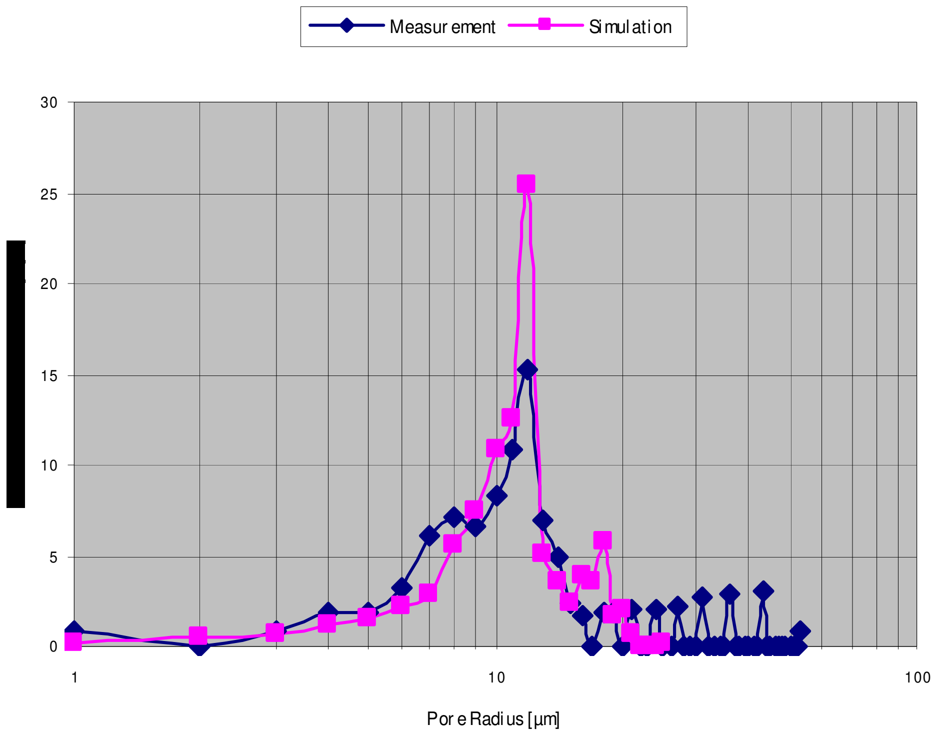
Measurement: MIP

Simulation:

• virtually created fibre structure using known values for porosity and fiber thickness distribution.

• simulated MIP



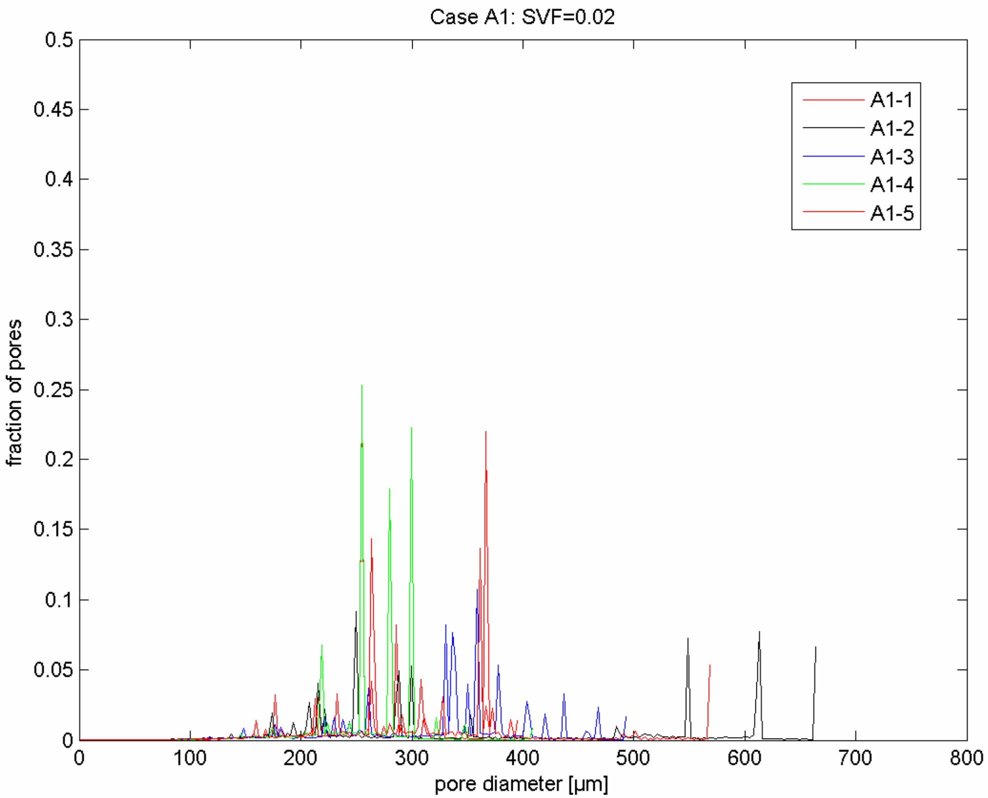


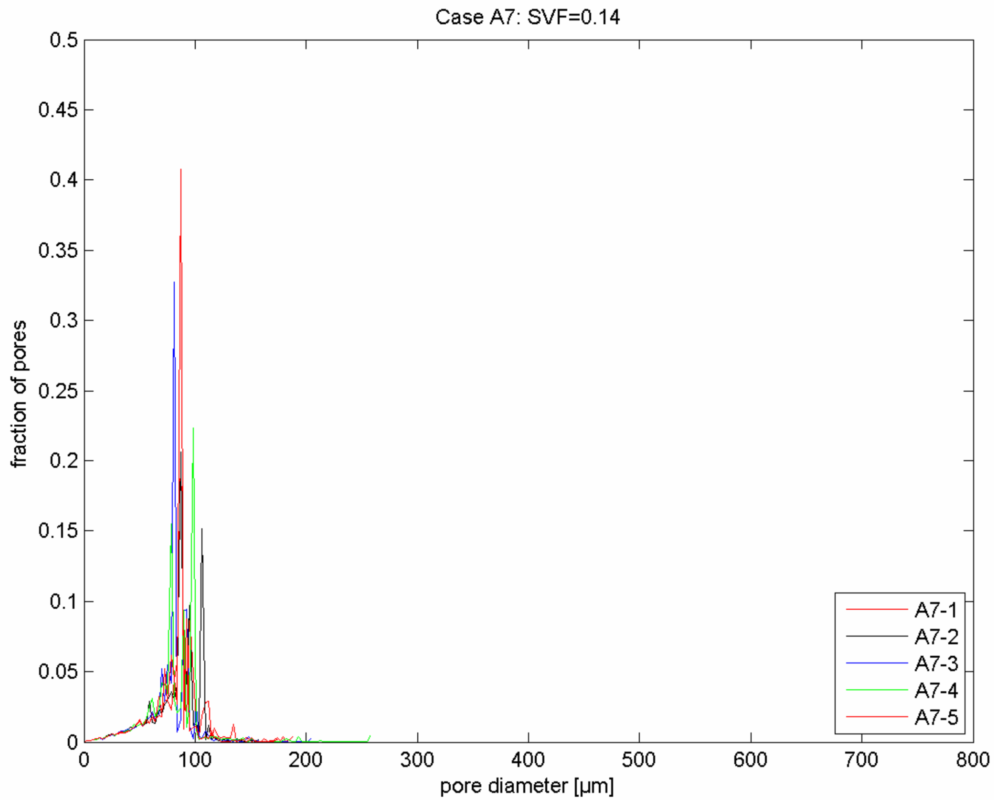
3. Two single-parameter studies

Exp. A	case 1	case 2	case 3	case 4	case 5	case 6	case 7
Fiber diameter	28μm	28μm	28μm	28μm	28μm	28μm	28μm
SVF	0.02	0.04	0.06	0.08	0.10	0.12	0.14

Exp. B	case 1	case 2	case 3	case 4	case 5	case 6	case 7
Fiber diameter	22μm	24μm	26μm	28μm	30μm	32μm	34μm
SVF	0.08	0.08	0.08	0.08	0.08	0.08	0.08

3. The need for an Representative Elementary Volume & multiple realizations





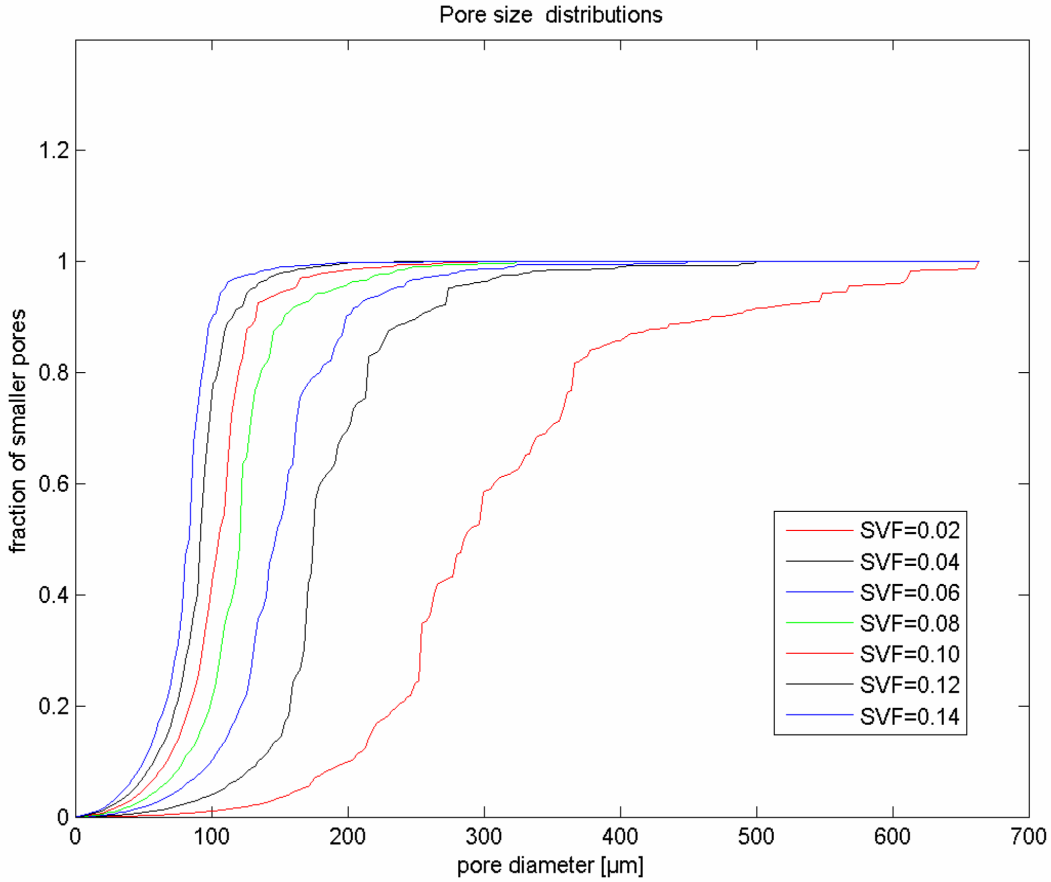
5 realizations, 98 % porosity:

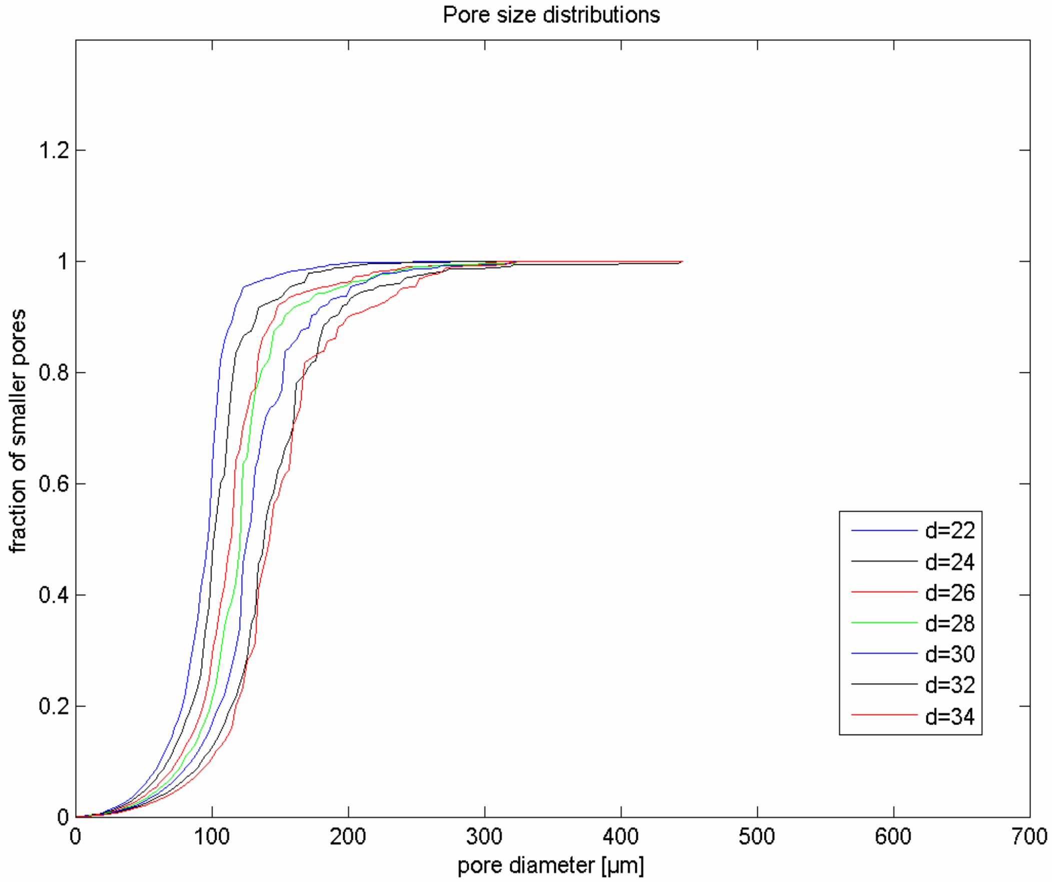
Large pore size variations

5 realizations, 86% porosity:

Little pore size variations

3. Pore size fractions – averaged over 5 realizations





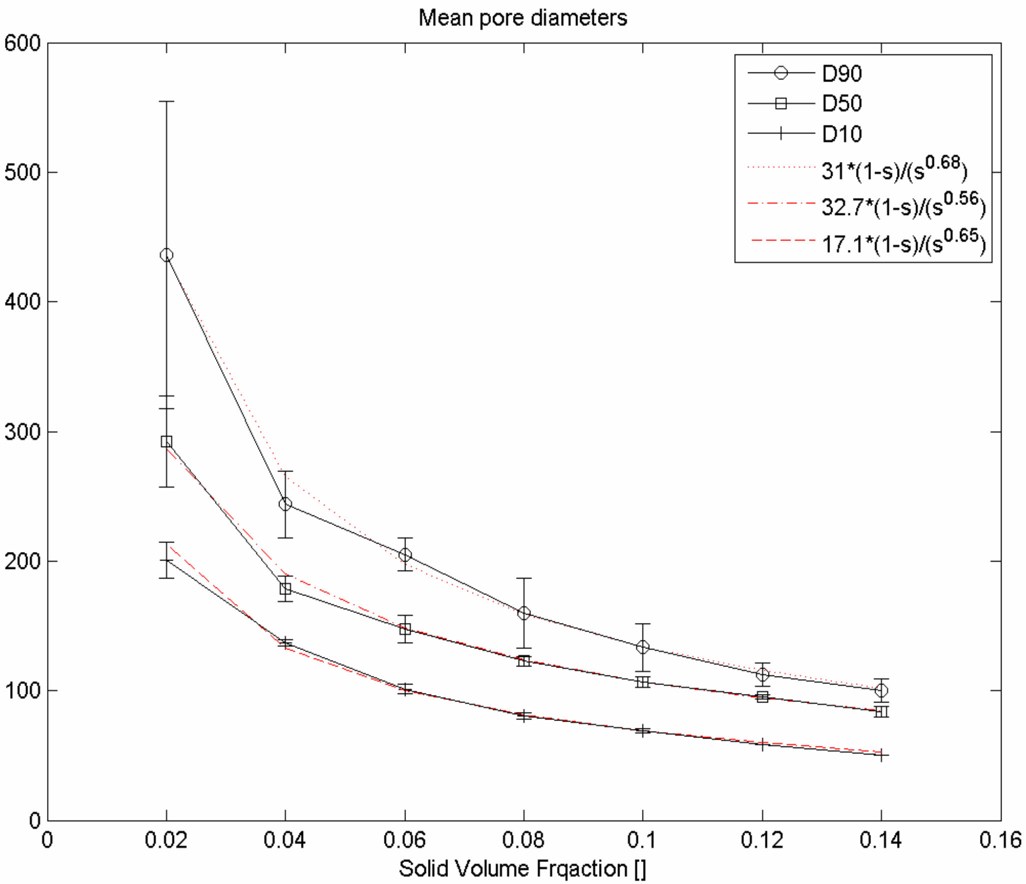
86% to 98 % porosity:

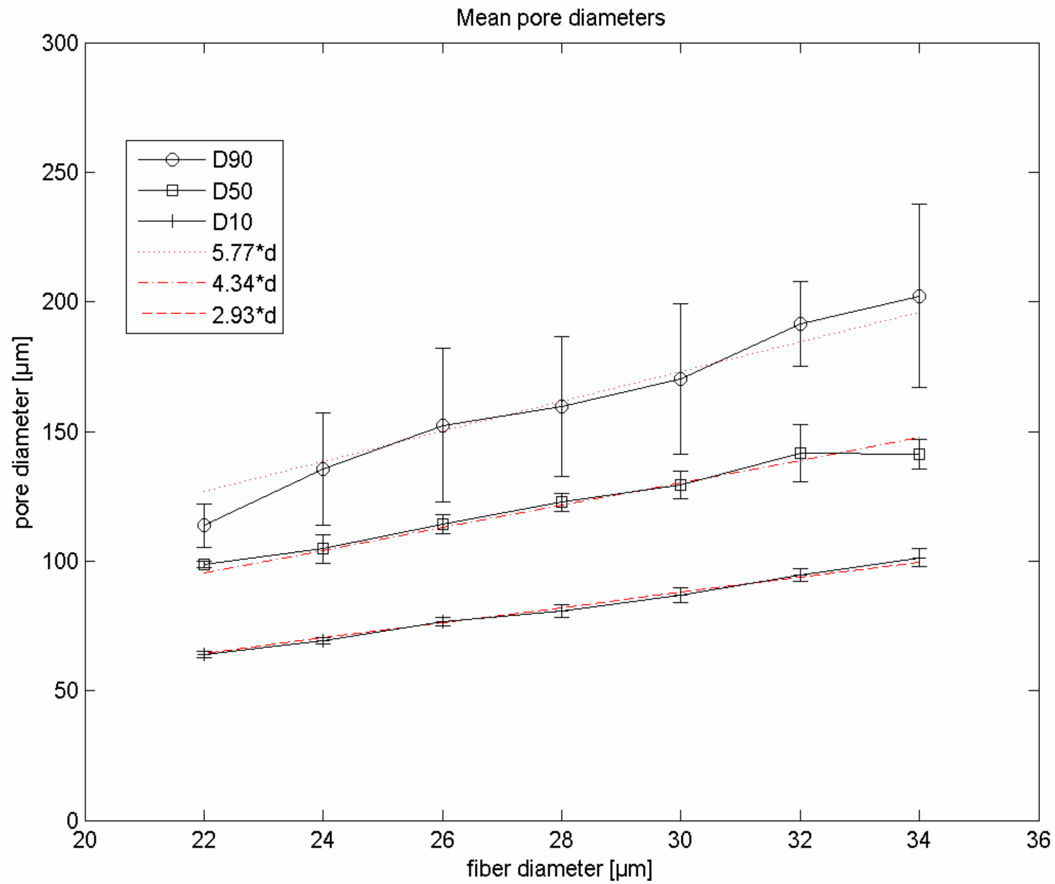
Large pore size variations

22µm to 34µm fiber diameter:

Little pore size variations

3. D10, D50 and D90 and fit formulas





$$f = \alpha \frac{1-s}{s^{\beta}}$$

$$f = \lambda d$$

A. Wiegmann
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3. Next steps: multiple parameters, i.e. more complex nonwoven

The data for these computations can be found completely automatically, once the choices of parameters are determined, including variations of more than one parameter at a time.

The “Ansatz” or “shape of the function” of the fit has to be guessed, and should be combined over the single parameter studies to derive formulas for more complex nonwoven structures.

Experimental validation for the single phase parameters should probably happen first, but cannot be done by Fraunhofer Institute for Industrial Mathematics.

4. Summary

It is the **the pores that matter**

⇨ *simple nonwoven model works*

Virtual pore size measurements *follow* **measurement technology**

⇨ *observe same caveats*

Simulations show **clear trends for pore size distributions**

⇨ **analytic formulas are derived for single variable experiments**

Next:

validate

find analytic formulas for multiple parameters

Different measurement techniques measure different "Pore Size Distributions": A. Jena, K. Gupta, Fluid Particle Separation J. 4, 2002, pp. 227-241.

Virtual pore size measurements: J. Becker, A. Wiegmann, V. Schulz, Filtech 2007.

Software for Generation, Simulation, Visualization:

GEO DICT

www.geodict.com

Thank you for attending this presentation.