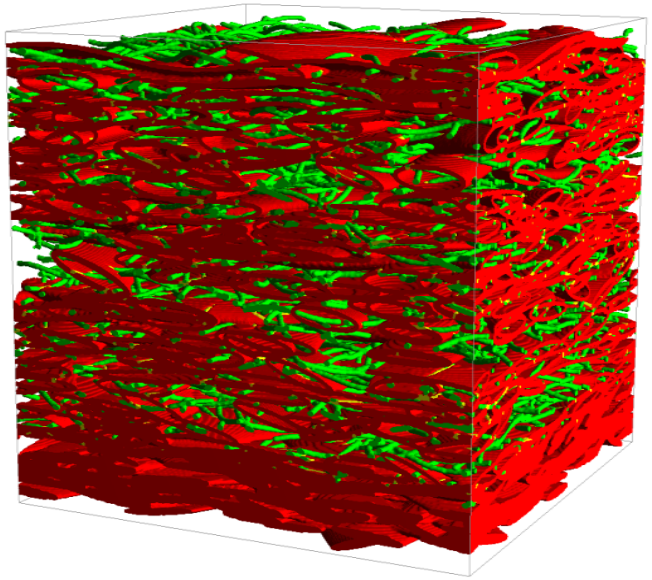
Determination of the capillary pressure – saturation relation for paper based on its 3D microstructure



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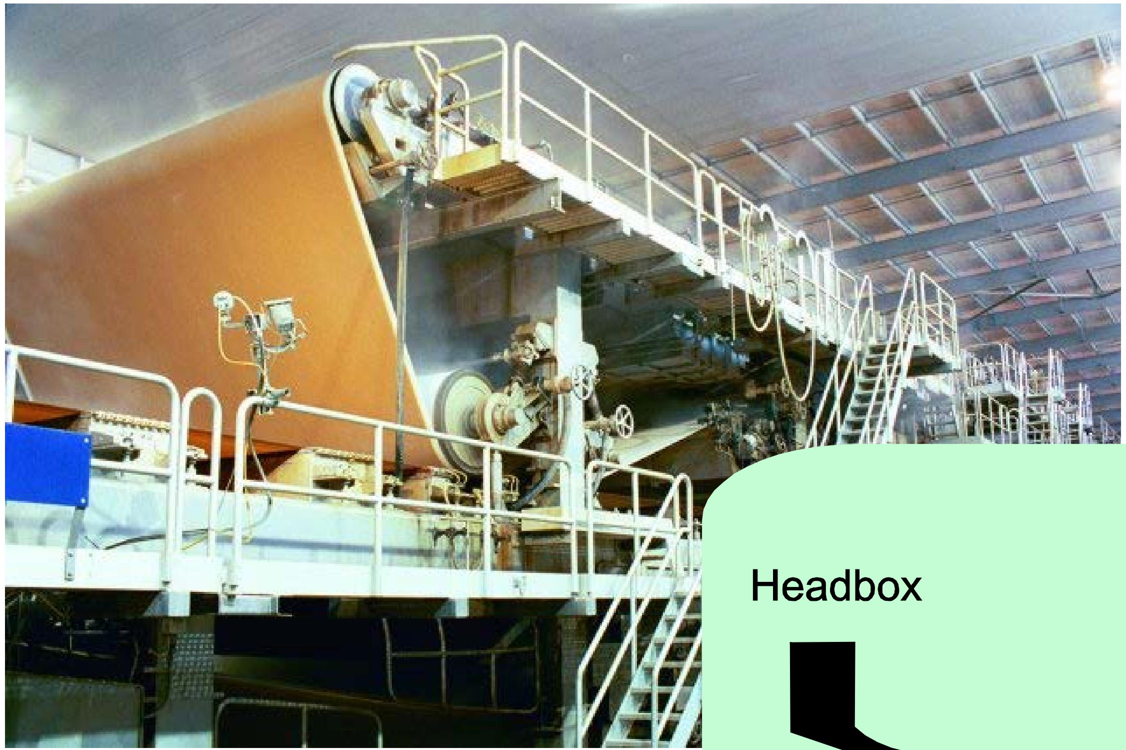
May 18-21, 2015

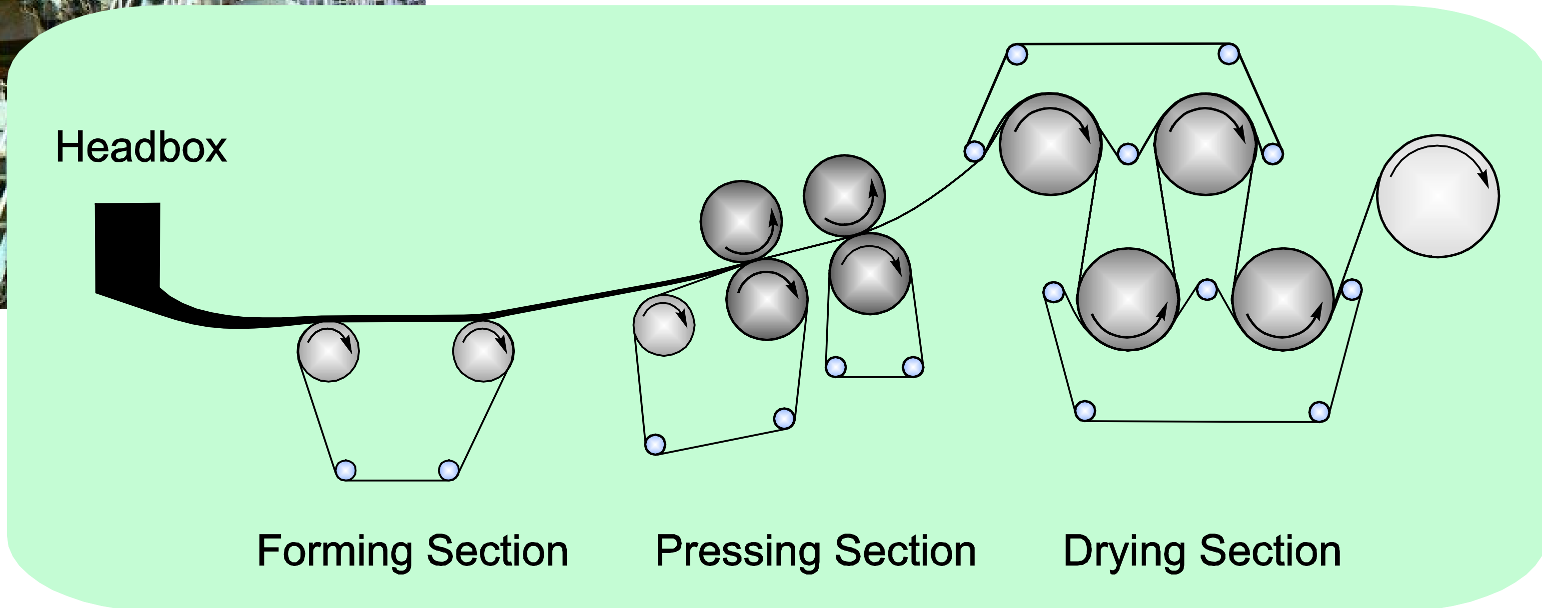
Overview

- Motivation: Paper Research at Fraunhofer ITWM
- Virtual Paper Generation
- New Multiple Contact Angle Pore Morphology Method
- Capillary Pressure – Saturation Curves of Virtual Paper
- Application and Summary

Paper Research at Fraunhofer ITWM

Paper Machine





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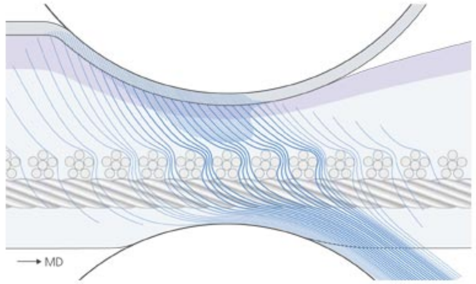
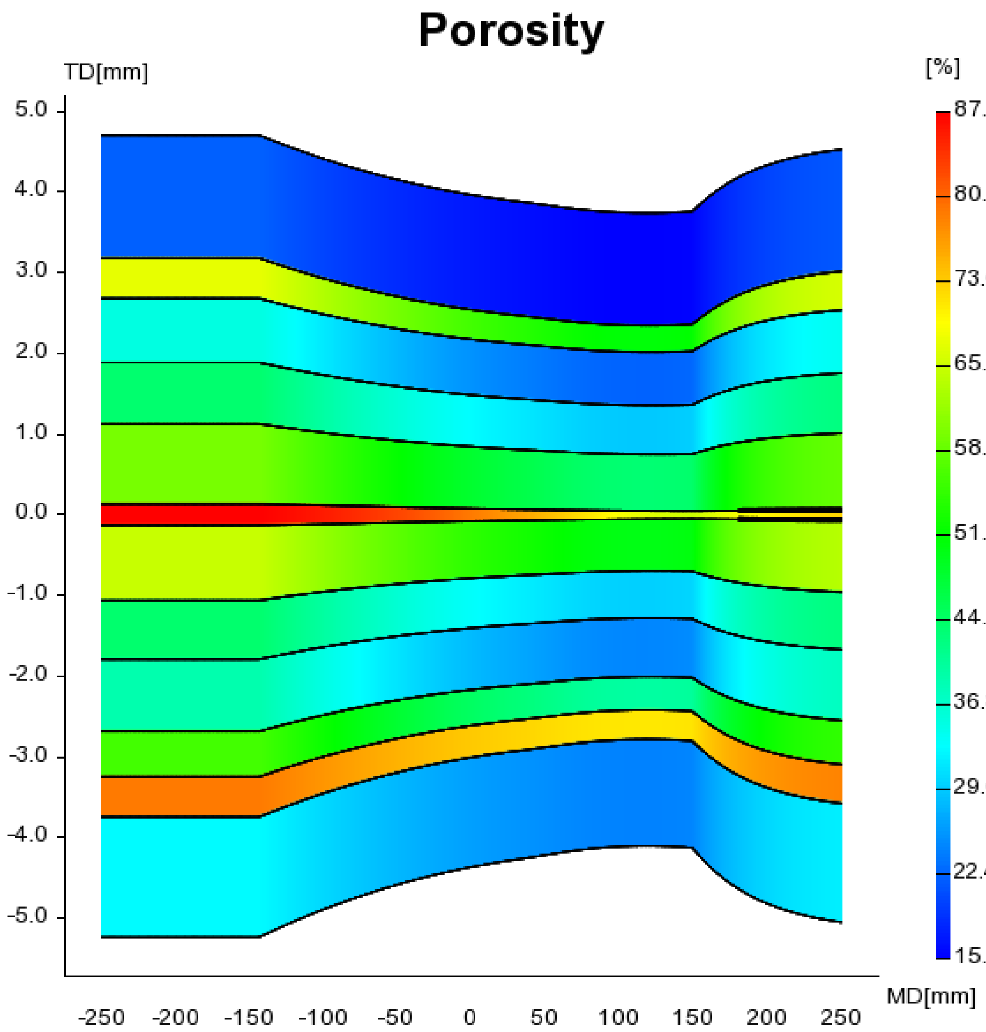
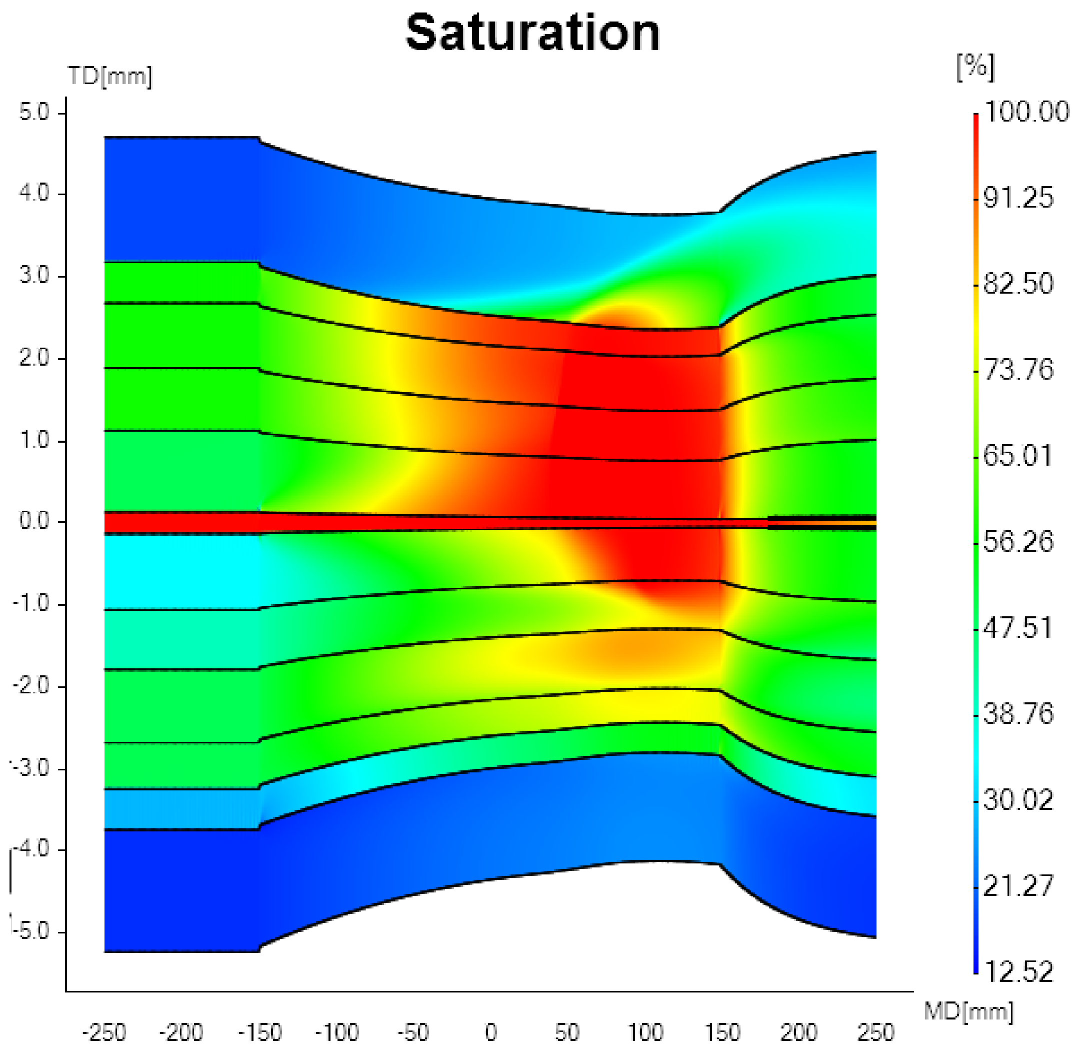
Paper Research at Fraunhofer ITWM

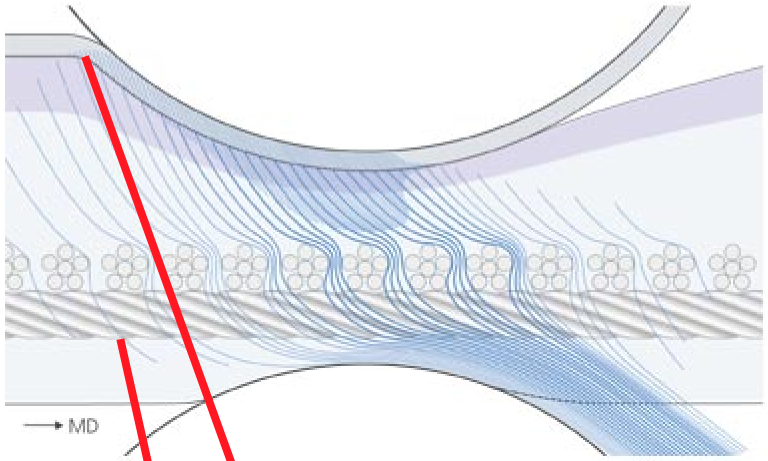
Macro simulation of the press nip



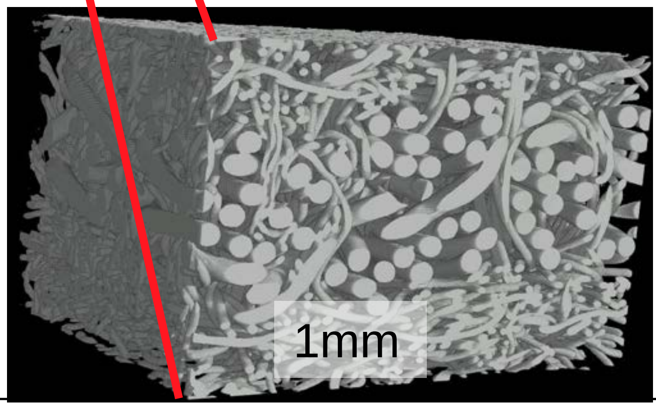


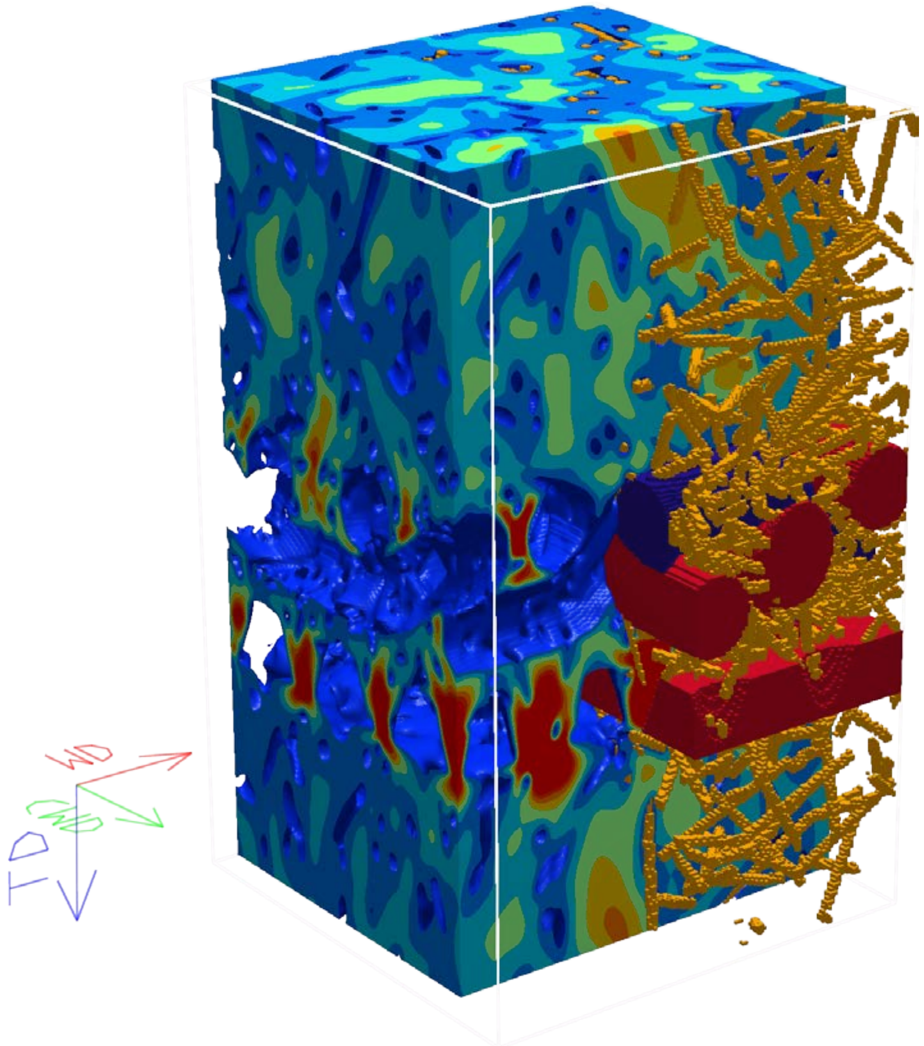


Paper Research at Fraunhofer ITWM



Press Nip





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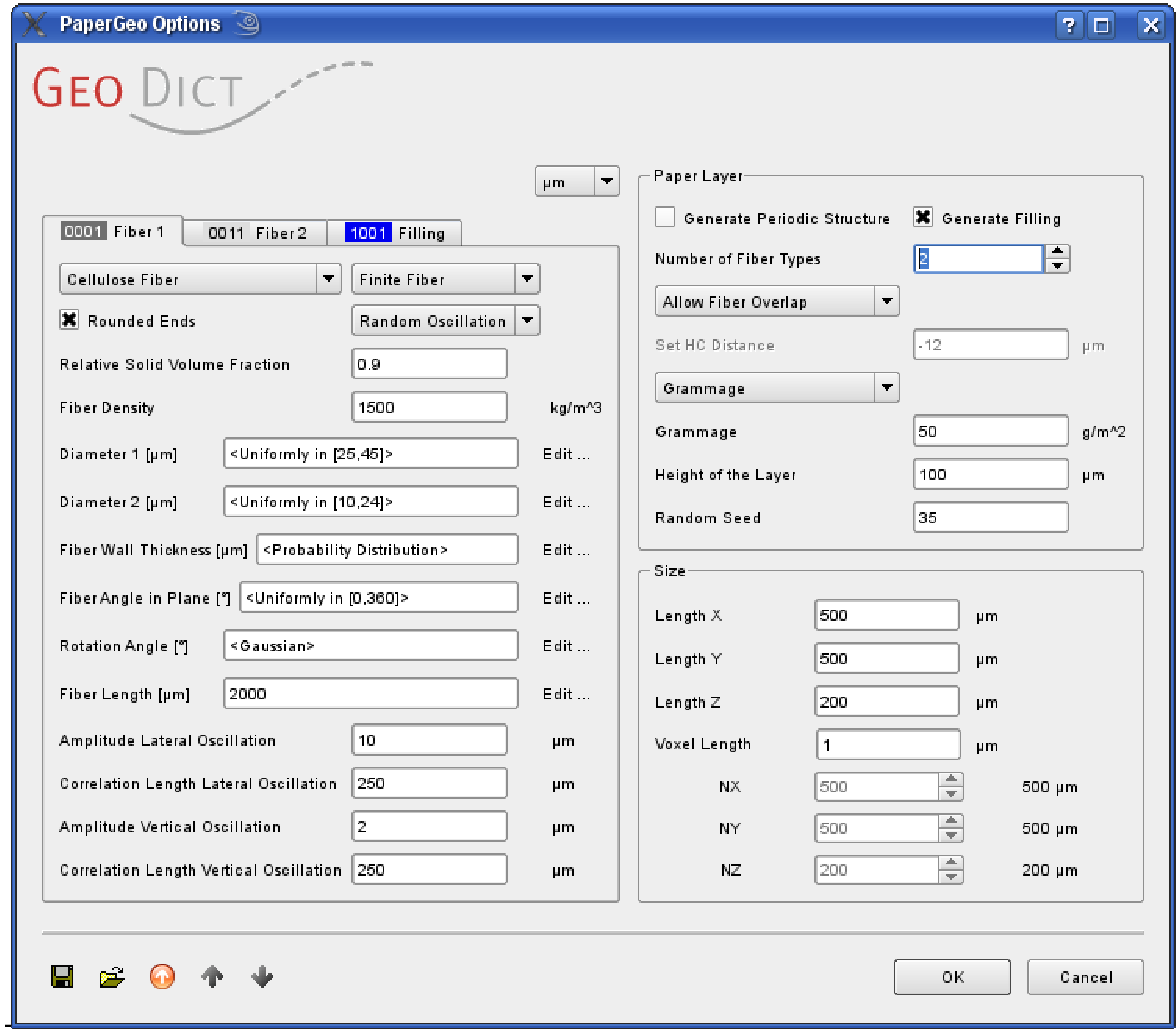
Virtual Paper Generation



Use **PaperGeo** to generate realistic paper models

Parameters

- Cellulose, ellipsoidal, and circular fibers
- Fillers and fines
- Random structure
- Fiber lay down

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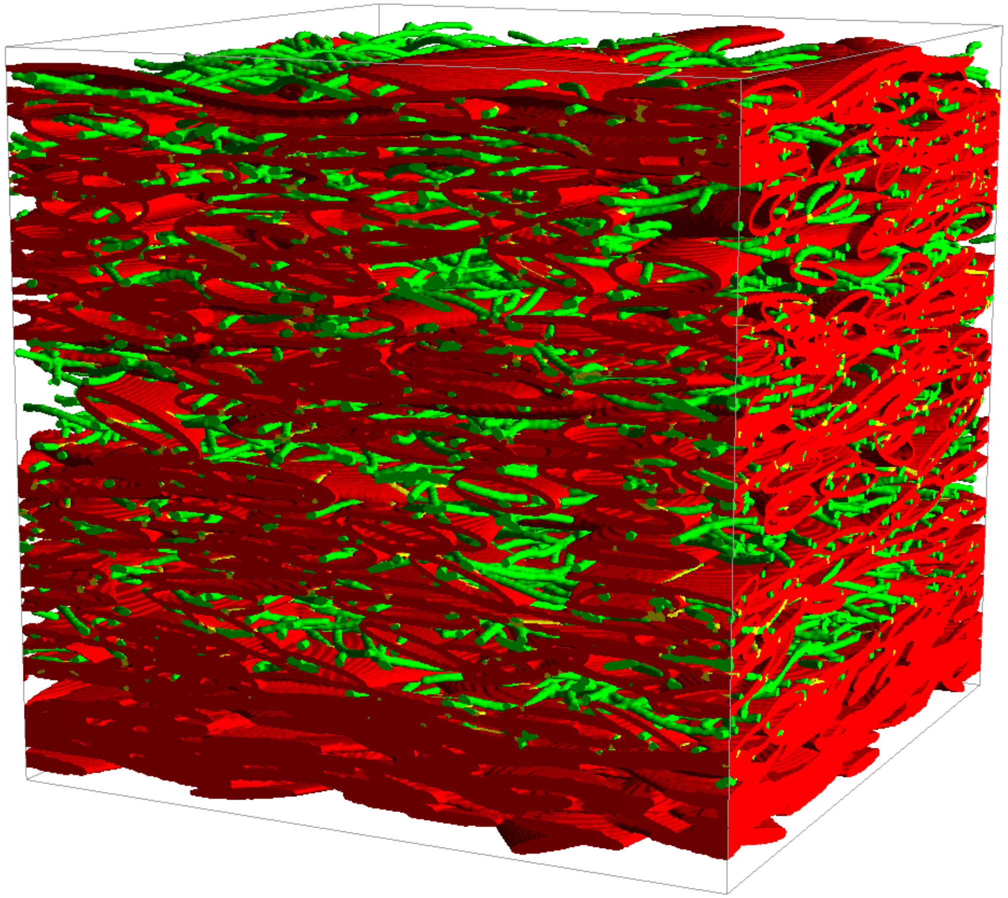
Virtual Paper Generation



Simulation of wetting and non-wetting phase distribution

- Solving two-phase Navier-Stokes equation requires large ressources
- We use a morphological operations are used to simulate the phase distribution according to a drainage experiment (Hilpert et al. 2001)
- Drainage of the wetting phase if

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

- Initial conditions:
  Void space is completely filled with wetting phase
- Algorithm based on the calculation of the Euclidean distance

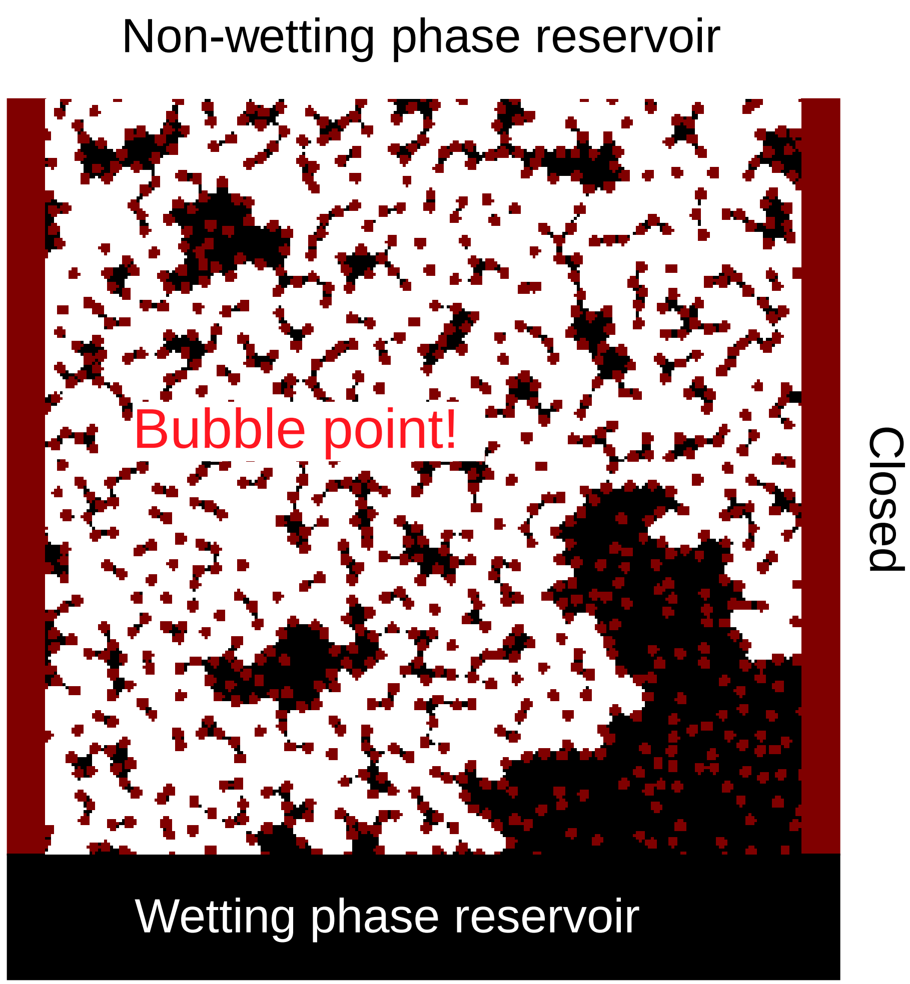


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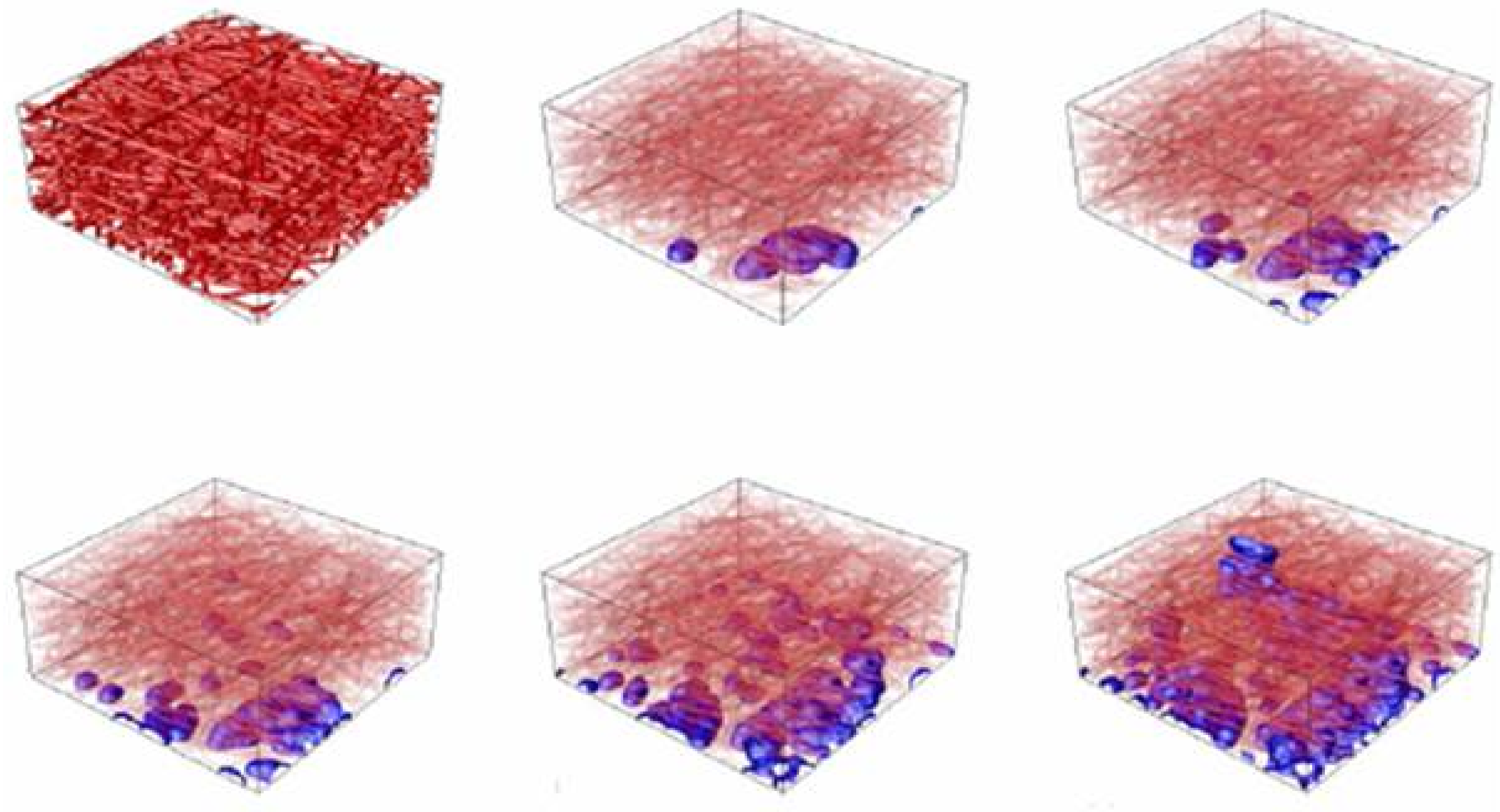
Illustration of the wetting phase distribution



V.P.Schulz, P.P. Mukherjee, J. Becker, A. Wiegmann, and C.Y. Wang: “Modeling of Two-phase Behavior in the Gas Diffusion Medium of Polymer Electrolyte Fuel Cells via Full Morphology Approach,” *Journal of the Electrochemical Society*, 154, B419 (2007).

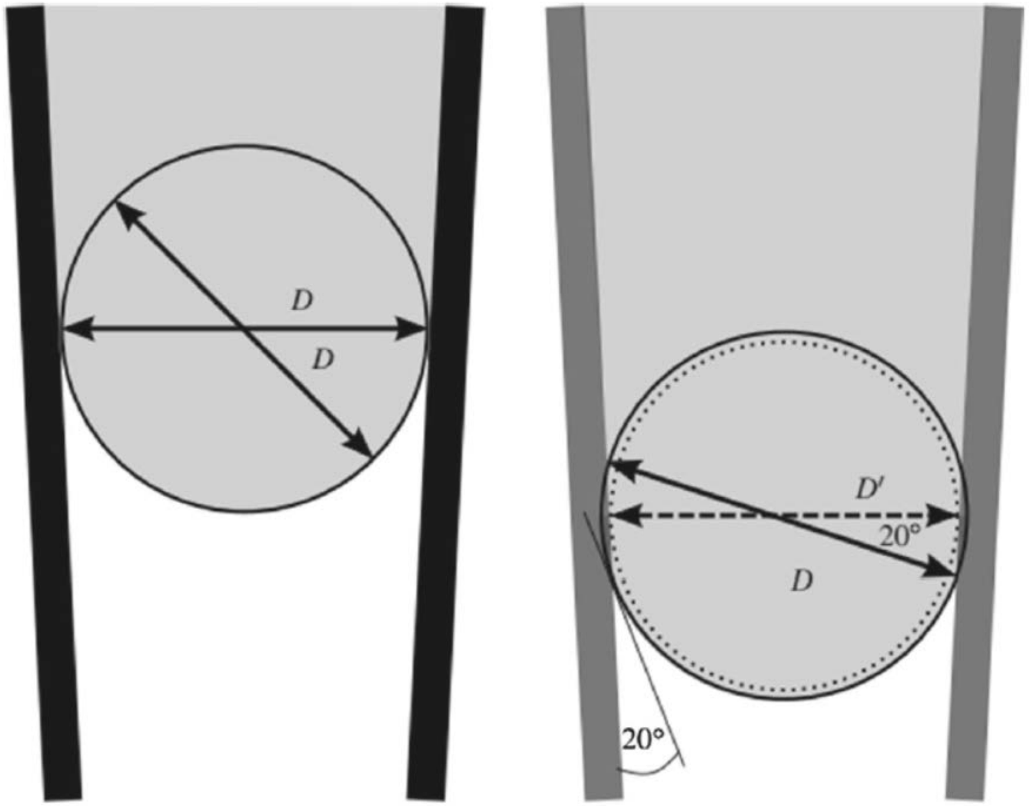
New Multiple Contact Angle Pore Morphology Method

- For totally wetting (left hand side), the meniscus is determined by a sphere of diameter D

$$p_c = \frac{4\sigma}{D}$$

- For partially wetting (right hand side), the meniscus is determined by a sphere of diameter D', where

$$p_c = \frac{4\sigma}{D}\cos\theta \qquad D' = D \cdot |\cos\theta|$$



Volker P. Schulz, Eric A. Wargo and Emin C. Kumbur: „Pore-Morphology-Based Simulation of Drainage in Porous Media Featuring a Locally Variable Contact Angle“, Transp Porous Med (2015) 107:13–25

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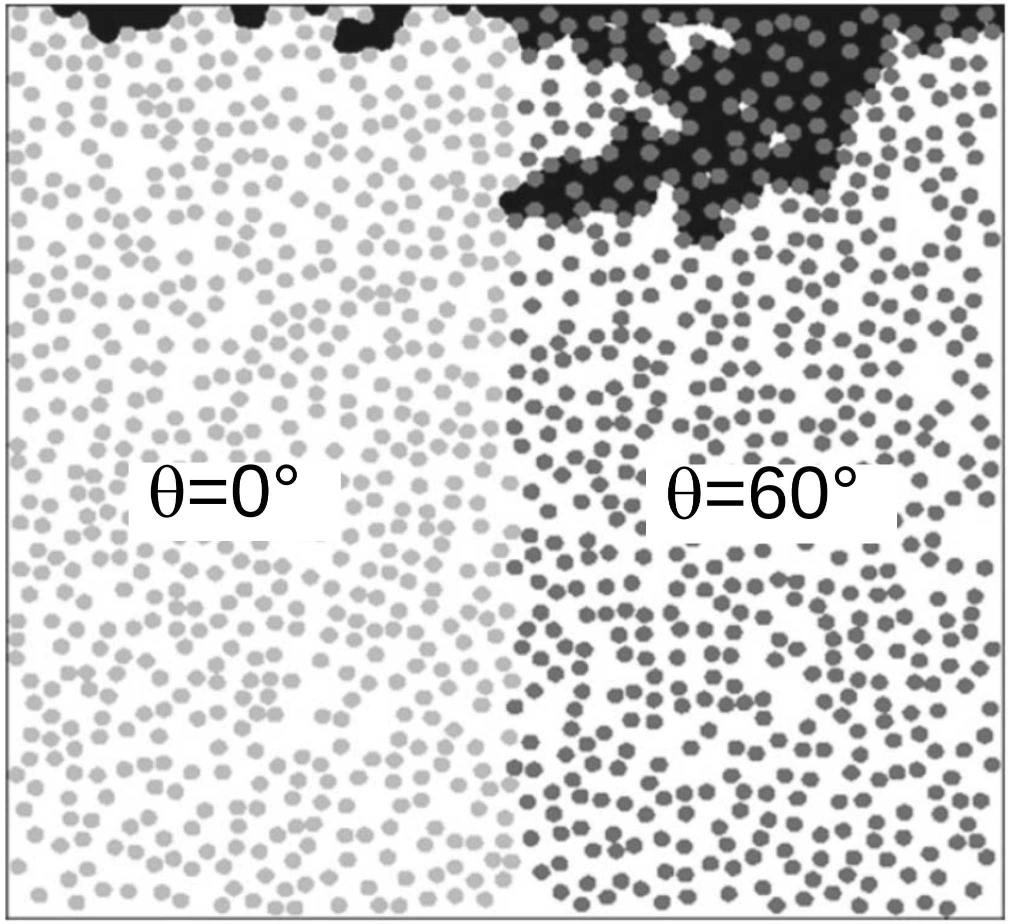
Porous media with locally different contact angle

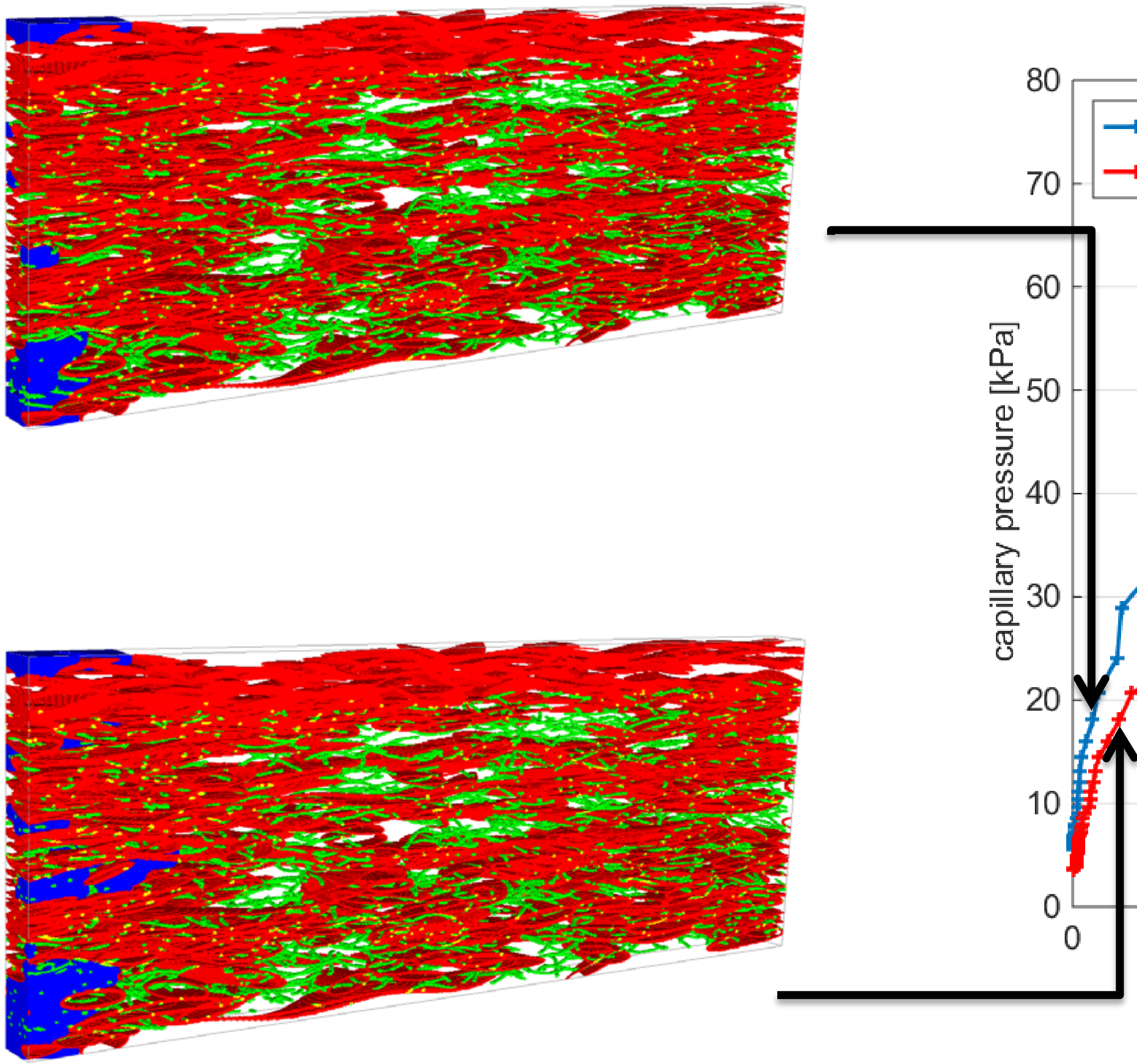
Locally variabl contact anlge leads to (locally) different satuaration at the same capillary pressure

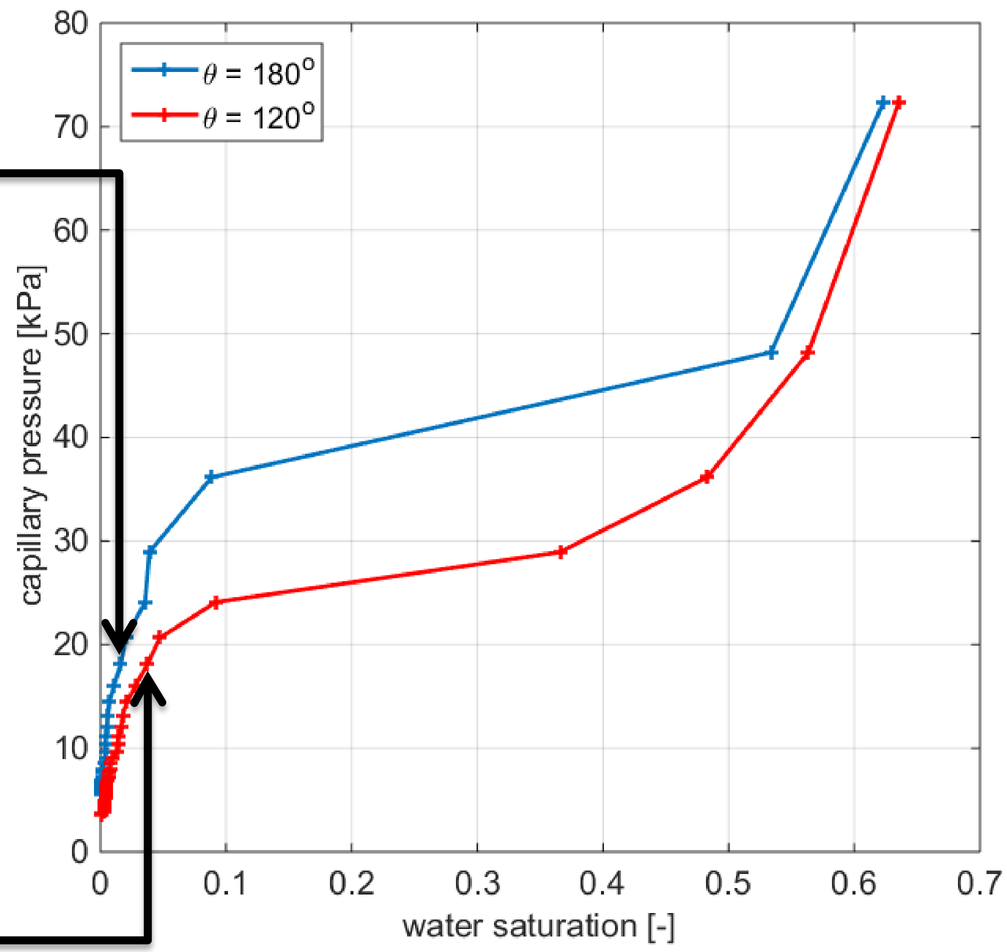


Application to 3D microstructures of paper

Two different fibers, 50x384x1000 voxel, resolution of 1µm/voxel

Contact angles are: 155° (red) and 120° (green, top), 180° (green, bottom)





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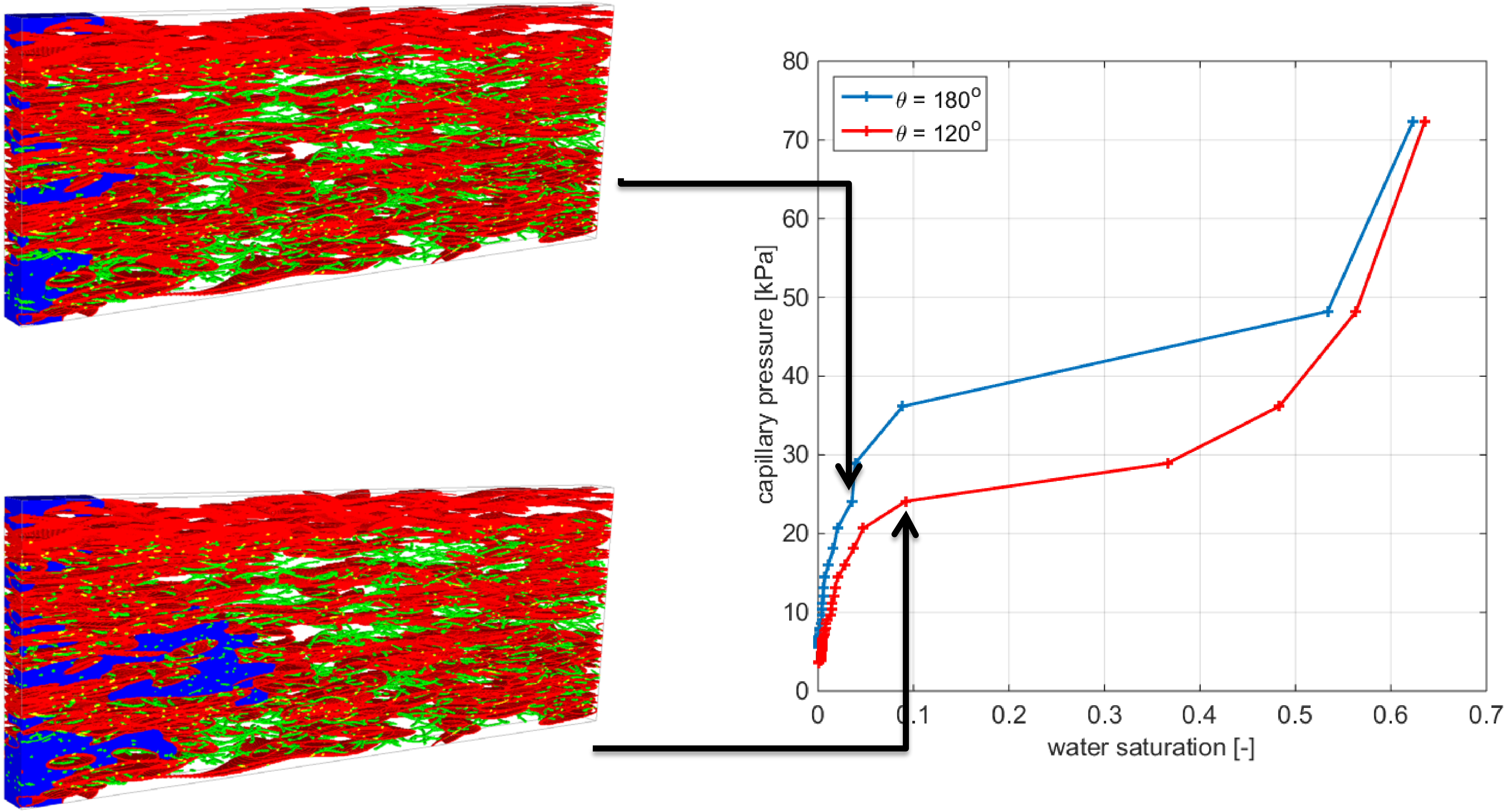

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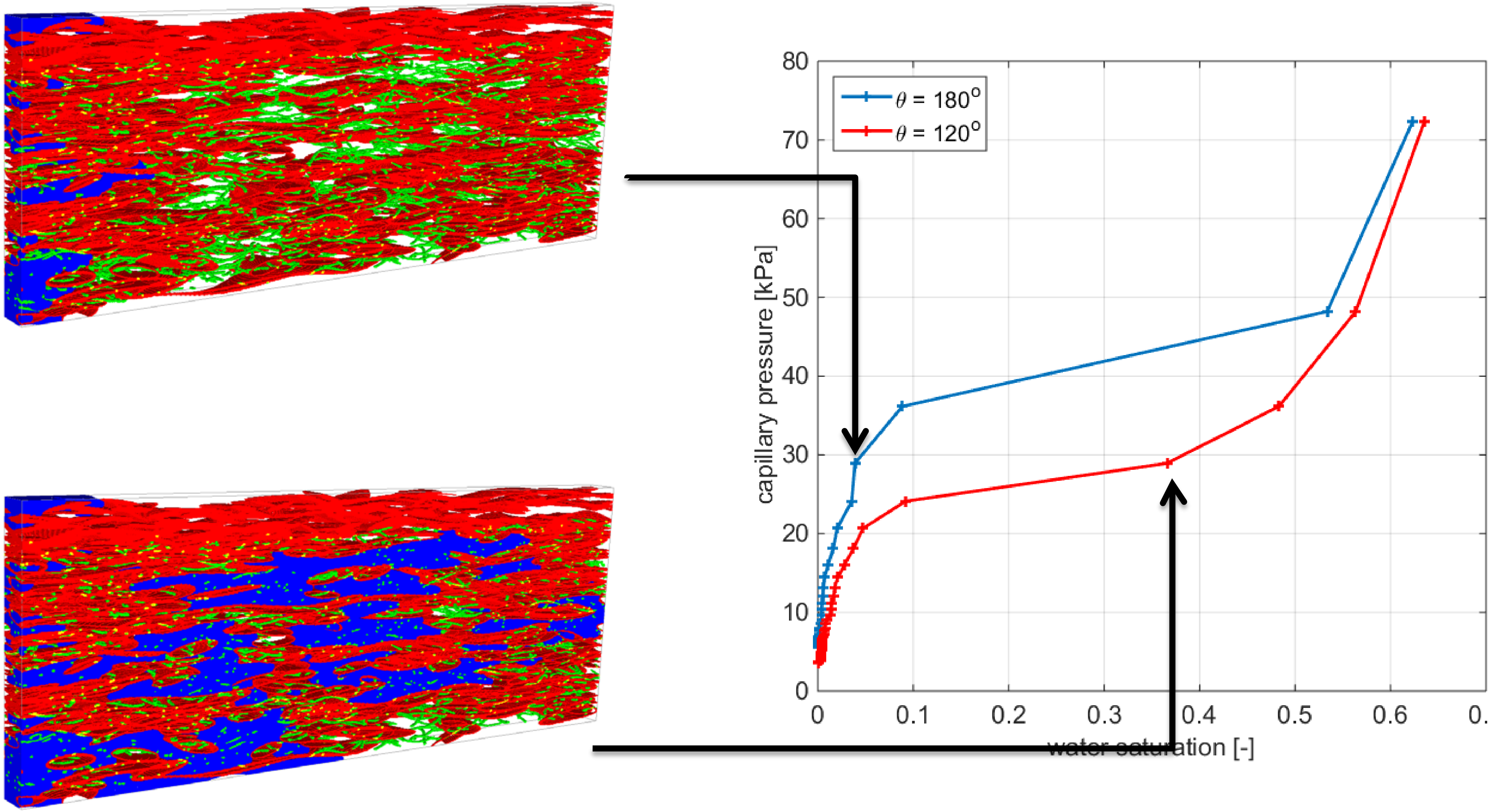

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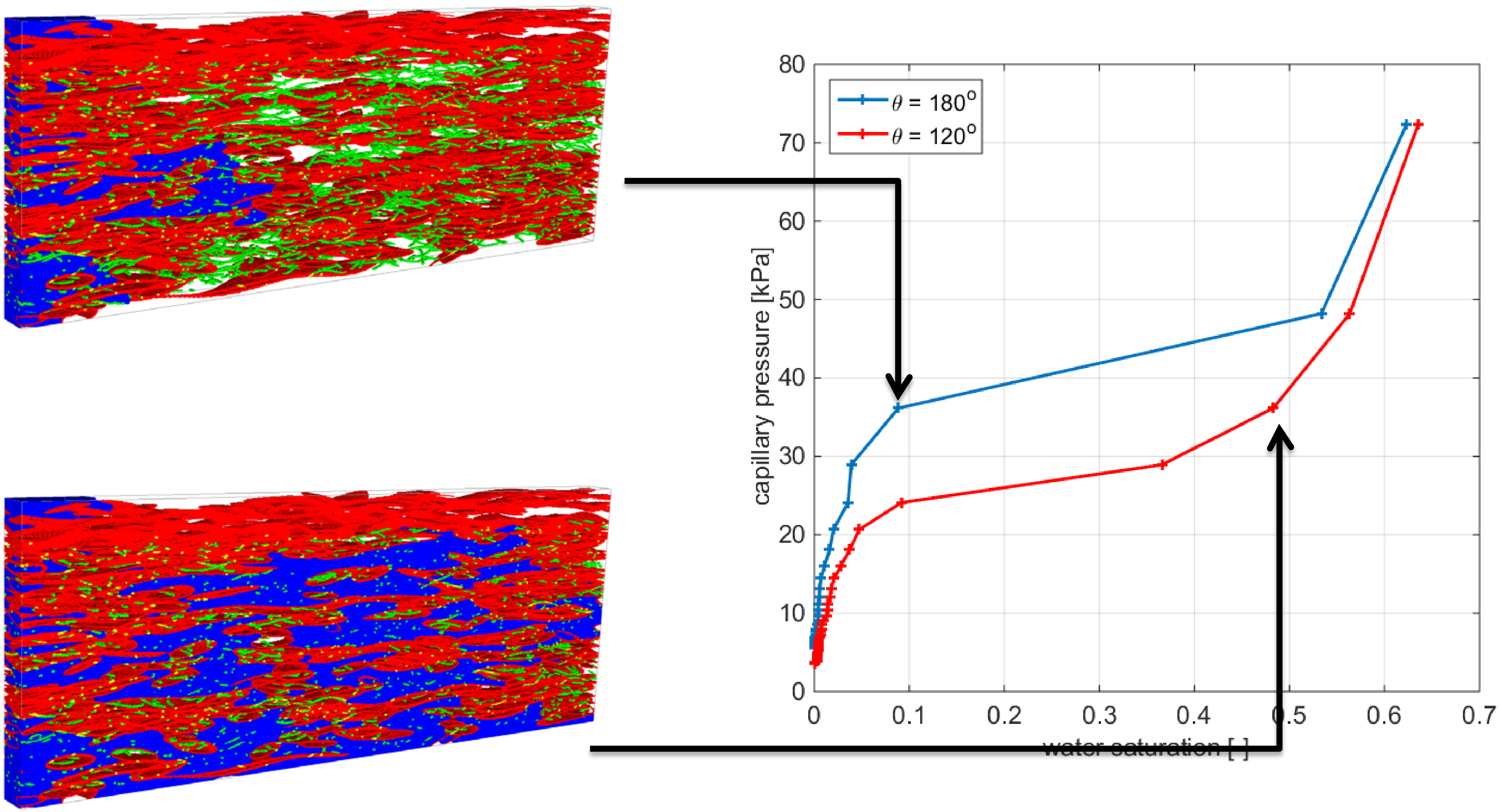

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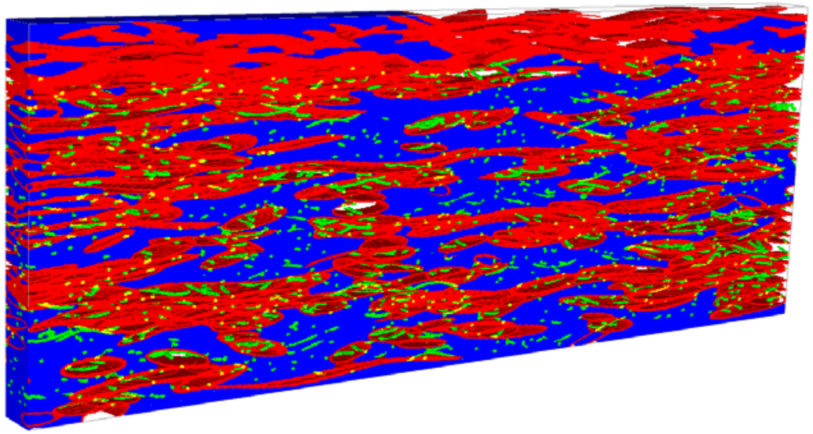

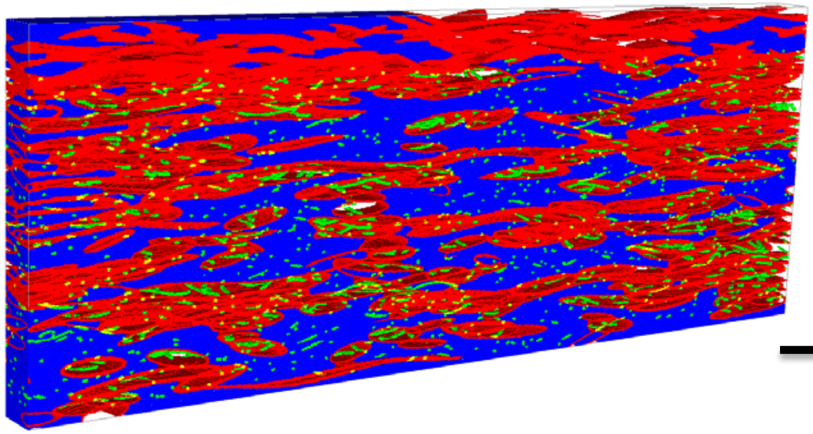

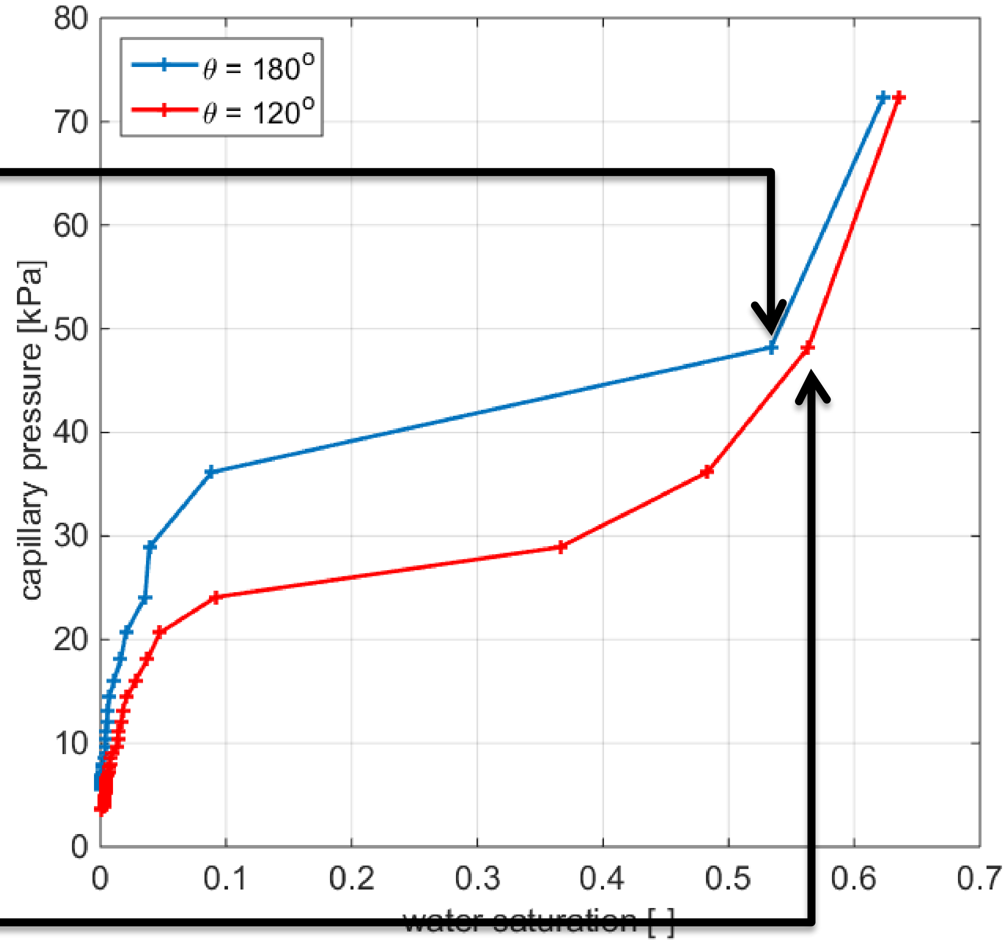

Application to paper and summary

•The pore morphology simulation has been already successfully used to simulate the paperboard edge wicking

A. Mark, J. Tryding, J. Amini, F. Edelvik, M. Fredlund, E. Glatt, R. Lai, L. Martinsson, U. Nyman, M. Rentzhog, S. Rief and A. Wiegmann: „Modeling and simulation of paperboard edge wicking", Nordic Pulp and Paper Research Journal, Vol 27, No.2/2012, pp. 397-402

•In this approach, the capillary pressure-saturation relation is used in a multi scale model

•With the shown extension, one can study 3D micro structures of paper featuring locally variable contact angles

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Thank you for your attention!