Pore network simulation and tomographic visualization of particle aggregates drying

Y.J. Wang, A. Kharaghani, E. Tsotsas

Thermal Process Engineering

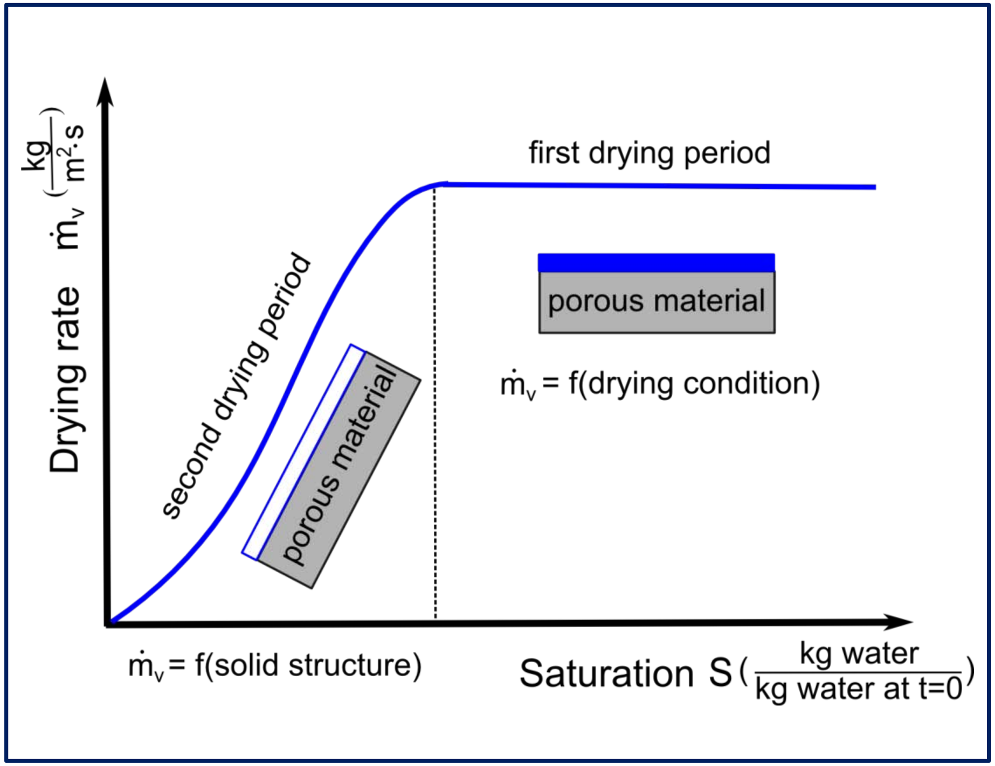
DFG - Graduiertenkolleg
Micro-Macro-Interactions
of Structured Media and Particle Systems

OTTO VON GUERICKE
UNIVERSITÄT
MAGDEBURG

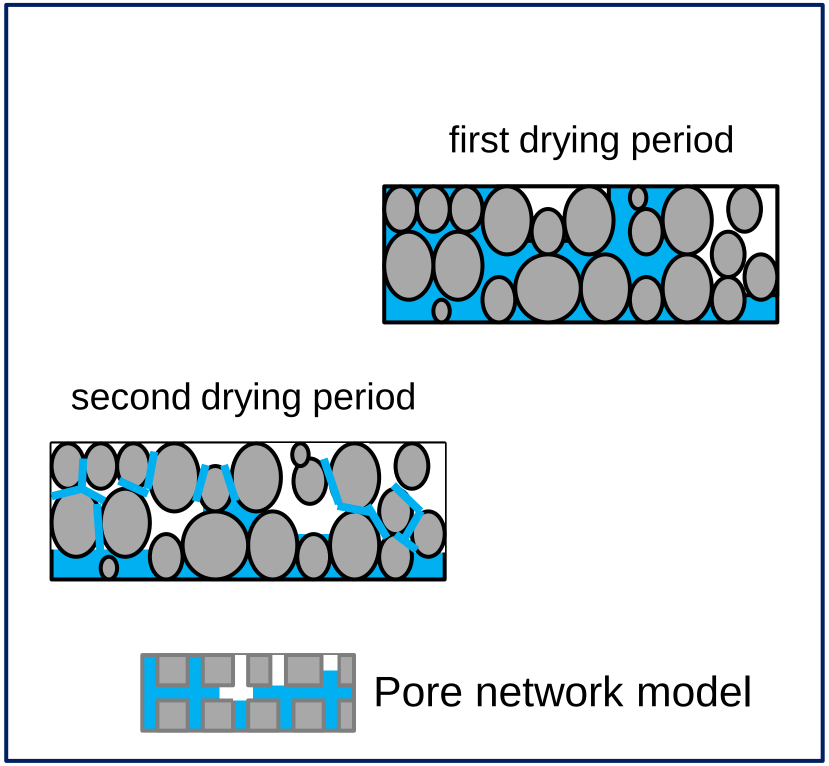
FAKULTÄT FÜR VERFAHRENS-
UND SYSTEMTECHNIK

14. 01. 2014

Problem definition



Macro



Micro

Pore network model is a suitable tool to examine the pore-scale behaviour of porous media.

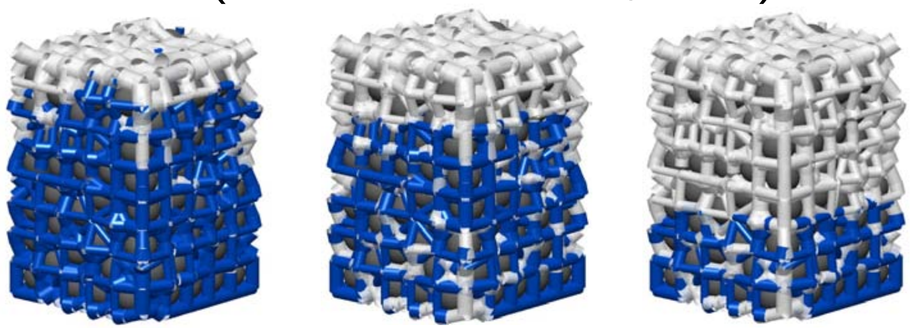
- some physical effects are still absence in the recent model
- lack of pore-scale experimental validation

Objective

- Use X-ray microtomography (µ-CT) to validate the pore network model by drying experiments with particle aggregates.

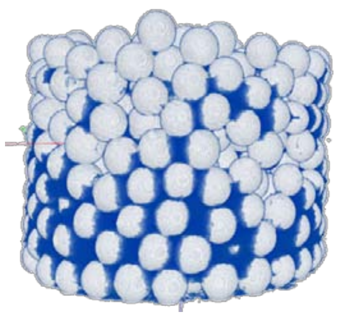
Pore network simulation

simulated particle packing
(voronoi tesselation, DEM)



µ-CT experiment

real particle packing



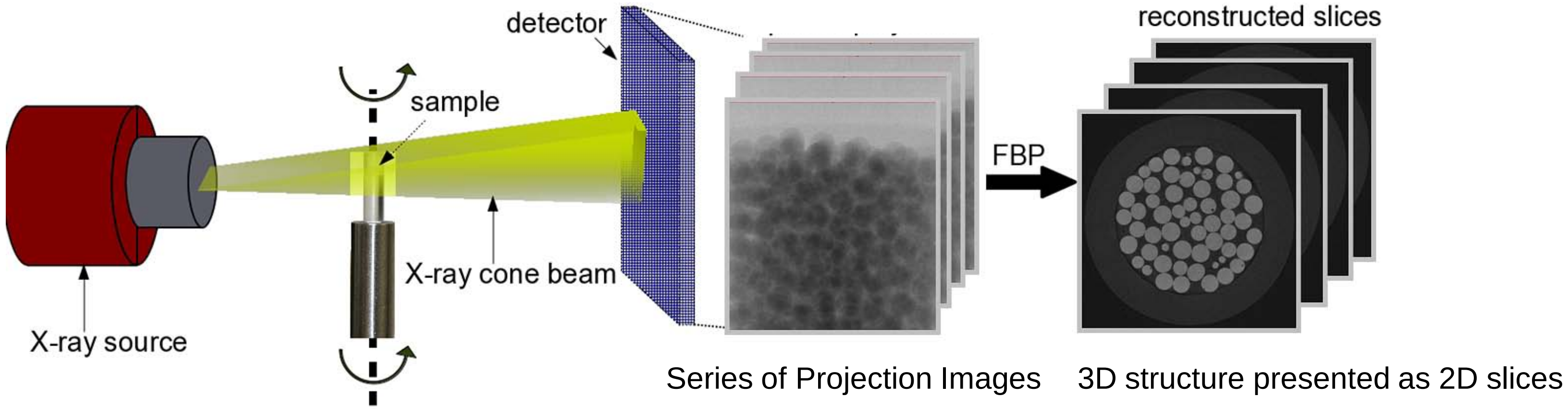
particle center coordinates

liquid distribution (pore scale)

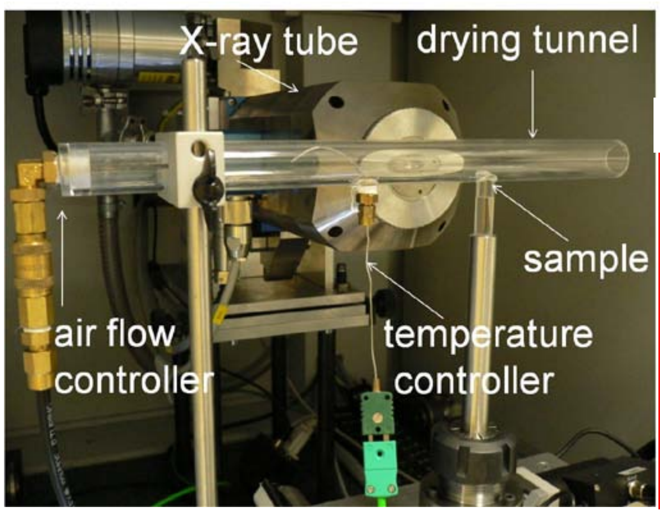
- Develop and implement liquid film effect in the pore network drying model

Material and experimental setup

Principle of X-ray microtomography



Experimental setup



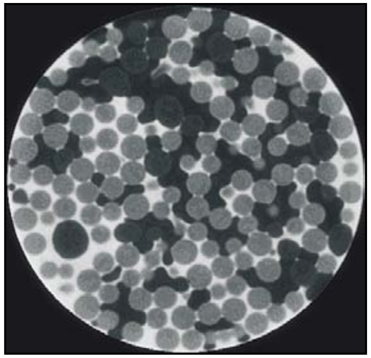
CT-ALPHA-160, ProCon X-Ray

- air flow rate: 1 m/s
- temperature: 25°C
- drying time interval: 30 mins
- number of projection: 400
- exposure time: 1000 µs
- voxel size: 6×16×16 µm^3
- scanning time: 30 mins

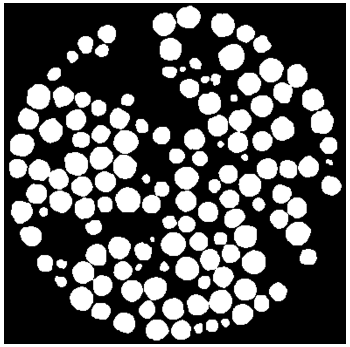
Drying from the top surface.
The sample dried inside the tomography.

Image processing

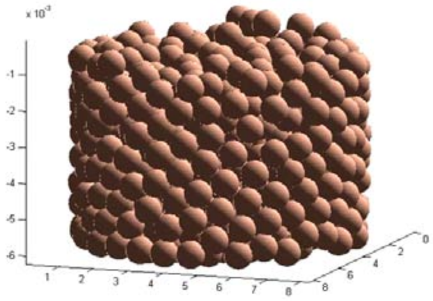
Cooperation with M.Sc. Maryam Sada Dadkhah



gray scale image

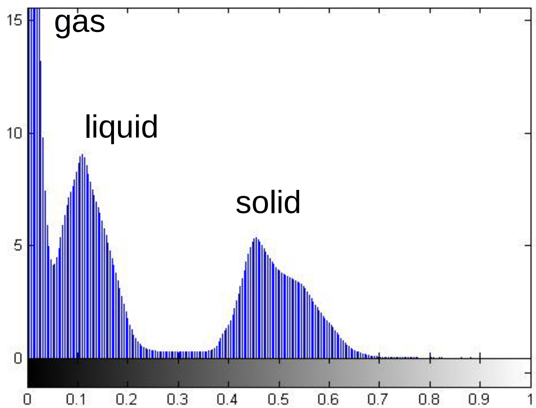


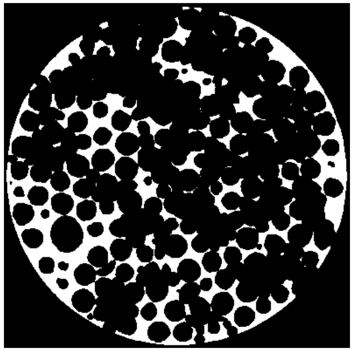
binary image
(solid phase)



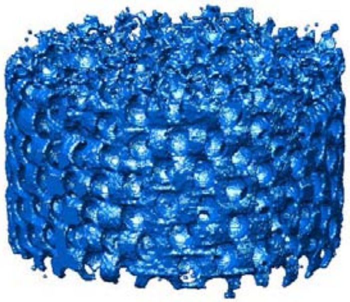
particle center coordinates

Histogram of gray values



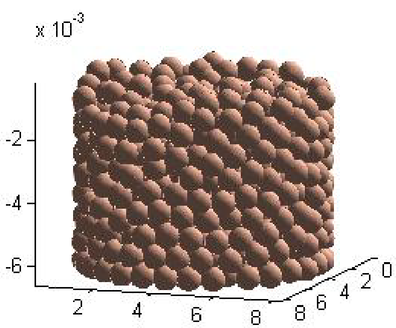


binary image
(liquid phase)

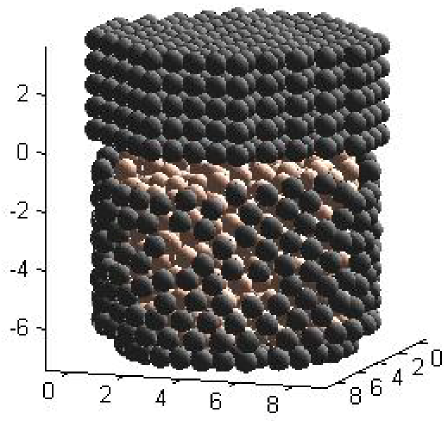


Saturation: S

Pore network drying model



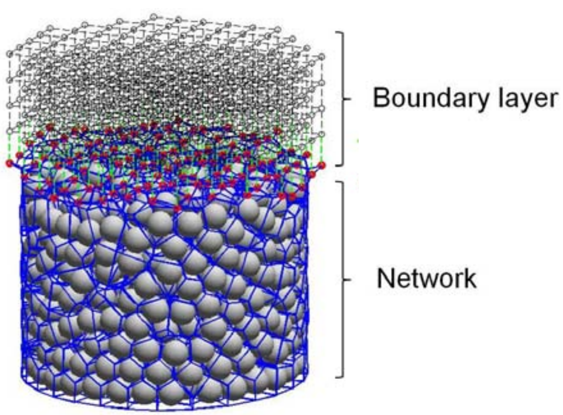
Original packing



Add virtual particles

M.Sc. Oleksandr Prygorniev

input → | Voronoi tessellation
Elimination
Node-merging | → output



Identify boundary layer, network, throats and nodes

evaporation at the liquid-gas interface

vapor diffusion in the gas phase

$$\sum_j \dot{M}_{v,ij} = \sum_j A_{ij} \frac{\delta}{L_{ij}} \frac{P\tilde{M}_v}{\tilde{R}T} \ln\left(\frac{p-p_{v,i}}{p-p_{v,j}}\right) = 0$$

viscous liquid flow

$$\sum_j \dot{M}_{w,ij} = \sum_j \frac{\rho_w \pi r_{ij}^4}{8\eta L_{ij}} \left(p_{w,i} - p_{w,j}\right) = 0$$

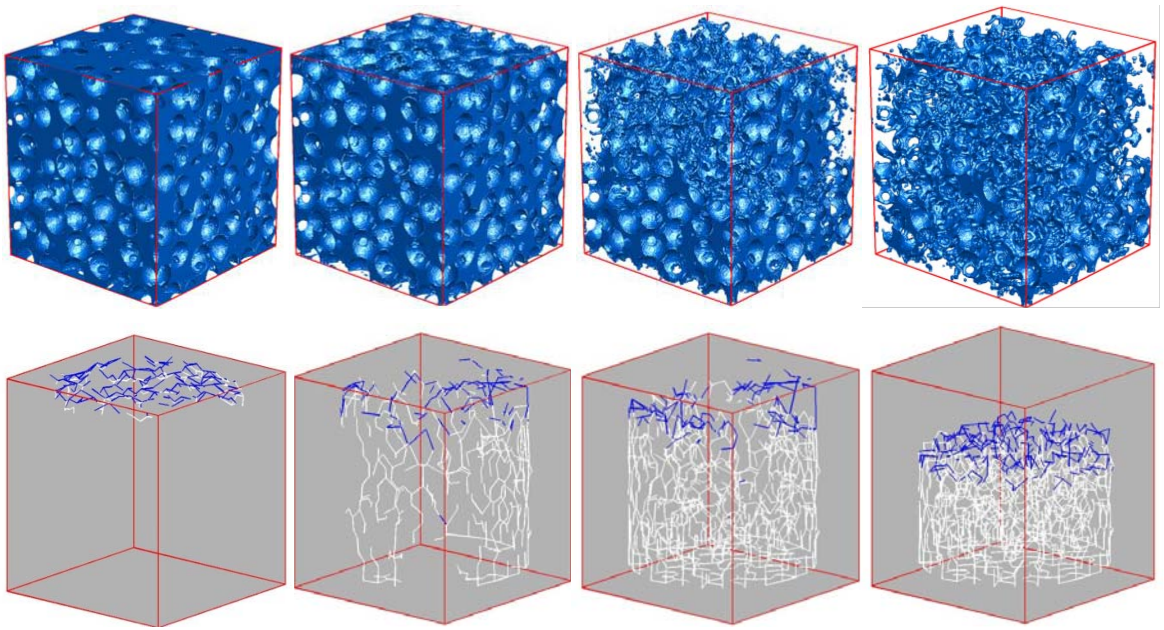
and balance gravity force

$$\Phi\left(r_{ij}, z_{ij}\right) = -\frac{2\sigma}{r_{ij}} + \left(\rho_w - \rho_a\right) g z_{ij}$$

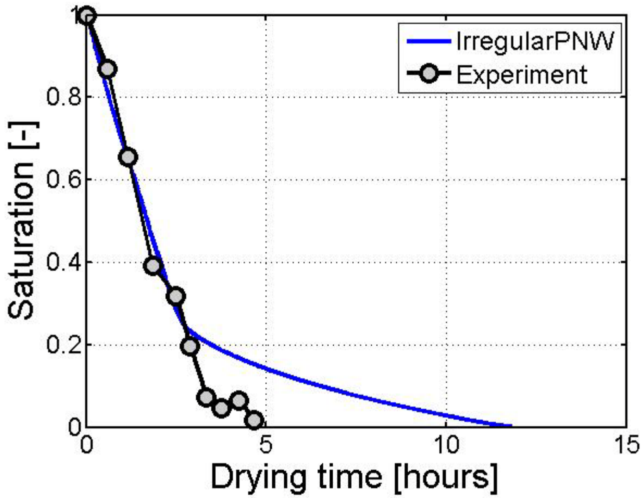
Comparison – total saturation

Evolution of liquid phase distribution

S=0.8 S=0.6 S=0.4 S=0.2



Drying curve



- Pore network model predicts fairly the first drying period.
- Drying time is overestimated by the pore network simulation.

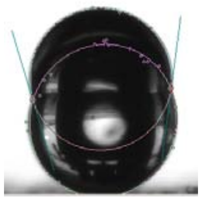
Which mechanism enhances drying rate and shorter drying time? ---> liquid film flow ?!

Existence of liquid film

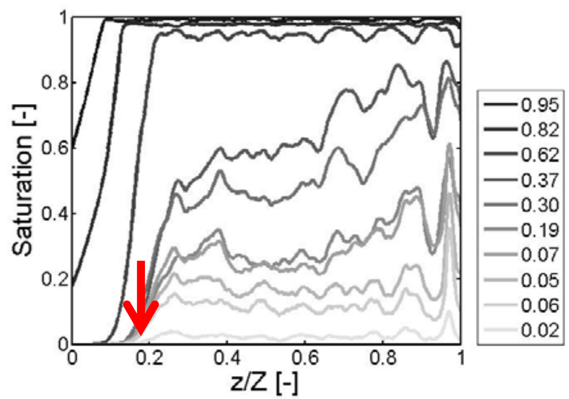
Hydrophilic (HI) glass beads are coated with a hydrophobic (HO) layer

Cooperation with M.Sc. Zinaida Kutelova

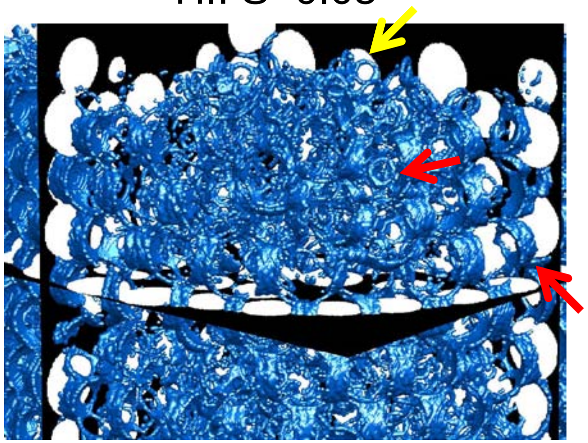
Hydrophilic particles (HI)



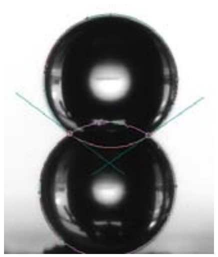
Contact angle = 32.2°



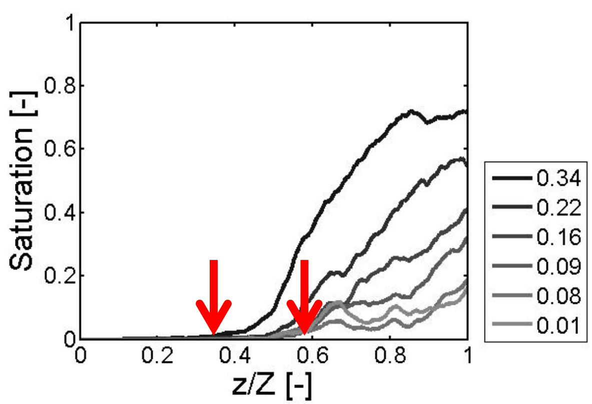
HI: S=0.05



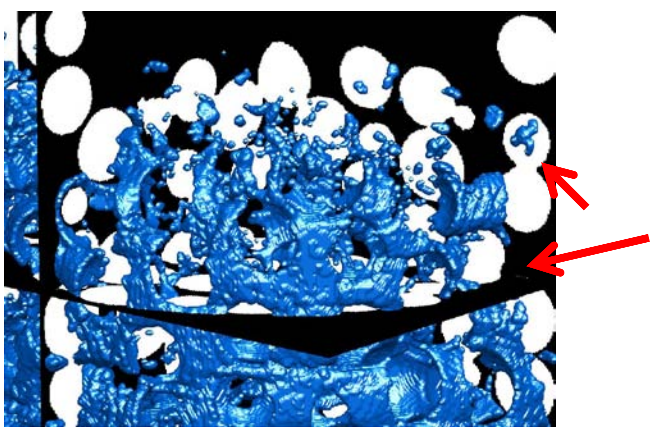
Hydrophobic particles (HO)



Contact angle = 109°



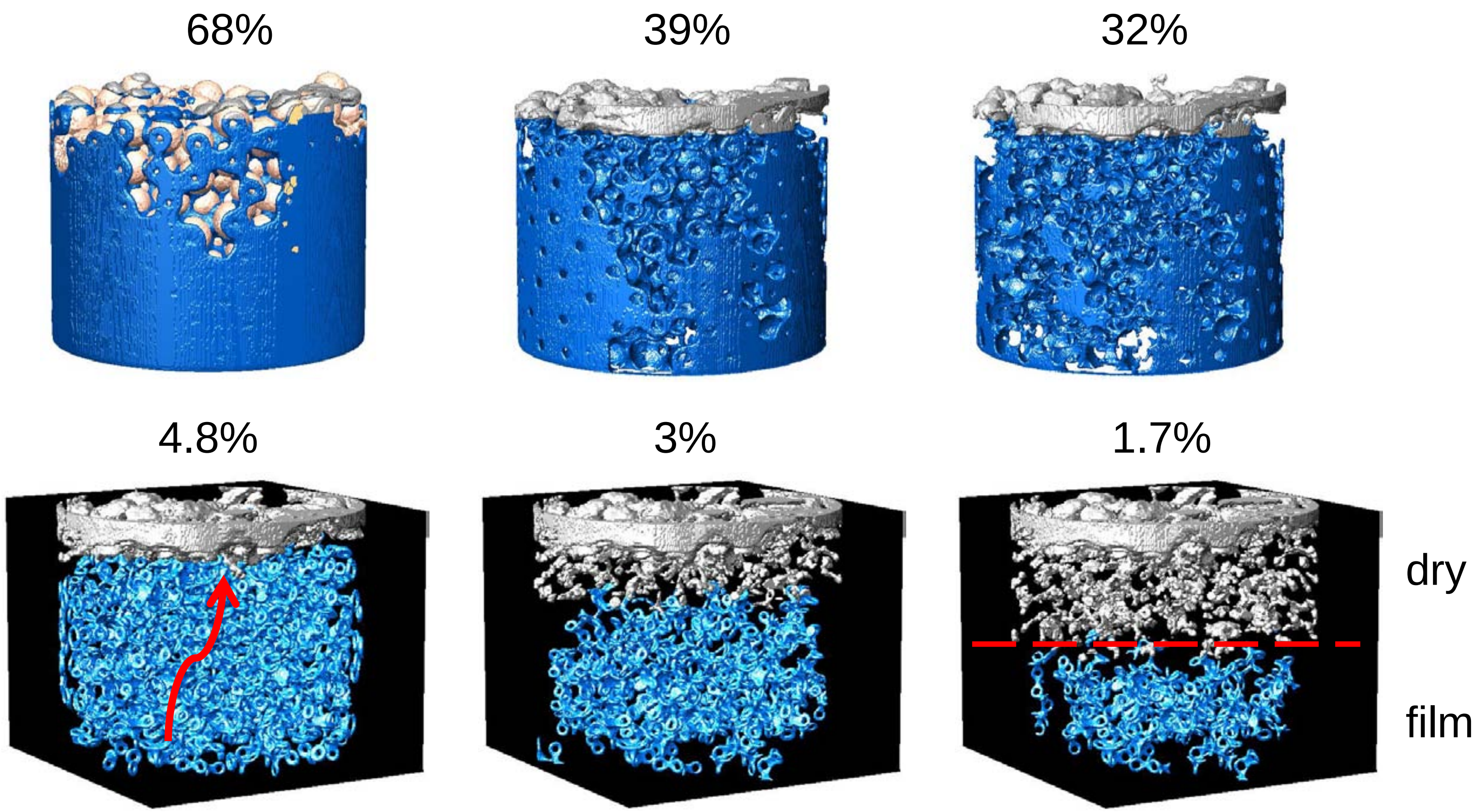
HO: S=0.05



Macroscopically isolated liquid or hydraulically connected?

Existence of liquid film

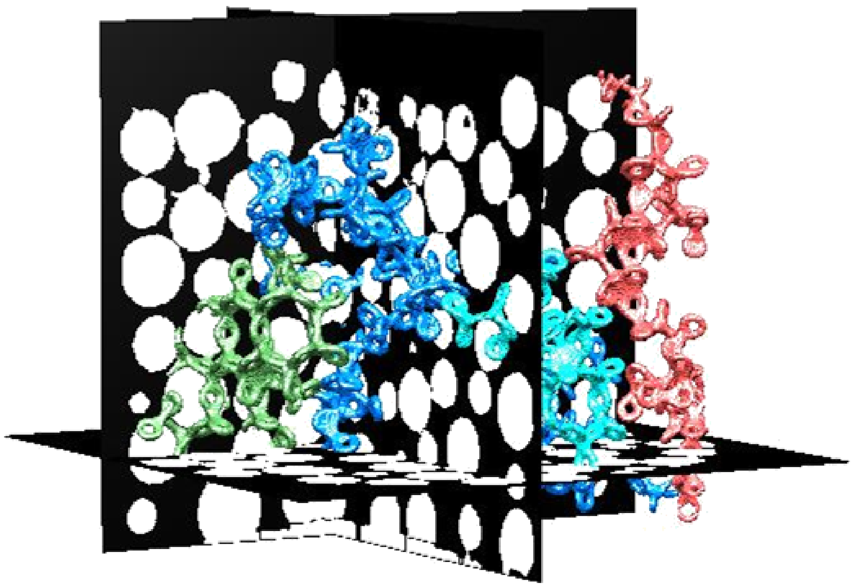
Drying of KI solution with concentration 73%



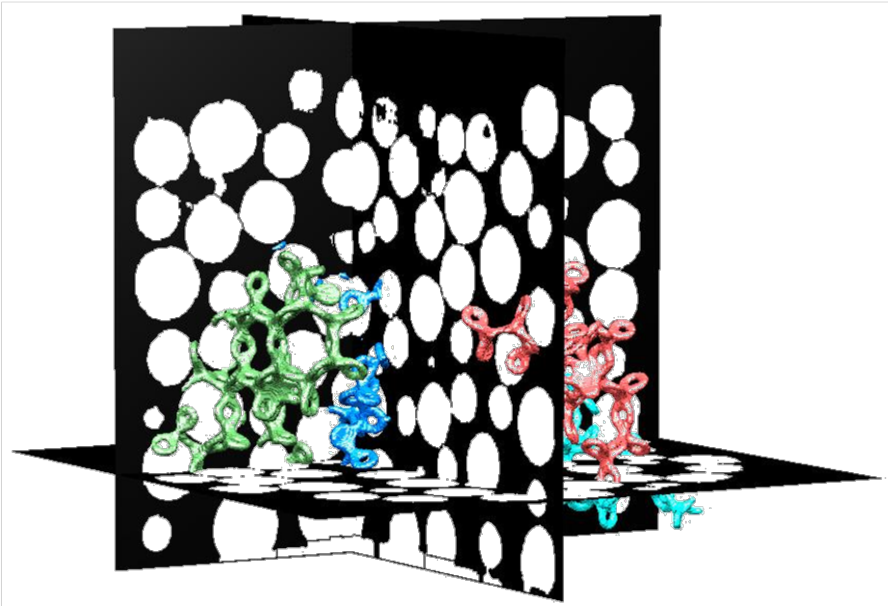
Due to the morphology difference between liquid film and salt crystals, the evaporation front is identified.

Connectivity of liquid film rings

S = 3%



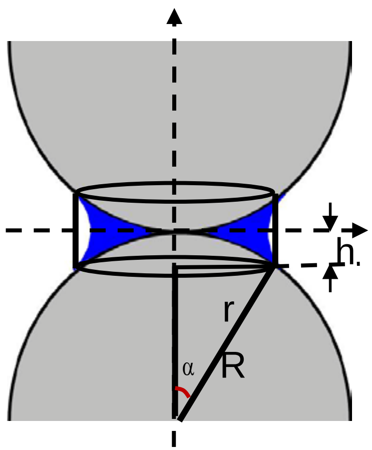
S = 1.7%



At low saturation, the liquid phase remains connected through liquid rings around the particle-particle contact points providing the liquid to the aggregate surface.

Incorporation of liquid rings into pore network model

Ring geometry

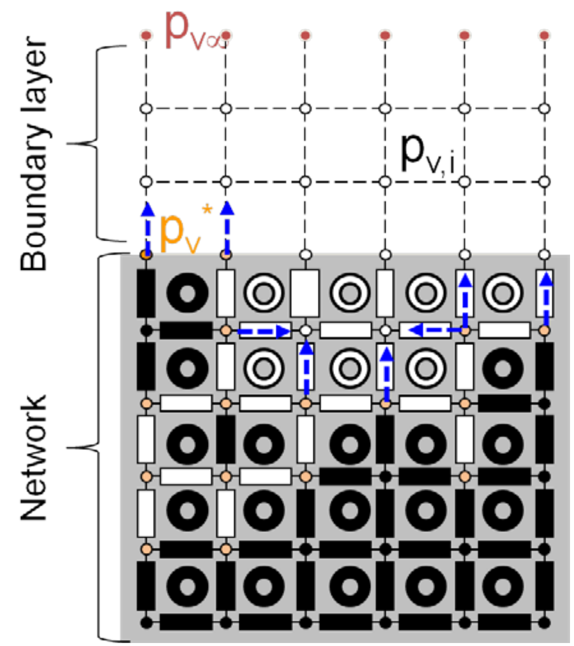


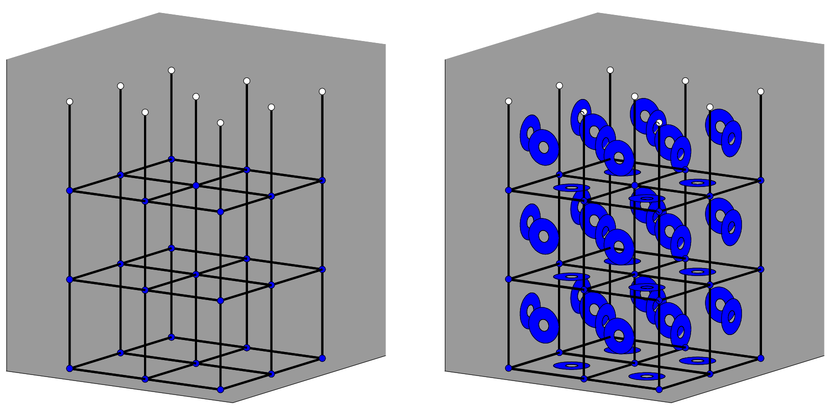
$$V_{Ring} = V_{Cylinder} - V_{spherical\ cap}$$

$$r = \left| R \sin \alpha \right|$$

$$h = R - \left| R \cos \alpha \right|$$

$$V_{Ring} = 2\left(\pi r^2 h - \frac{3}{\pi}(3R-h)h^2 \right)$$





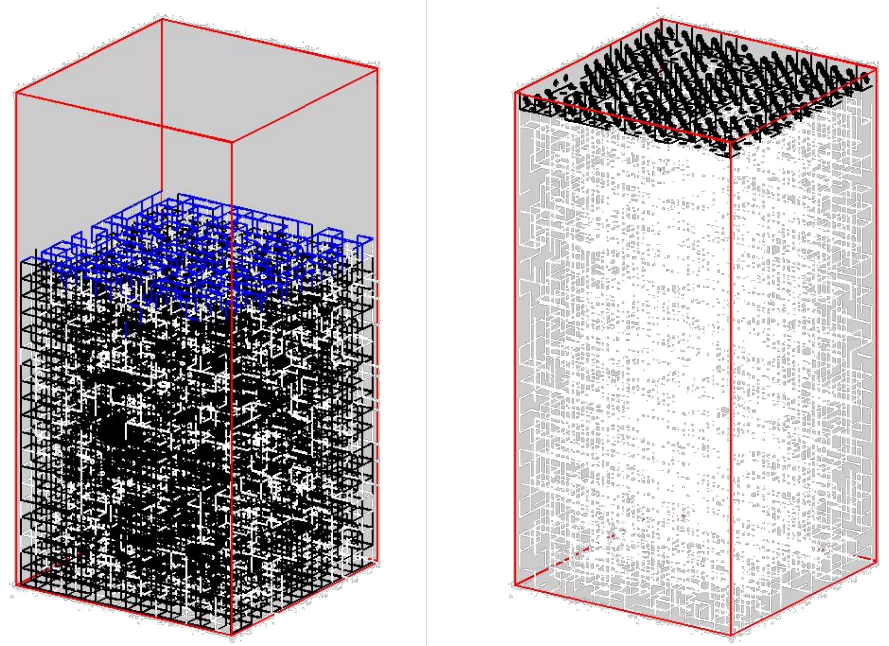
Regular pore network with liquid rings

An algorithm for liquid rings drying:

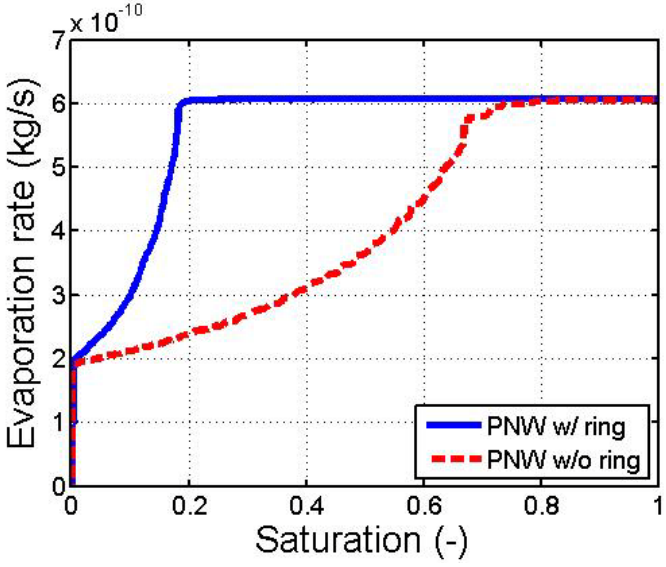
- The emptying sequence and disconnection of liquid rings are all decided by throats.
- There is no vapor diffusion in the network until a ring starts to dry.
- Ring starts to dry when it is isolated.
- Cluster labelling algorithm should change and take rings into account.

Comparison: PNW with ring and without ring

S=50%



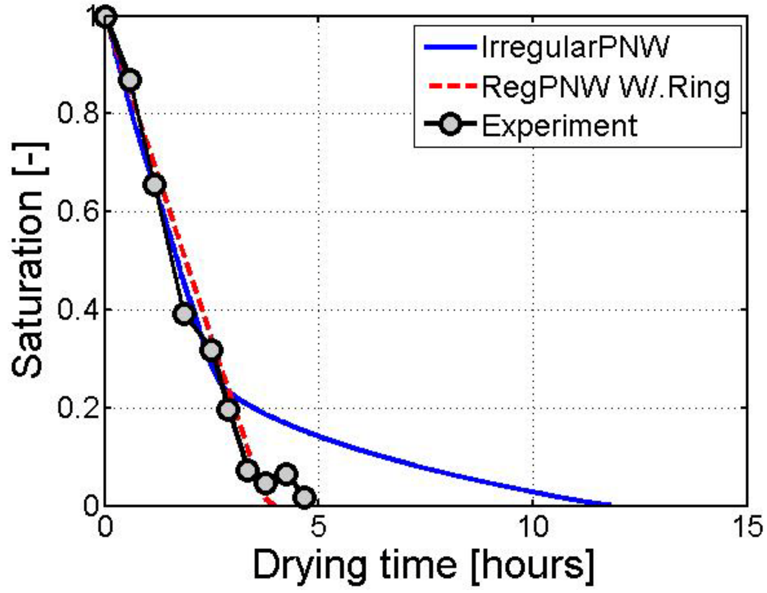
no ring　　　　with ring

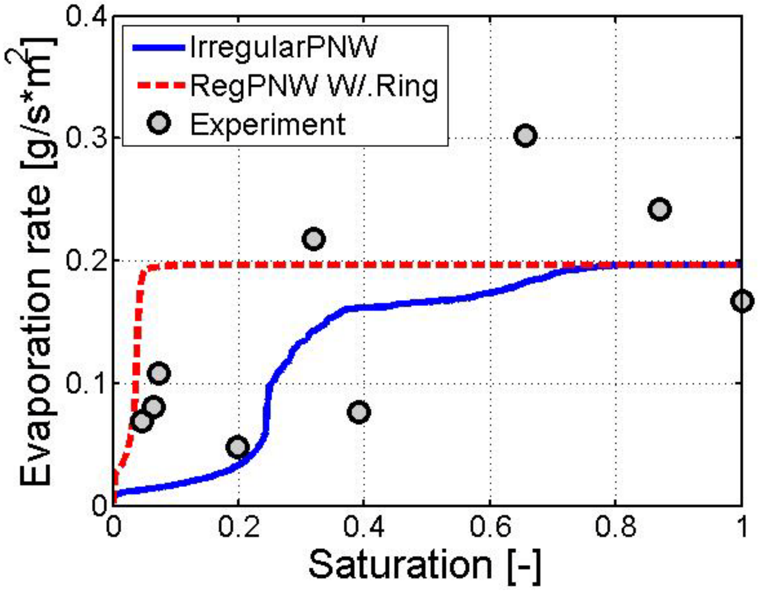


The film flow provides hydraulic connection between the bulk liquid region and the evaporation surface maintaining the surface partially wet for a longer time.

Comparison: experiment and PNW with ring

Based on the experimental data (geometry, initial drying rate) a 3D regular pore network with rings is generated.





CRP: lasts longer by the liquid rings.
FRP: begins once the liquid rings are detached from the network surface.

Summary

- A micro dryer has been set up inside the X-ray microtomography to perform online micro-scale drying measurements.
- Simulation results of 3D pore network drying model are compared with the experimental ones. The overestimation of drying time may be explained by the absence of liquid film effects.
- The existence and hydraulic connectivity of liquid film have been investigated and proved experimentally (surface wettability and salt solution).
- Pore network model with films leads to a very good agreement with the experimental results.

Thank you for your attention !

Graduate School for Micro-Macro-Interactions in Structured Media and Particle Systems – GRK 1554.

The X-ray micro tomographic device has been financed by EFRD European Fund for Regional Development (project no. 1211080002).

DFG - Graduiertenkolleg
Micro-Macro-Interactions
of Structured Media and Particle Systems

EUROPEAN UNION
European Regional
Development Fund