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Imperial College Consortium on Pore-Scale Modelling 2023

Modelling and analysis of multiphase flow in gas diffusion layers

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Presentation outline

- Predict breakthrough capillary pressure and water saturation
  - Pore network model and experimental CT data
- Characterize fluid distributions
  - Pore occupancy
- Predict contact angle *vs* experimental data

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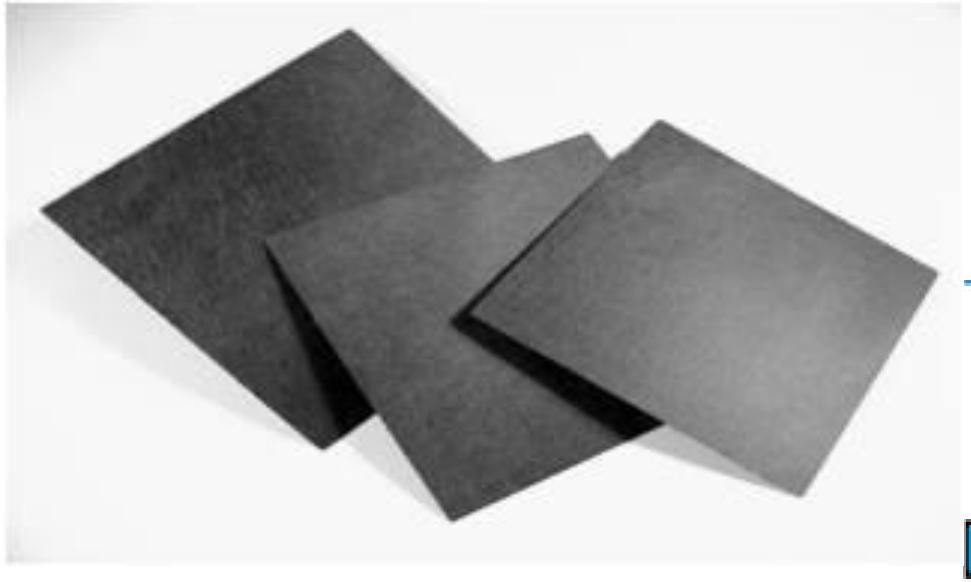
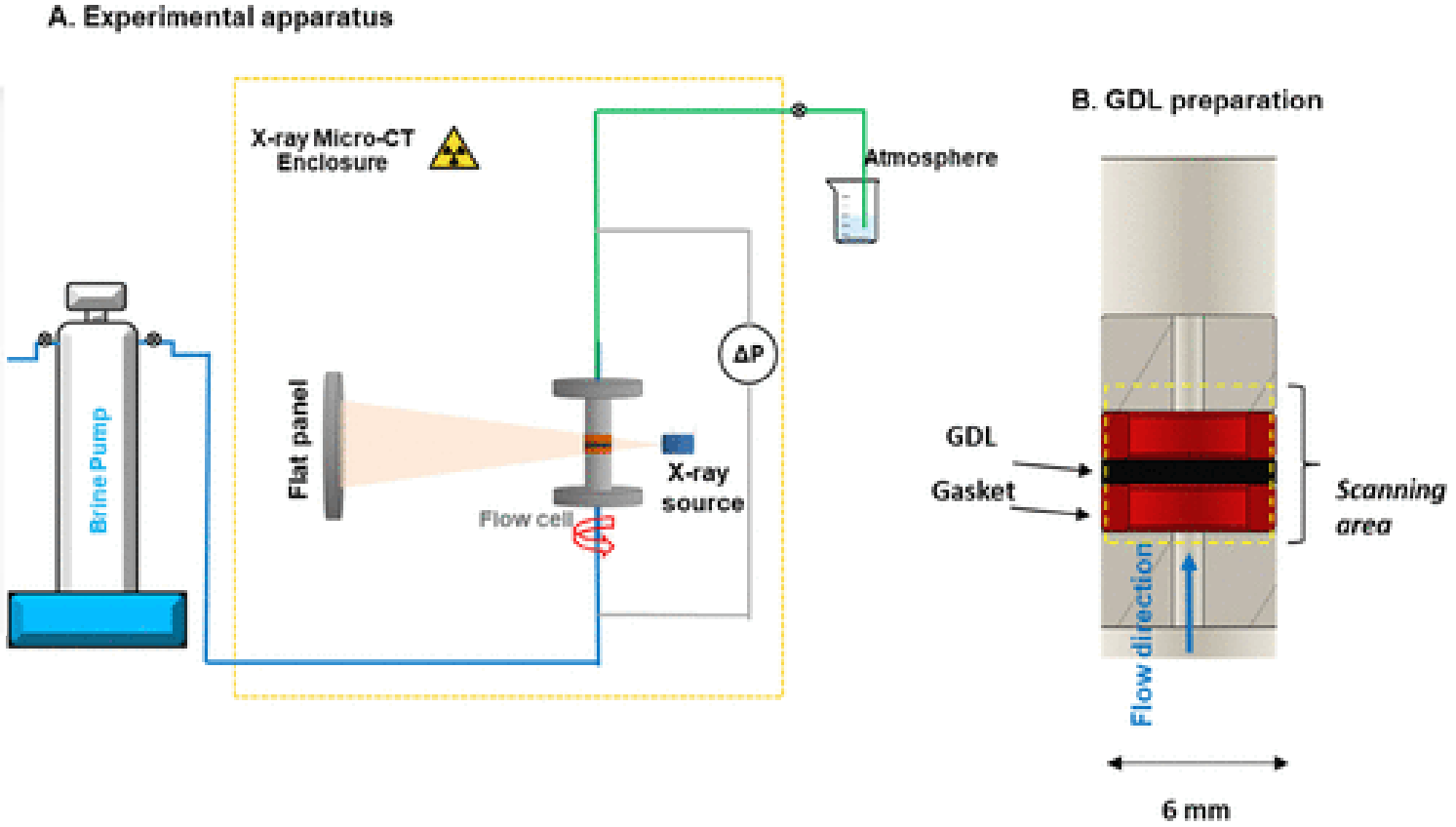
Gas diffusion layers: higher quality dry and wet images, voxel size = 2.05 µm

AvCarb MGL 370 Carbon Paper



(https://www.fuelcellearth.com/fuel-cell-products/avcarb%C2%A9-mgl370/)



(Shojaei et al., ACS Applied Energy Materials, 2022)

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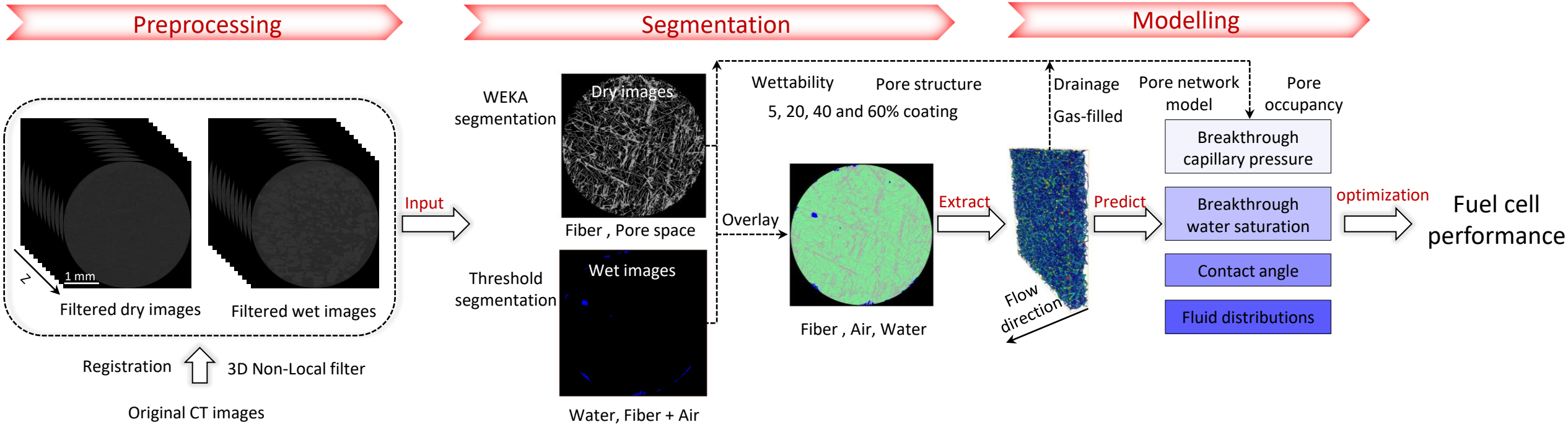
- It's difficult to distinguish between the water and gas diffusion layers in the wet images

Workflow



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Segmentation methods: Dry images (WEKA, Fiji), Wet images (Threshold, Avizo)

Dry images = $1_{Fiber} + 0_{Pore\ space}$

Wet images = $1_{Fiber + Air} + 0_{Water}$

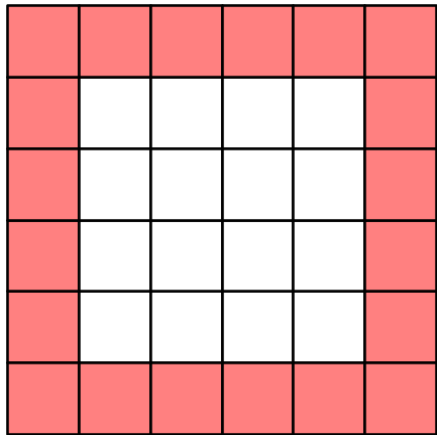
$0_{Water} = 0_{Water} \cap 0_{Pore\ space}$ (Arithmetic: a&&b) ⟶ 1_{Water}

$0_{Air} = 0_{Pore\ space} - 0_{Water}$: (Arithmetic: a - b) ⟶ 2_{Air}

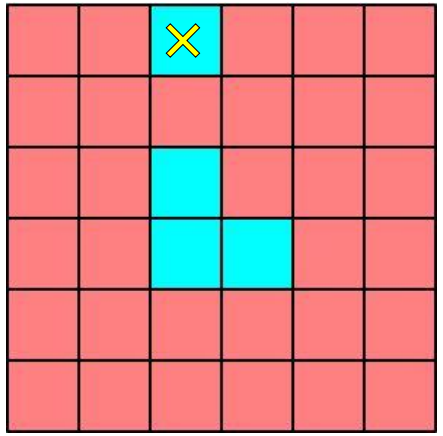
1_{Fiber} : (Arithmetic: 3*(a==1)) ⟶ 3_{Fiber}

Dry images = $1_{Water} + 2_{Air} + 3_{Fiber}$

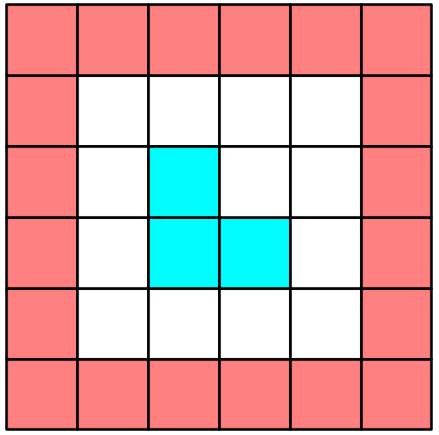
Dry image



Wet image



Final segmentation



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Trainable Weka Segmentation - Powerful tool in Fiji

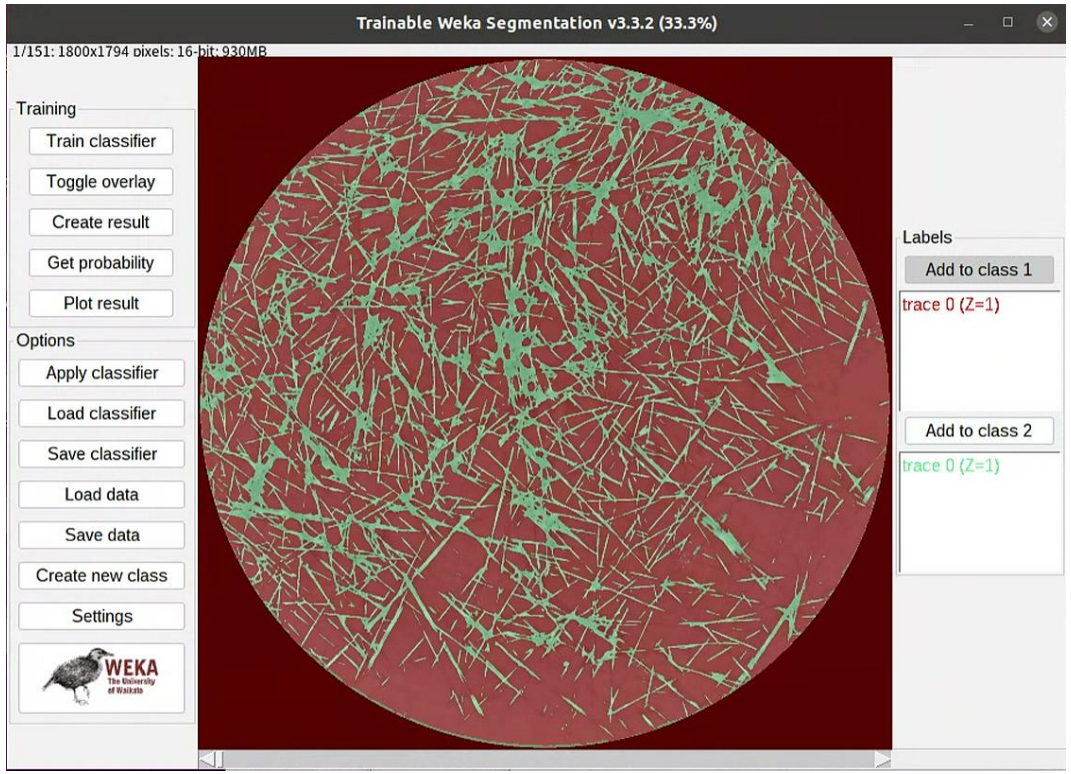
- Need computer resources (CPU)

Output information:

- Classified images
- Out of Bag (OOB) error (In this work < 4%)

This depends strongly on the selected voxels in the training dataset

- Selected voxels number (uniform, slice by slice)



Fiber morphology, porosity...

5% Coating classification model → input → 20, 40 and 60% Coating sample

NO!!!

(Carreras et al, Bioinformatics, 2017)

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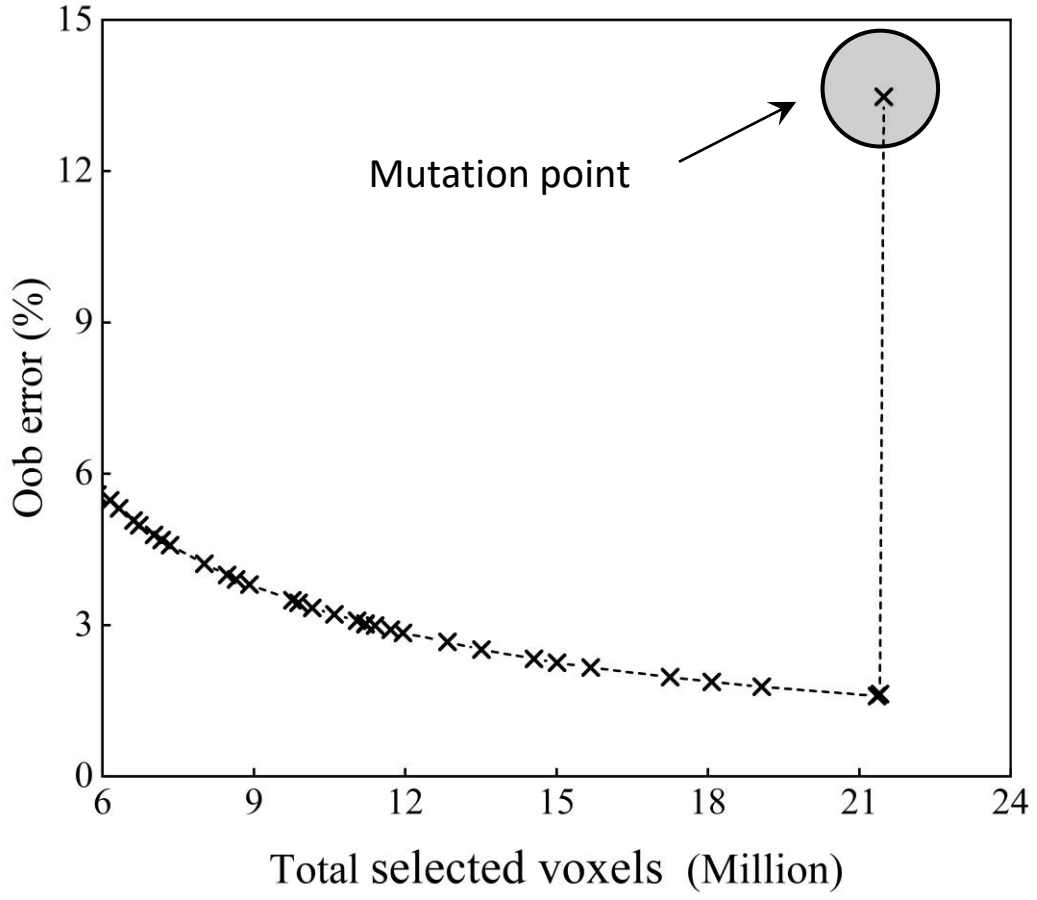
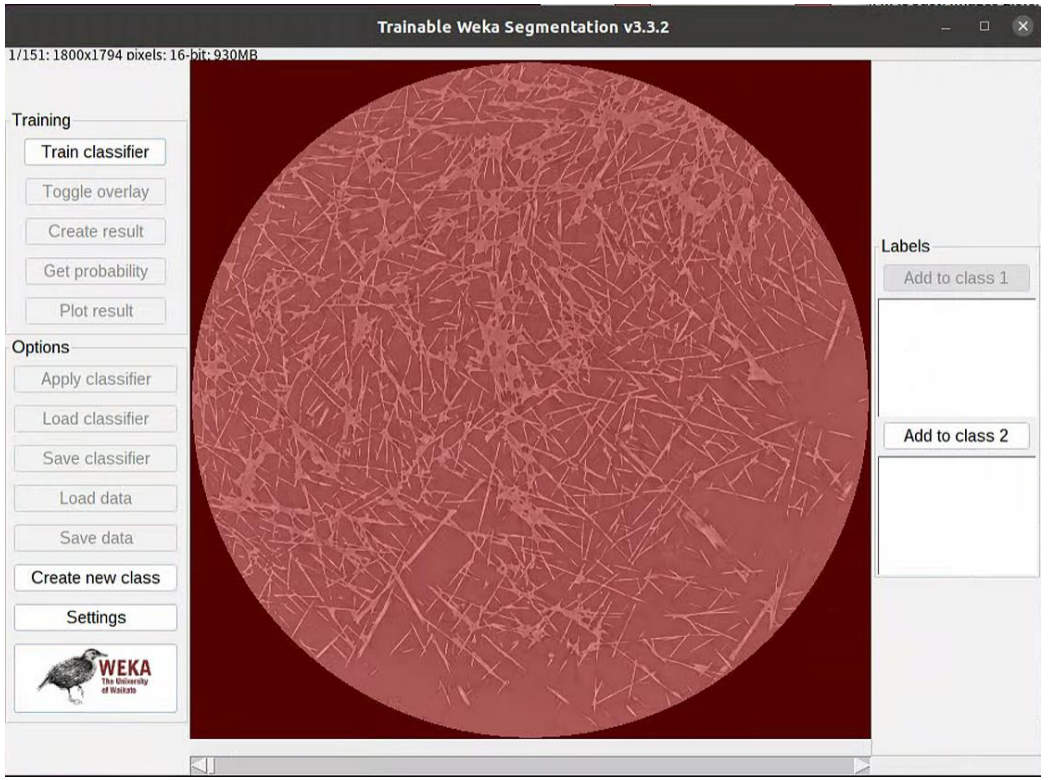
Trainable Weka Segmentation - Powerful tool in Fiji





- Mutation point: The corresponding independent classification model is better for different coating sample segmentation

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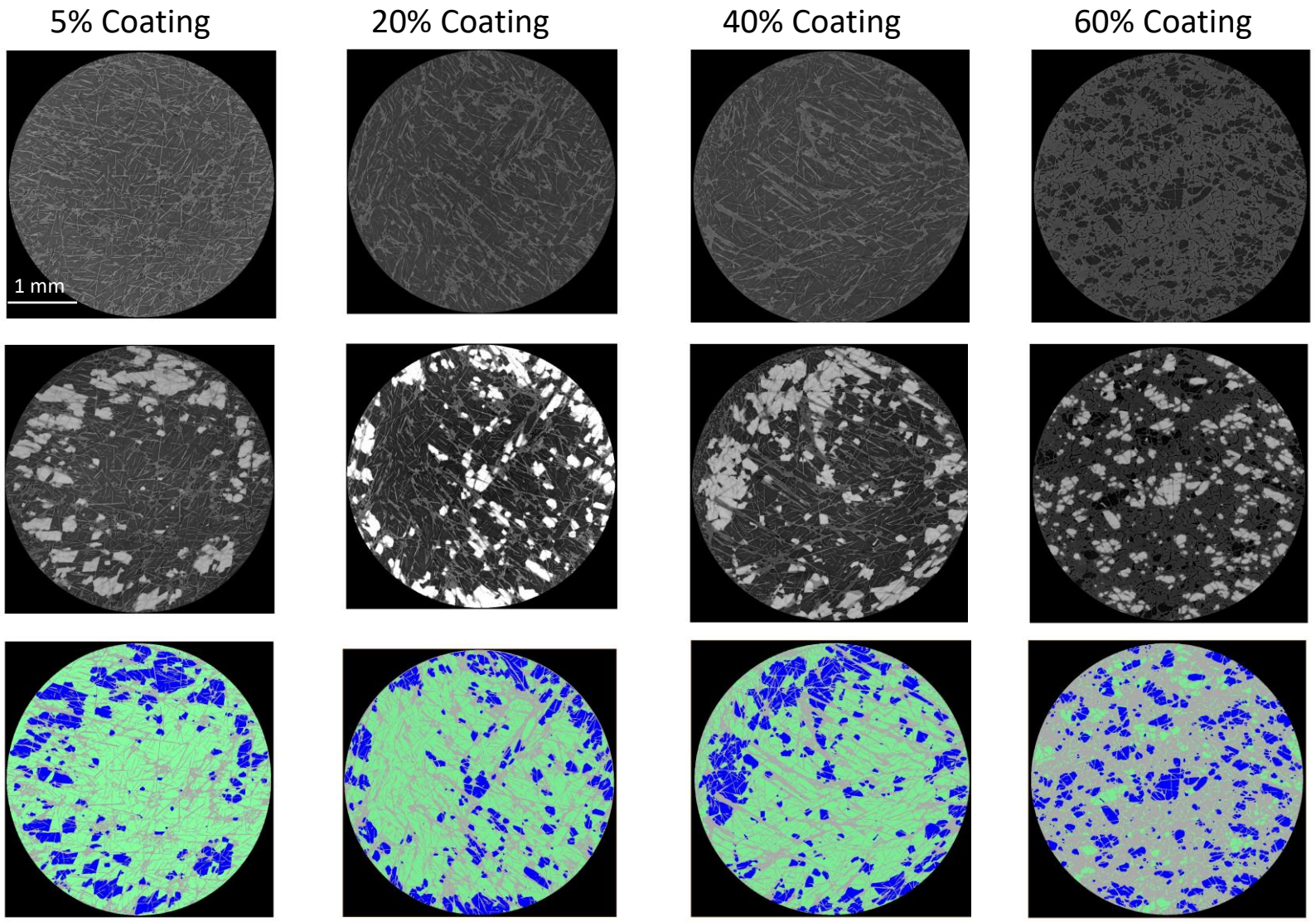
Segmentation results



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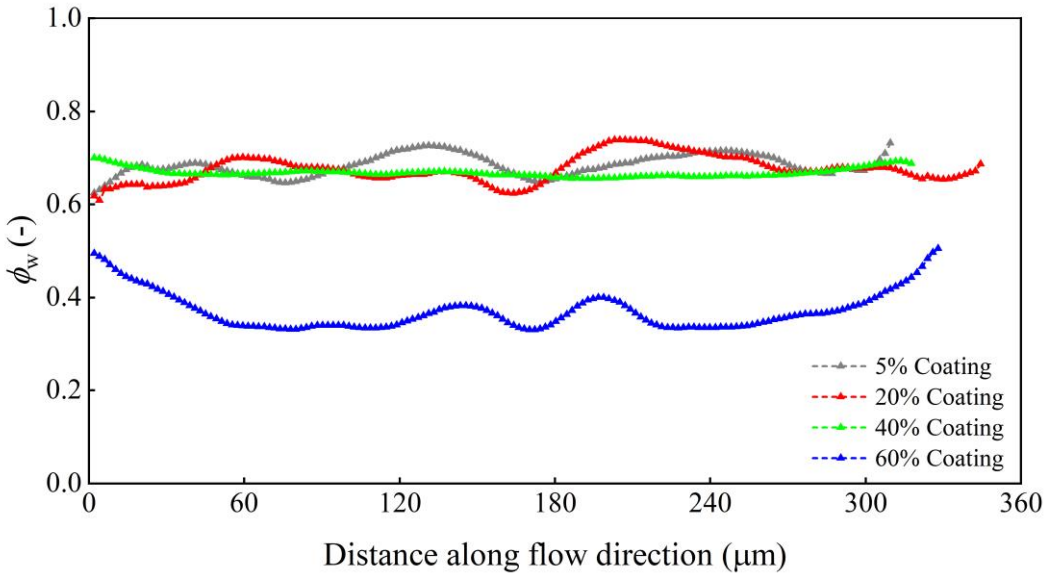
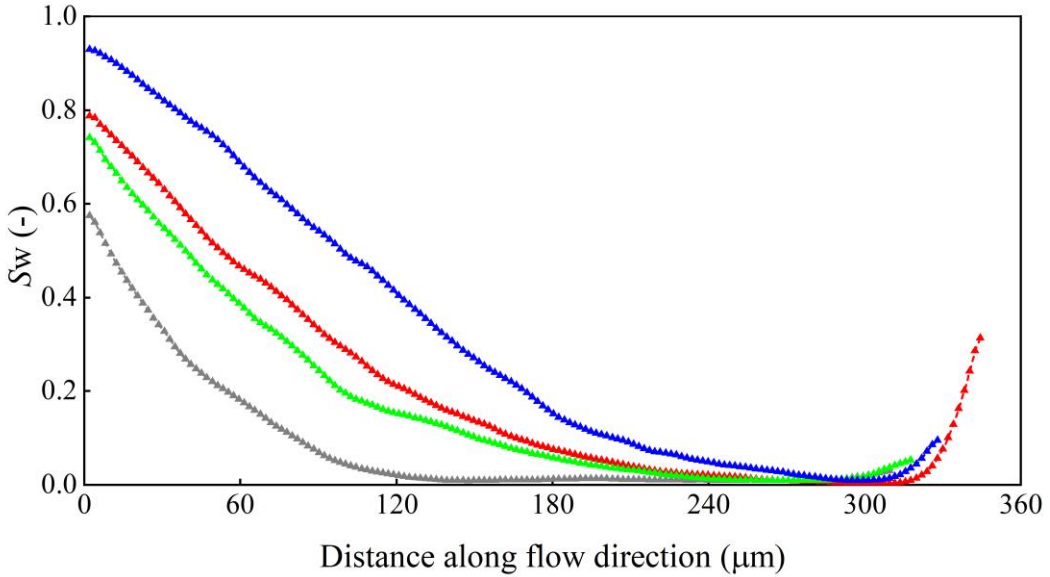
Porosity ϕ and water saturation S_w





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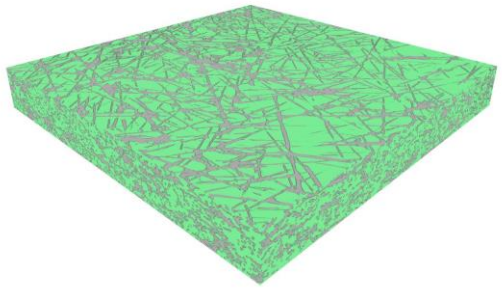
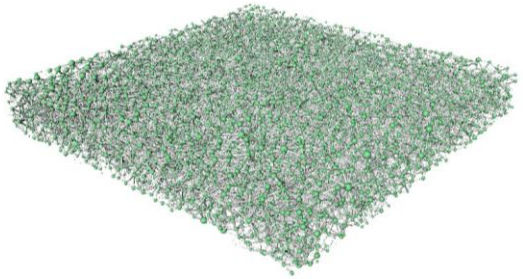
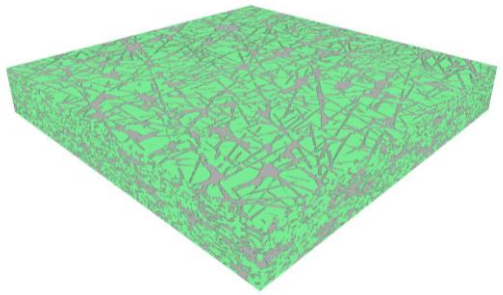
Visualize 3D images and pore networks

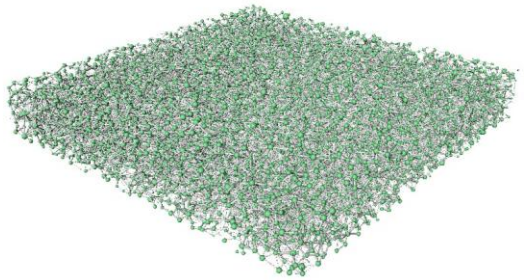
5% Coating



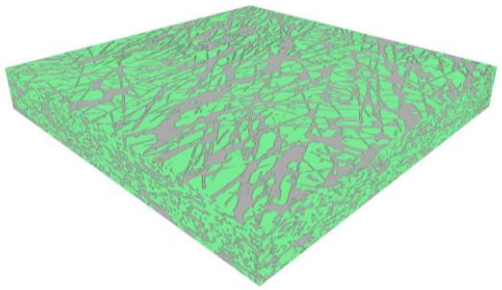


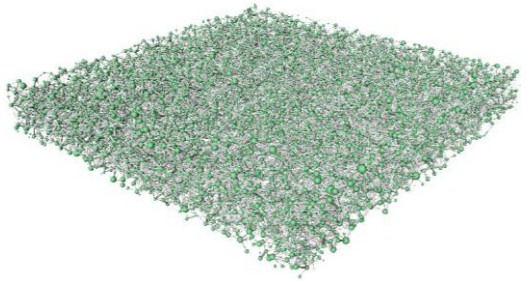
20% Coating



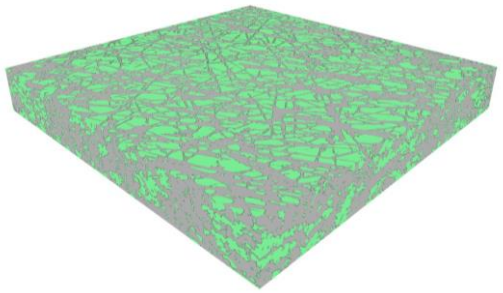


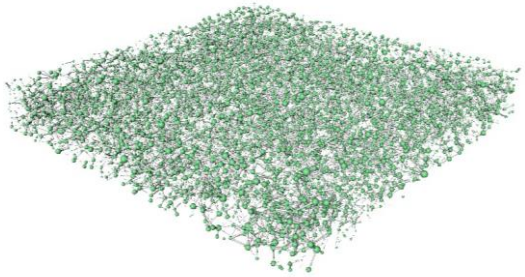
40% Coating





60% Coating





More hydrophobic

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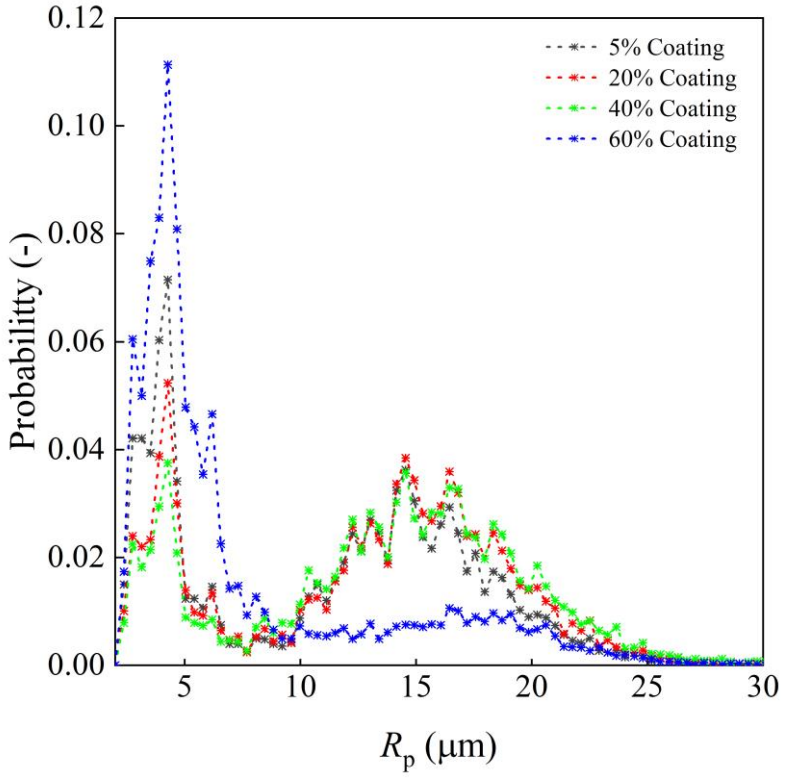
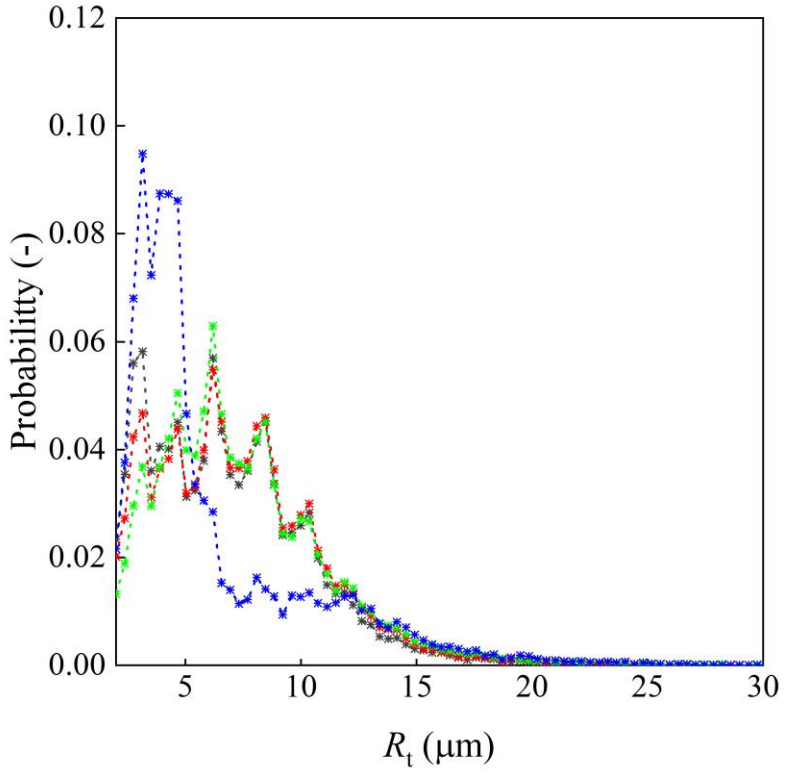
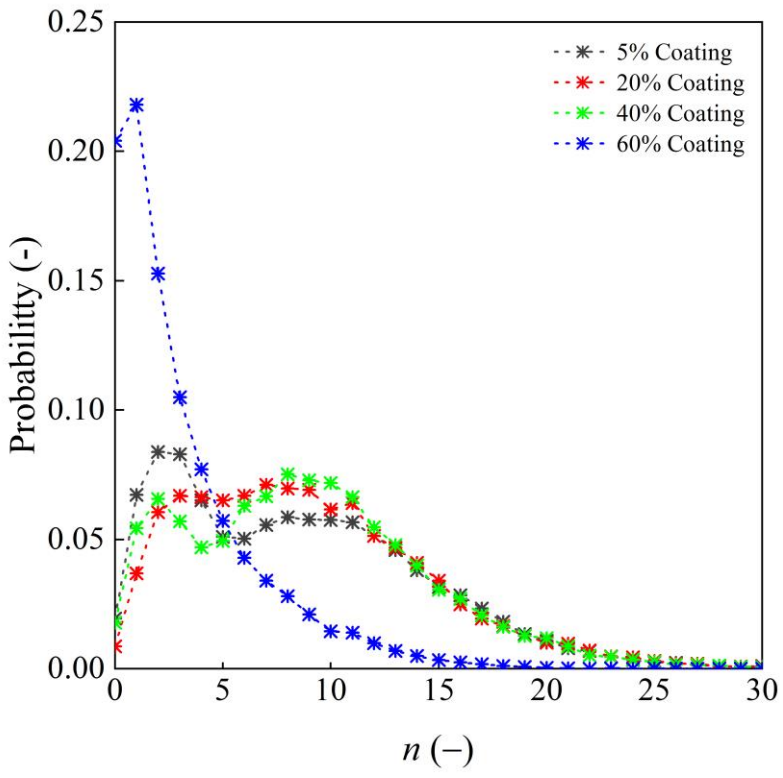
Pore network statistics







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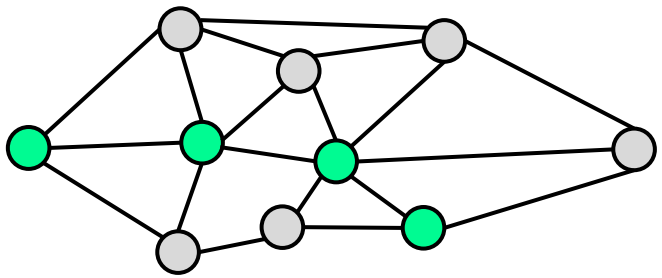
Breakthrough capillary pressure P_{cb} and S_{wb}

$P_c = P_g - P_w$

Before water breakthrough

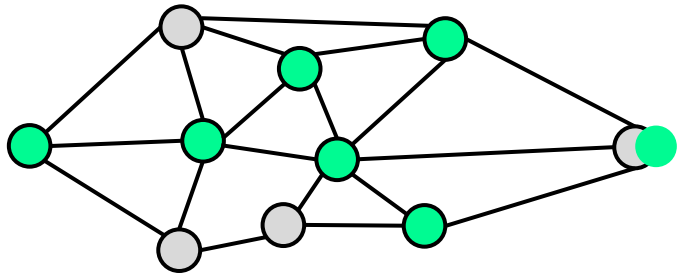
$S_{w1} \sim P_{c1}$



Water flow direction

After water breakthrough

$S_{wb} \sim P_{cb}$



- "Drainage process": water (non-wetting phase) displace air
- Breakthrough point: $k_{rw} > 0$ (first point)

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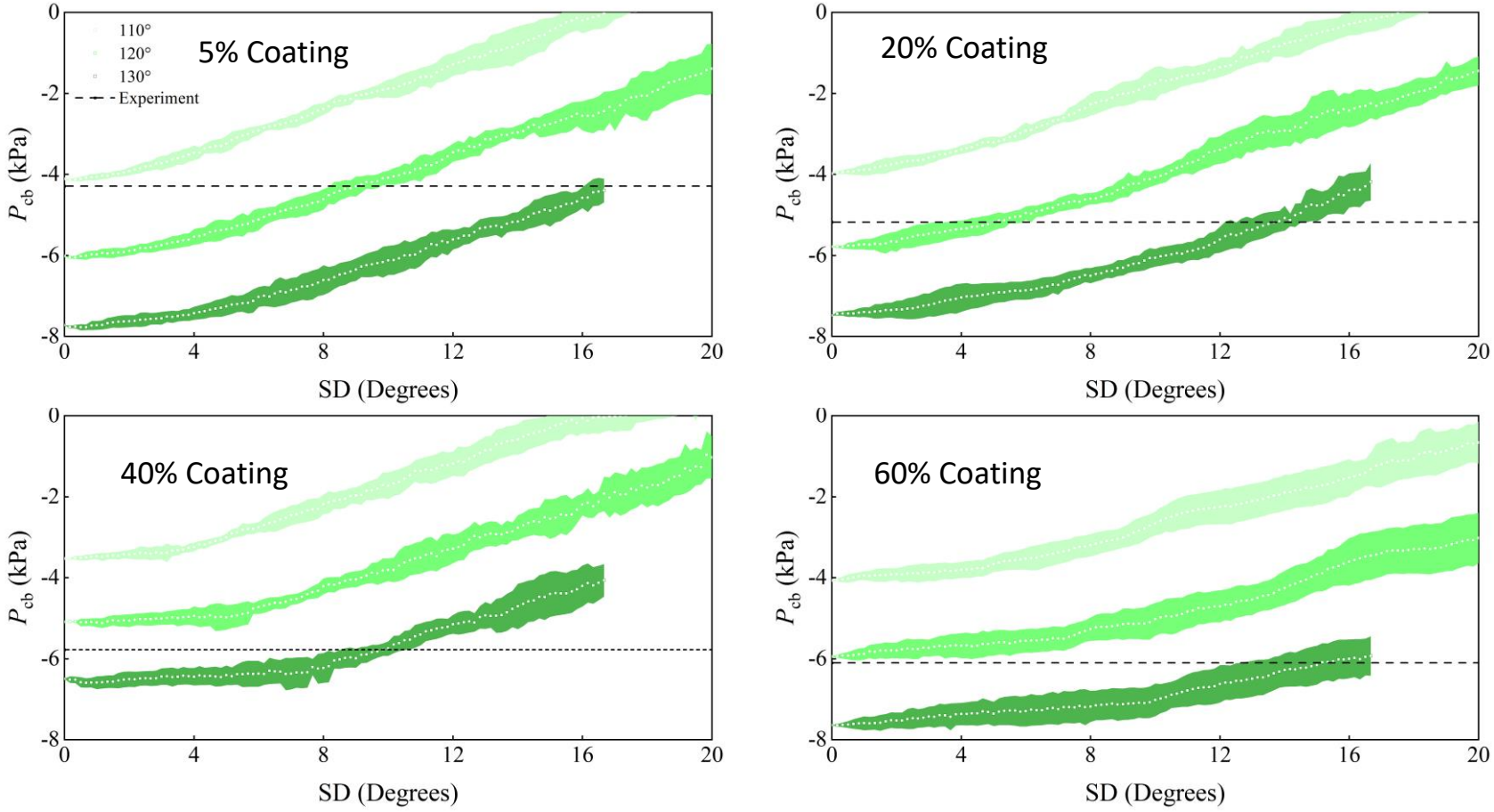
Sensitivity analysis: Breakthrough capillary pressure P_{cb} ~ contact angle



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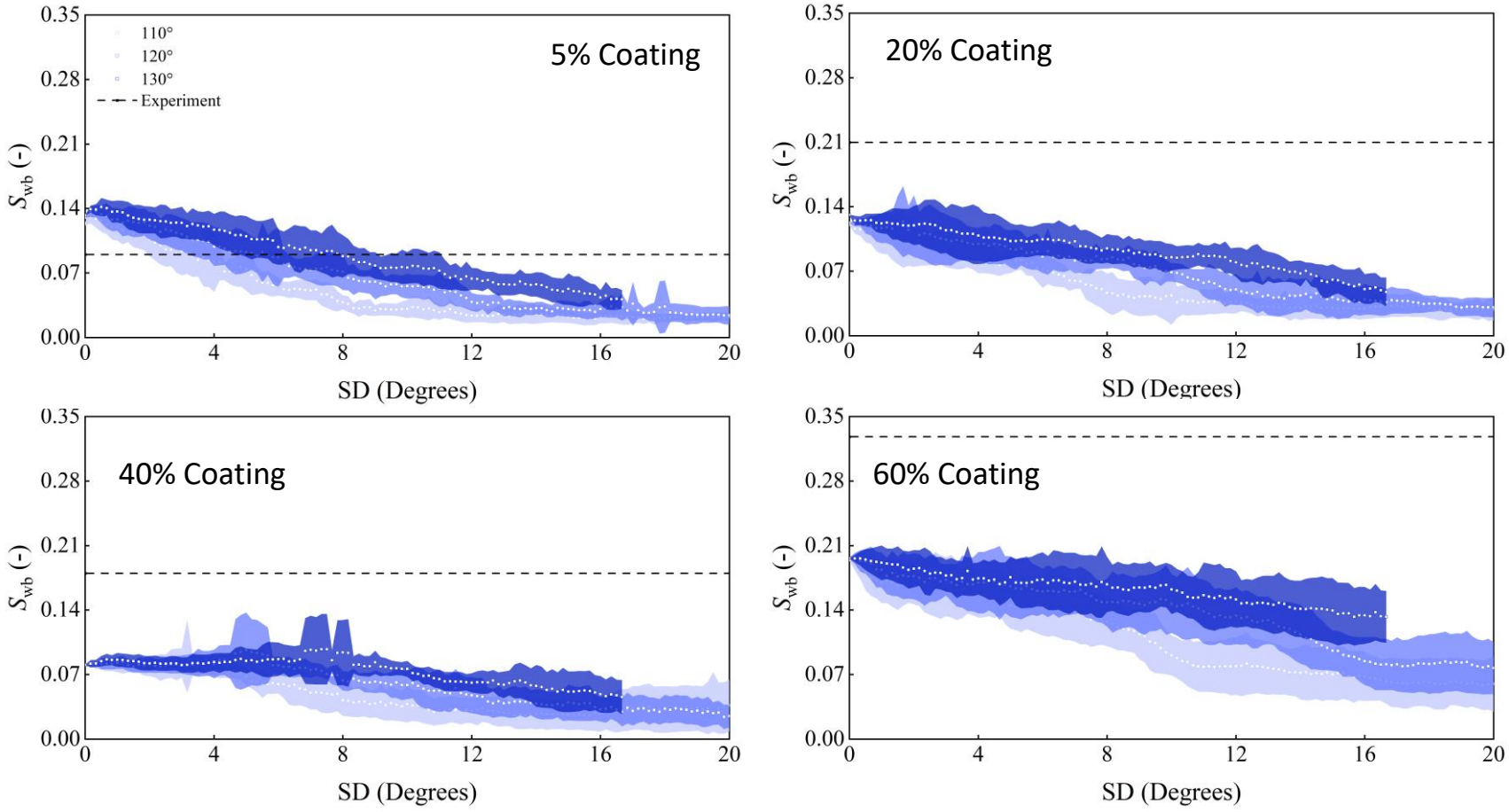
Sensitivity analysis: Breakthrough water saturation S_{wb} *vs* contact angle



- Why the simulated S_{wb} is smaller than the experimental S_{wb} from CT images?

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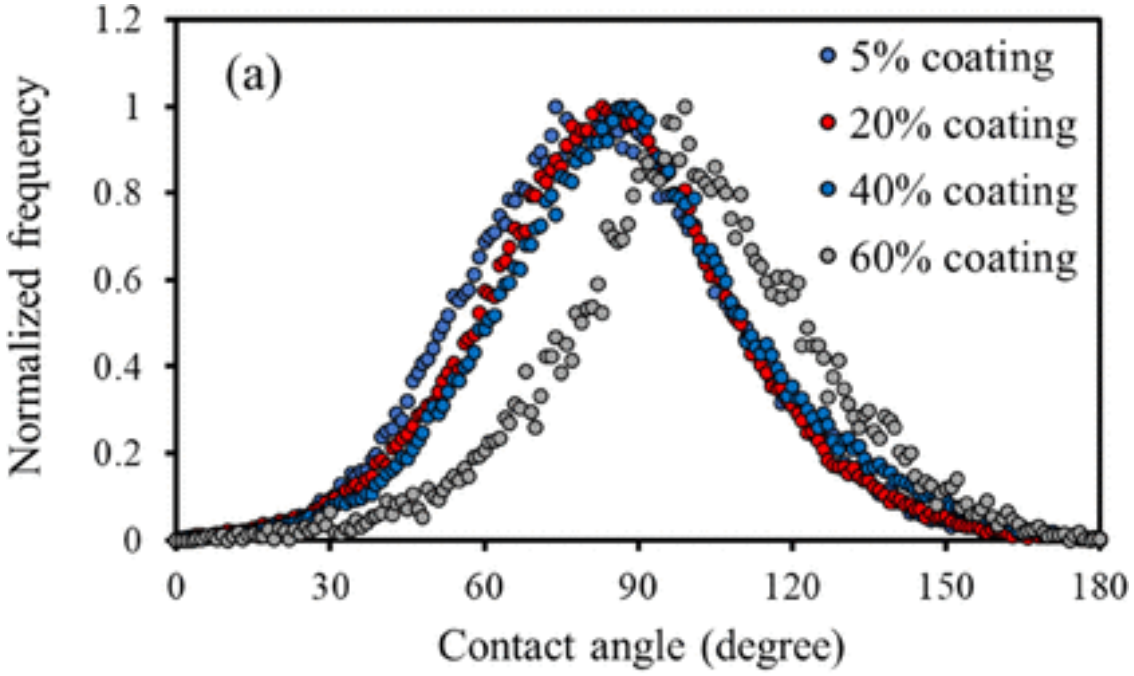
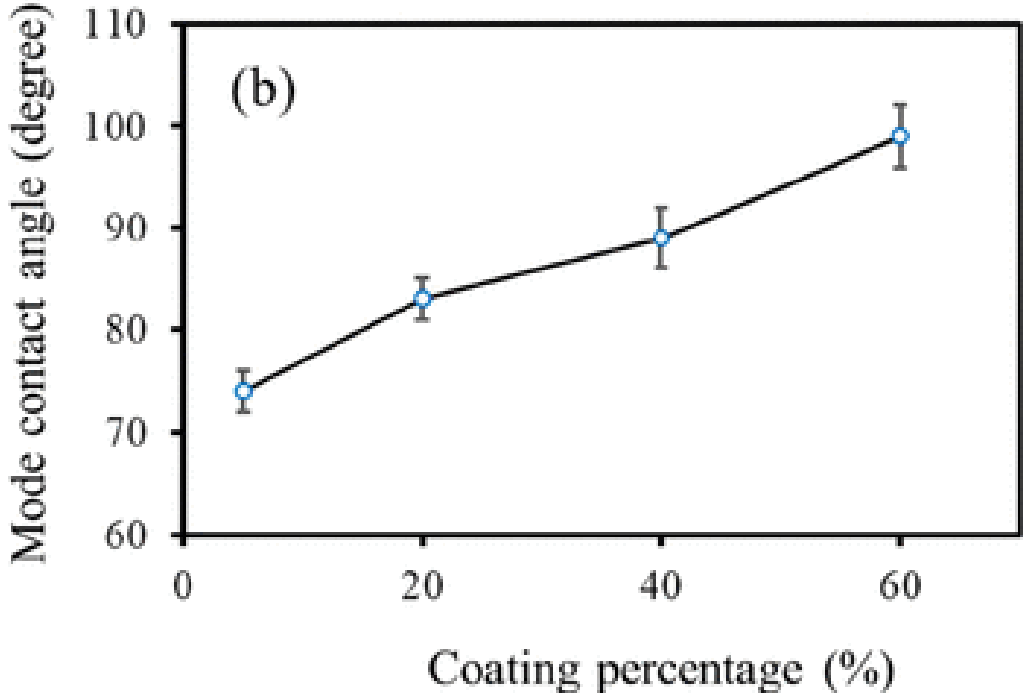
Contact angle (distribution) from images

- Geometric contact angle (image resolution, image quality and segmentation)





(Shojaei et al., ACS Applied Energy Materials, 2022)

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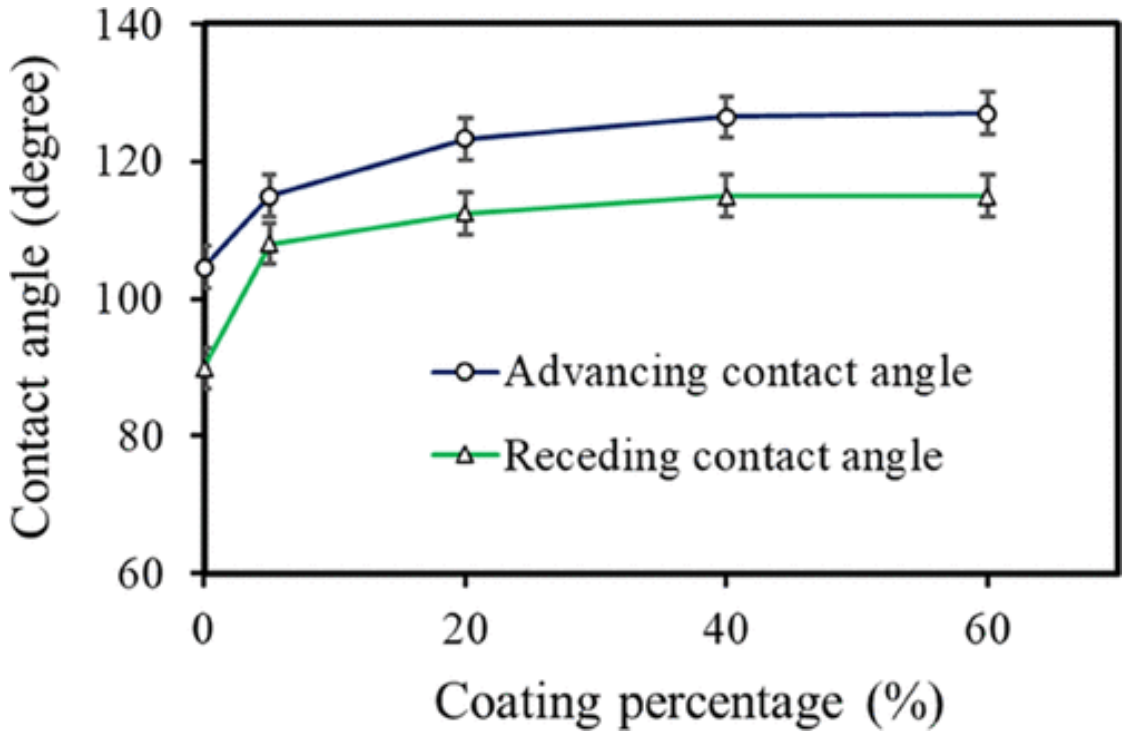
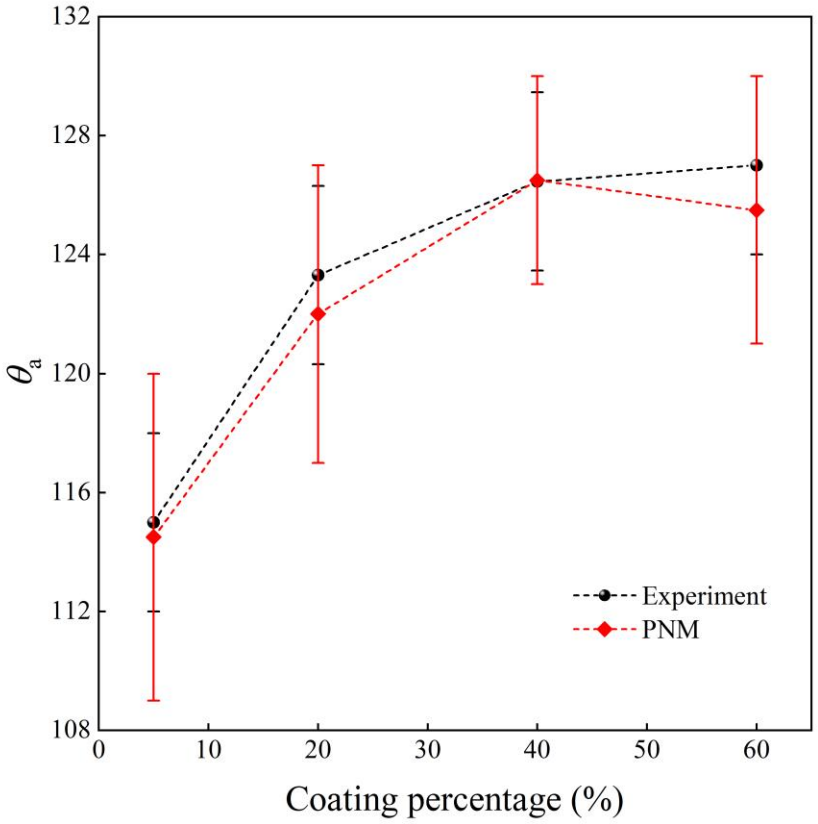
Advancing contact angle θ_a: Experiment *vs* PNM

- The advancing or receding contact angle measured in gas diffusion layers surface





(Shojaei et al., ACS Applied Energy Materials, 2022)

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Conclusion and future work

- The pore network extraction method provides representative networks for fibrous porous media and can predict P_{cb} and S_{wb}
- Characterize pore occupancy
- Consider different flow directions (x and y)

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Thanks for you attention