



煤矿灾害动力学与控制全国重点实验室

State key laboratory of coal mine disaster dynamics and control

SKL-CMD



Road to Net Zero: UK-China Workshop on CO₂ Geological Storage, 15th of November, 2025

Pore-scale studies on capillary trapping of carbon dioxide in carbonate rocks

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Bo Guo (University of Arizona, USA)

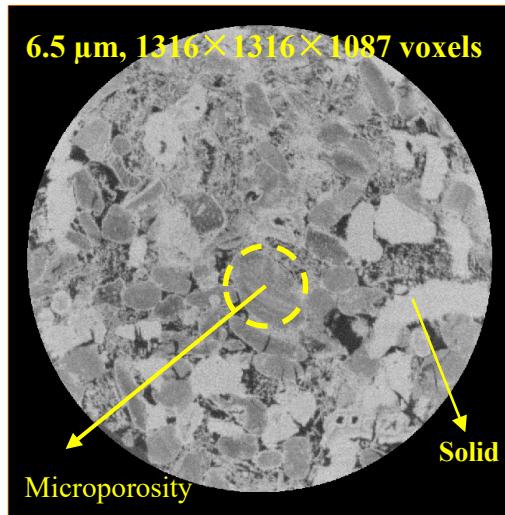
S. Majid Hassanizadeh (Utrecht University, The Netherlands)

- 1. Multiscale pore structures of carbonate rocks**
- 2. The multiscale pore-network model and verification**
- 3. Predictions of capillary trapping**
- 4. Conclusions and outlook**

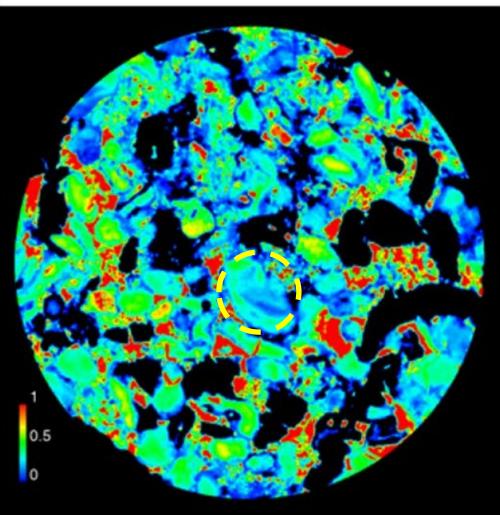


Multiscale pore structures of carbonate rocks

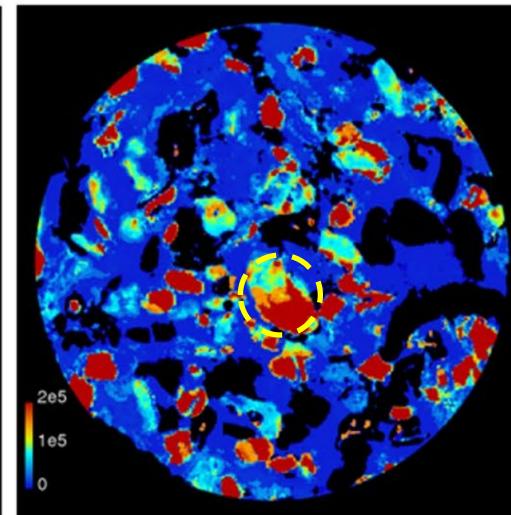
(Wang et al., WRR, 2022)



CT grey-scale map

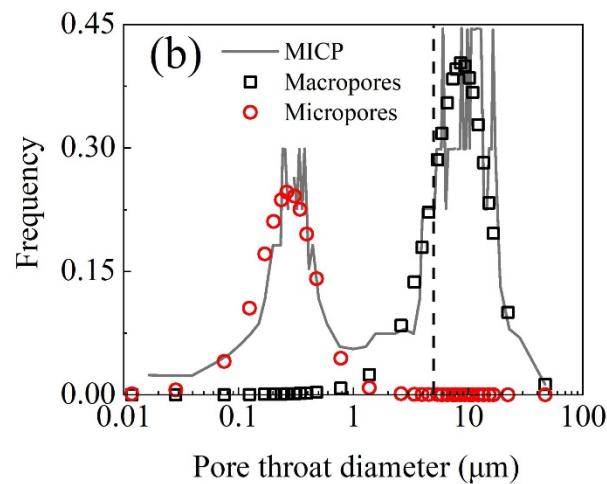
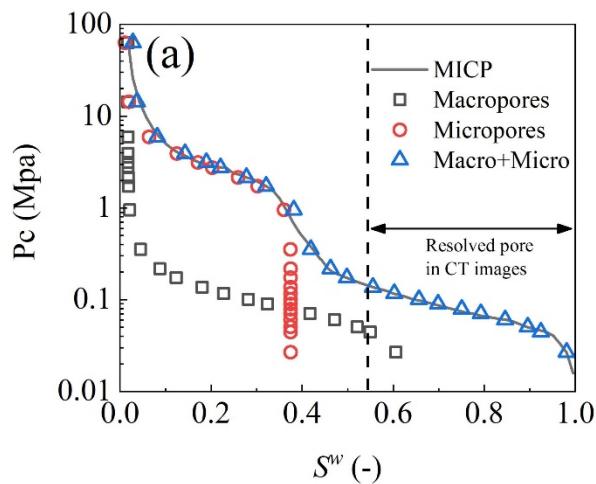


Porosity map



Entry pressure map

In-situ CT scanning of quasi-static drainage process



Bimodal of VG

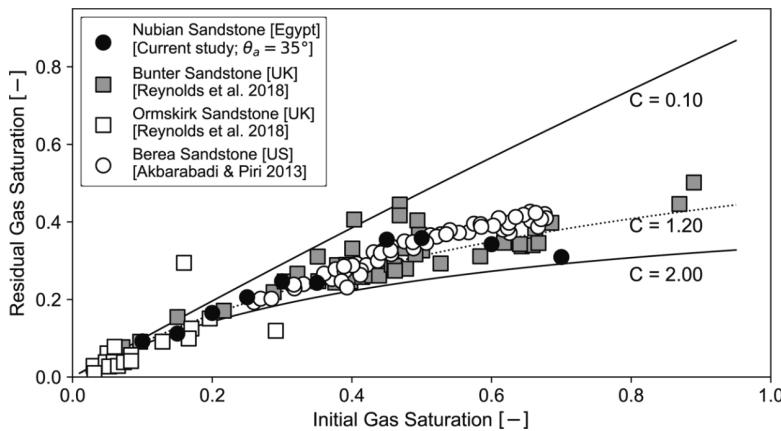
$$S_e^w = \sum_{i=1}^2 w_i \left[1 + (\alpha_i P_c)^{N_i} \right]^{-M_i}$$

(Durner, WRR, 1994)



Questions

1. How does the **heterogeneity** of pore structures influence Land trapping coefficient?
2. How does **wettability** influence Land trapping coefficient?

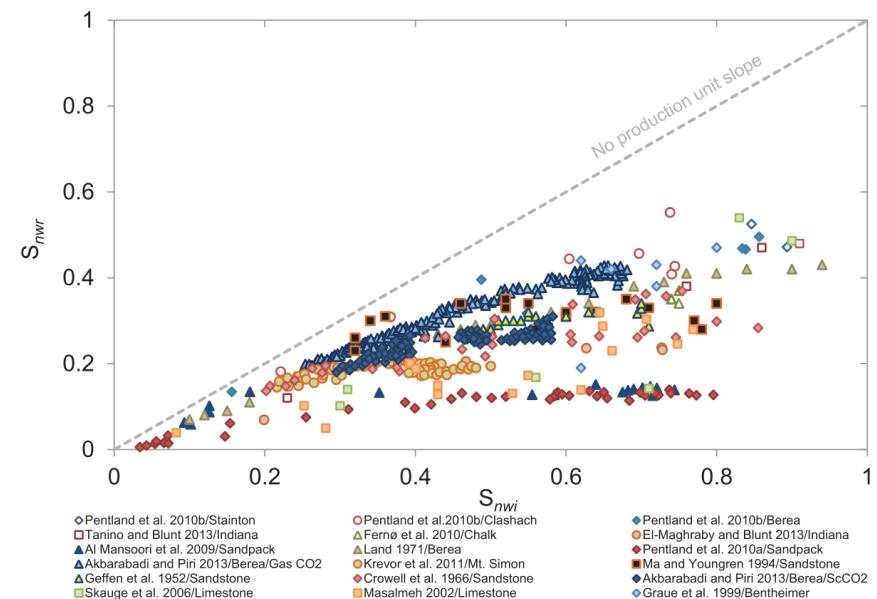


(Hefny, Qin, Saar, and Ebigbo, Int. J. Greenhouse Gas Control, 2020)

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$$S_{nw,r} = \frac{S_{nw,i}}{1 + CS_{nw,i}}$$

Land trapping coefficient
(Land, 1968)

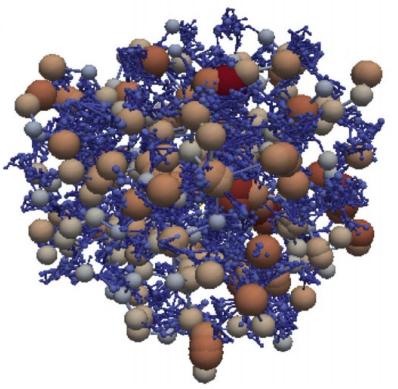
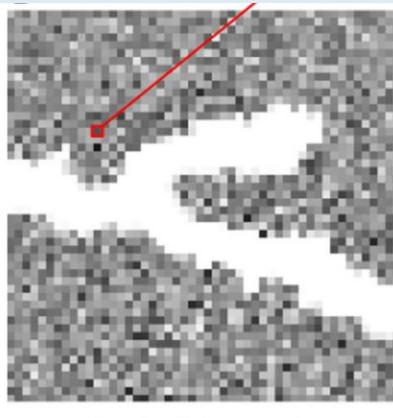
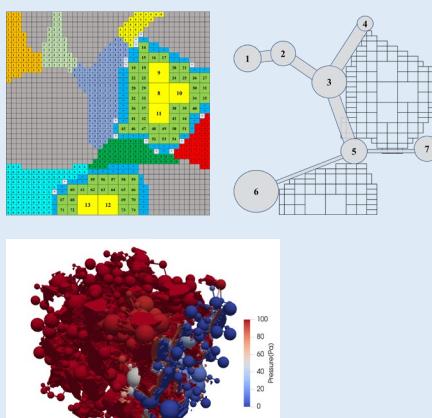
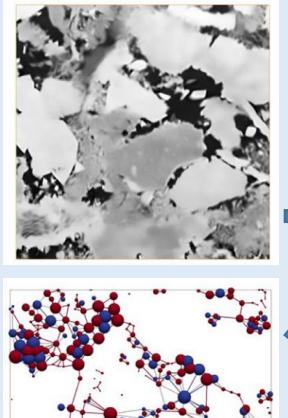


(Alyafei and Blunt, AWR, 2016)

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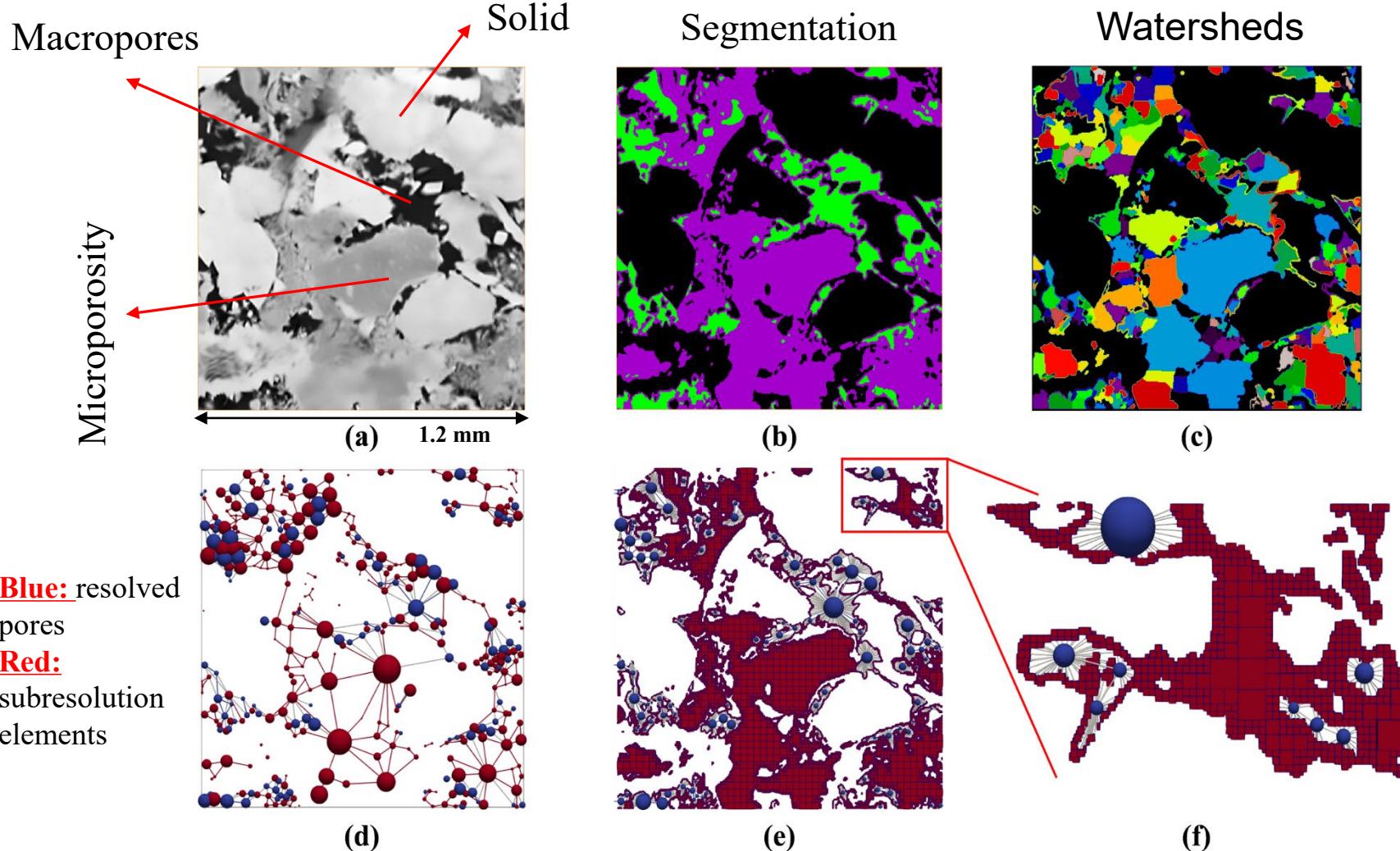
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Numerical models for multiscale porous media

Dual-pore-network model (DPNM)	Micro-continuum model (MCM)	Pore-network-continuum model (PNCM)	Multiscale pore-network model (MPNM)
	 hybrid-scale	 Qin, 2024	 Mehmani, 2014 Soulaine, 2023

- The MPNM is most efficient, but it needs calibration and verification.
- The PNCM can balance efficiency and accuracy.

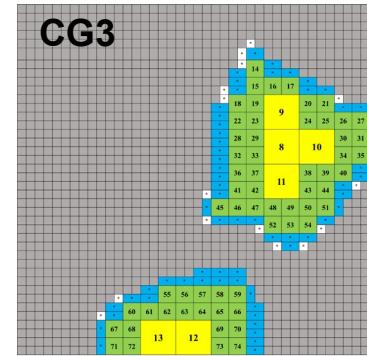
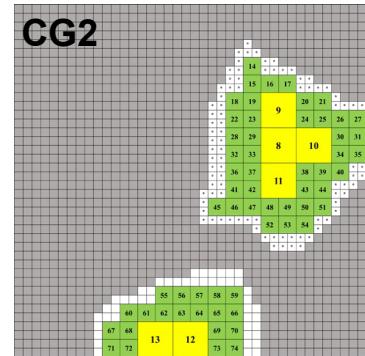
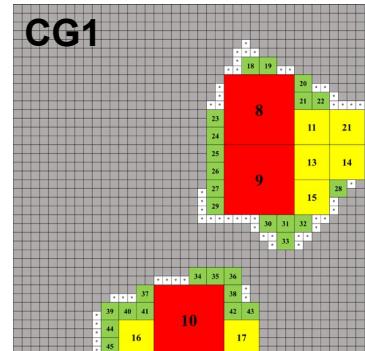
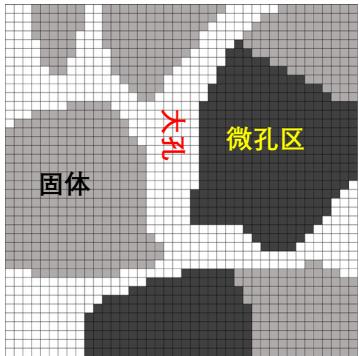
The multiscale pore-network model (MPNM)



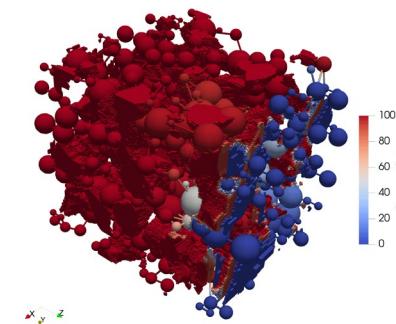
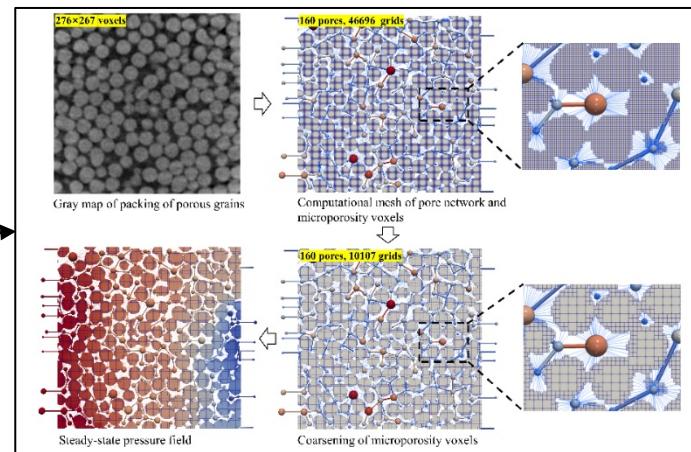
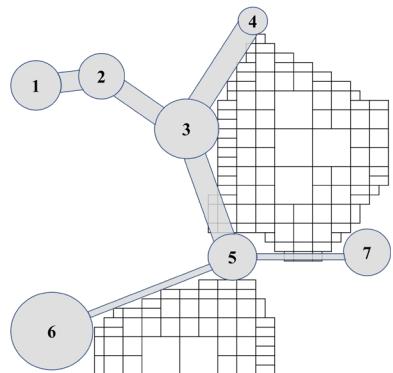
<https://digitalporousmedia.org/>

1. Modeling of permeability and formation factor of carbonate digital rocks: dual-pore-network and pore-network-continuum models. *Transport in Porous Media*, 152:37, 2025
2. Modeling of flow and transport in multiscale digital rocks aided by grid coarsening of microporous domains. *Journal of Hydrology*, 633:131003, 2024

Pore-network-continuum model – coarsening algorithm



(AWR, 2024; JoH, 2024)



Depressurization process

Packing of porous particles

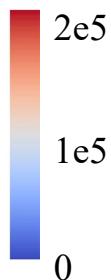
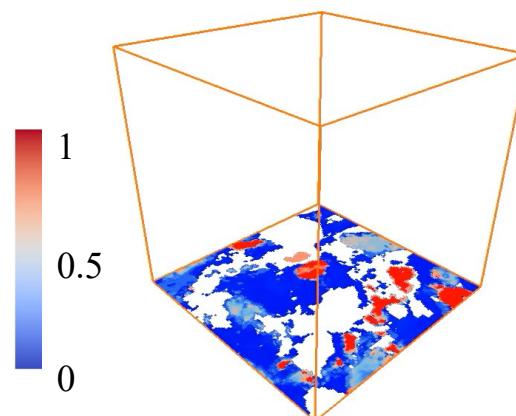
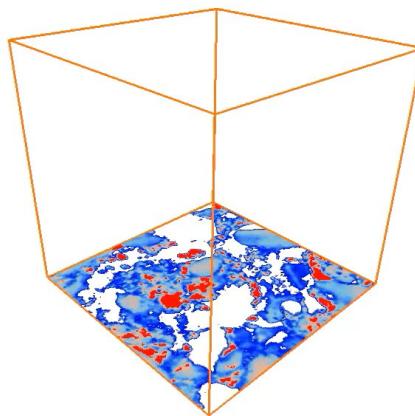
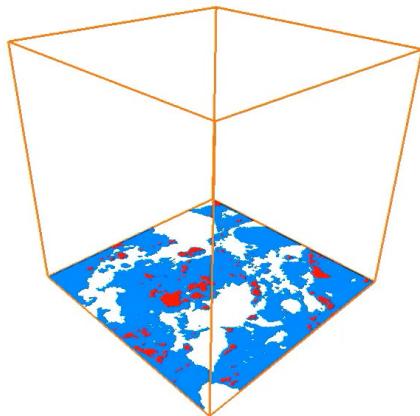


Verification of MPNM: rock sample

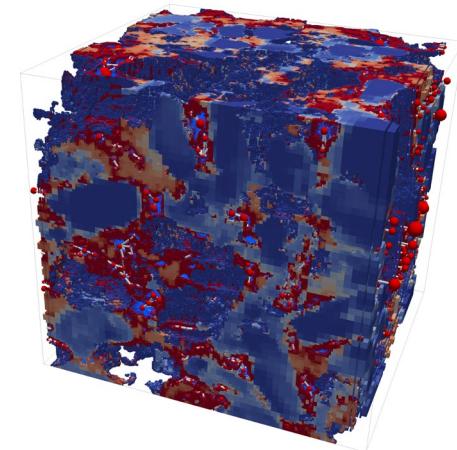
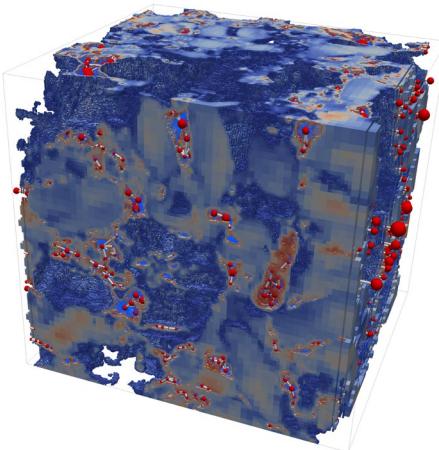
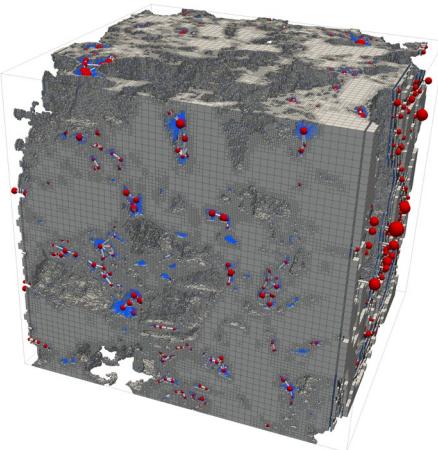
(Wang et al., WRR, 2022)

400³的测试岩心

<https://www.digitalrocksportal.org/>

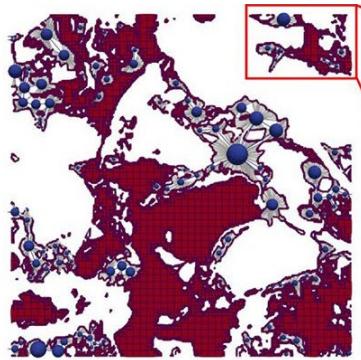
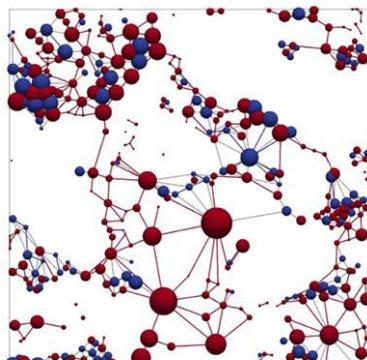
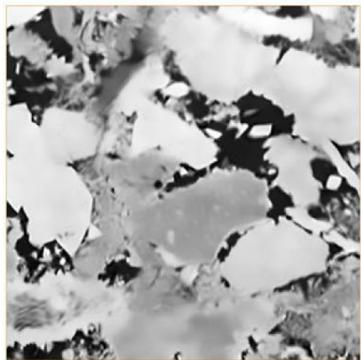


Computational mesh for the PNCM modeling





Verification of MPNM: mean pore size of watershed



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① Average based on sphere-assumption

$$\bar{r}_i = \left(\frac{3}{4\pi} \frac{\sum_{k=1}^{N_i} V_k \varepsilon_k}{\sum_{k=1}^{N_i} M_k} \right)^{1/3}$$

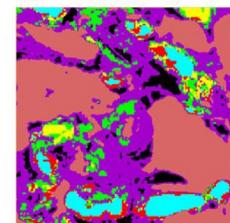
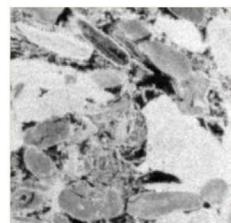
$$M_k = V_k \varepsilon_k / (4\pi r_k^3 / 3)$$

② Average based on voxel-counting

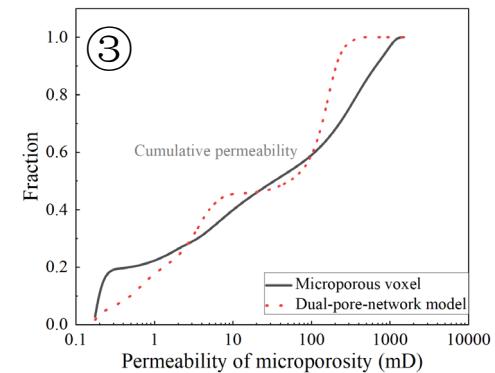
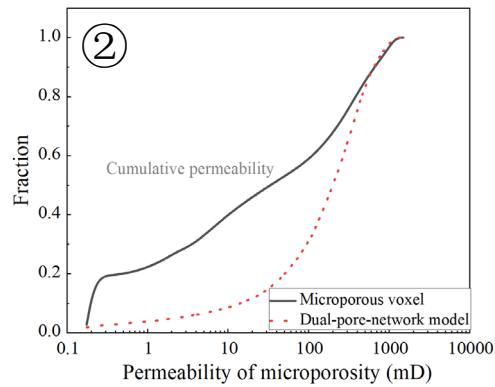
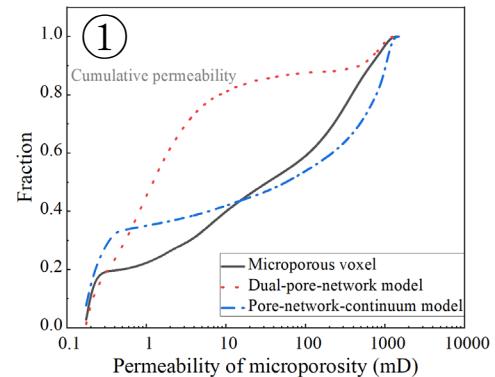
$$\bar{r}_j = \frac{\sum_{k=1}^{N_i} \sum r}{N_i}$$

③ Entry-pressure-based sub-rock typing (*Wang et al., 2022*)

Macro pore RT1 RT2 RT3 RT4 RT5 Solid grain



Estimation of microporosity permeability distribution



Verification of MPNM: absolute permeability and formation factor

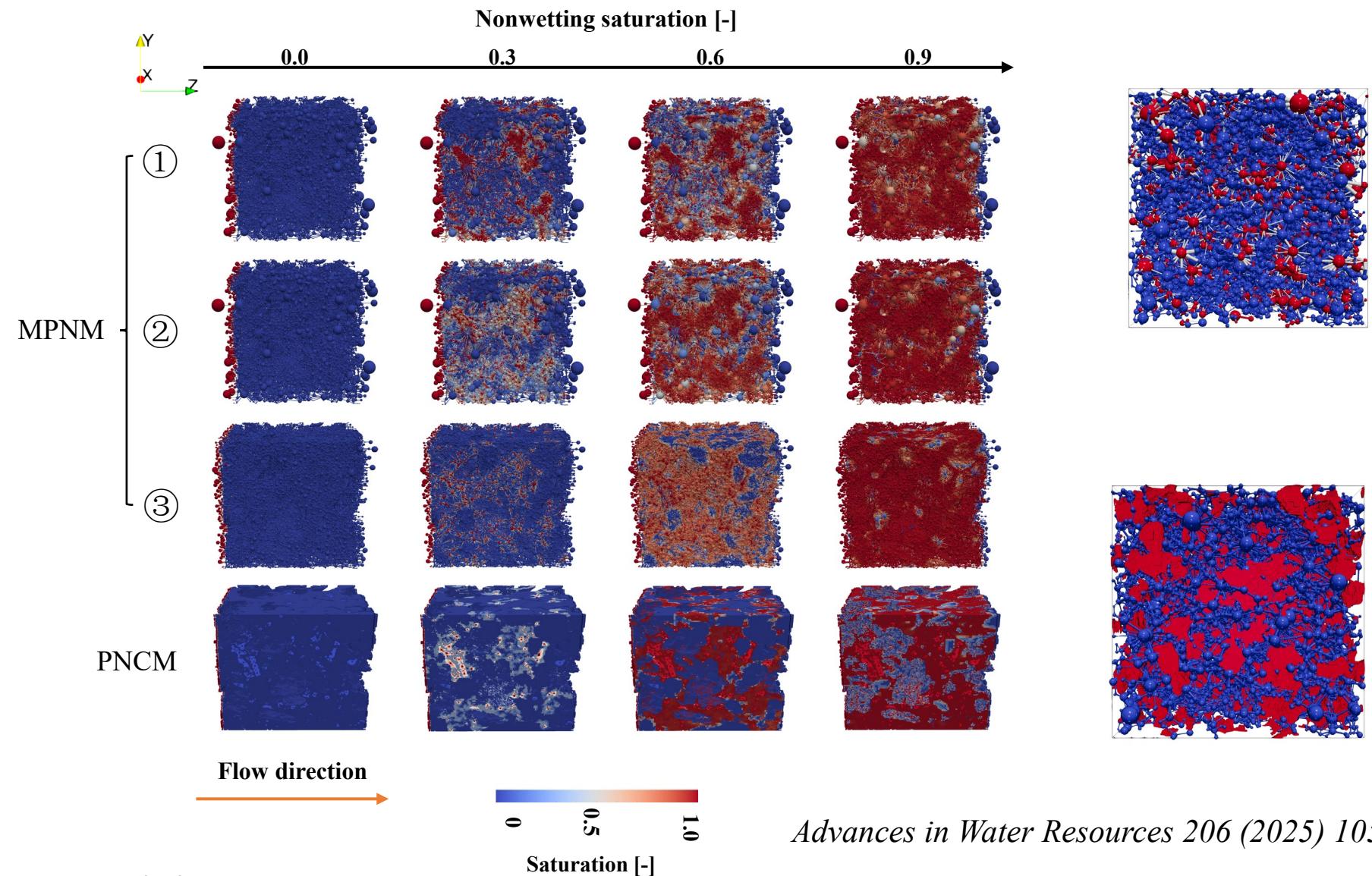
Digital rock	Mean pore size (μm)	By the MPNM (mD)	By the PNCM (mD)	By the reference model (mD)
ES3.1	0.61	109	116	117
ES3.6	0.74	34	37	37
ES6.5-1	1.81	28	18	18
ES6.5-2	Estimated by entry pressure	12 ^① / 205 ^② / 112 ^③	128	174

The sub-rock typing is essential to the MPNM

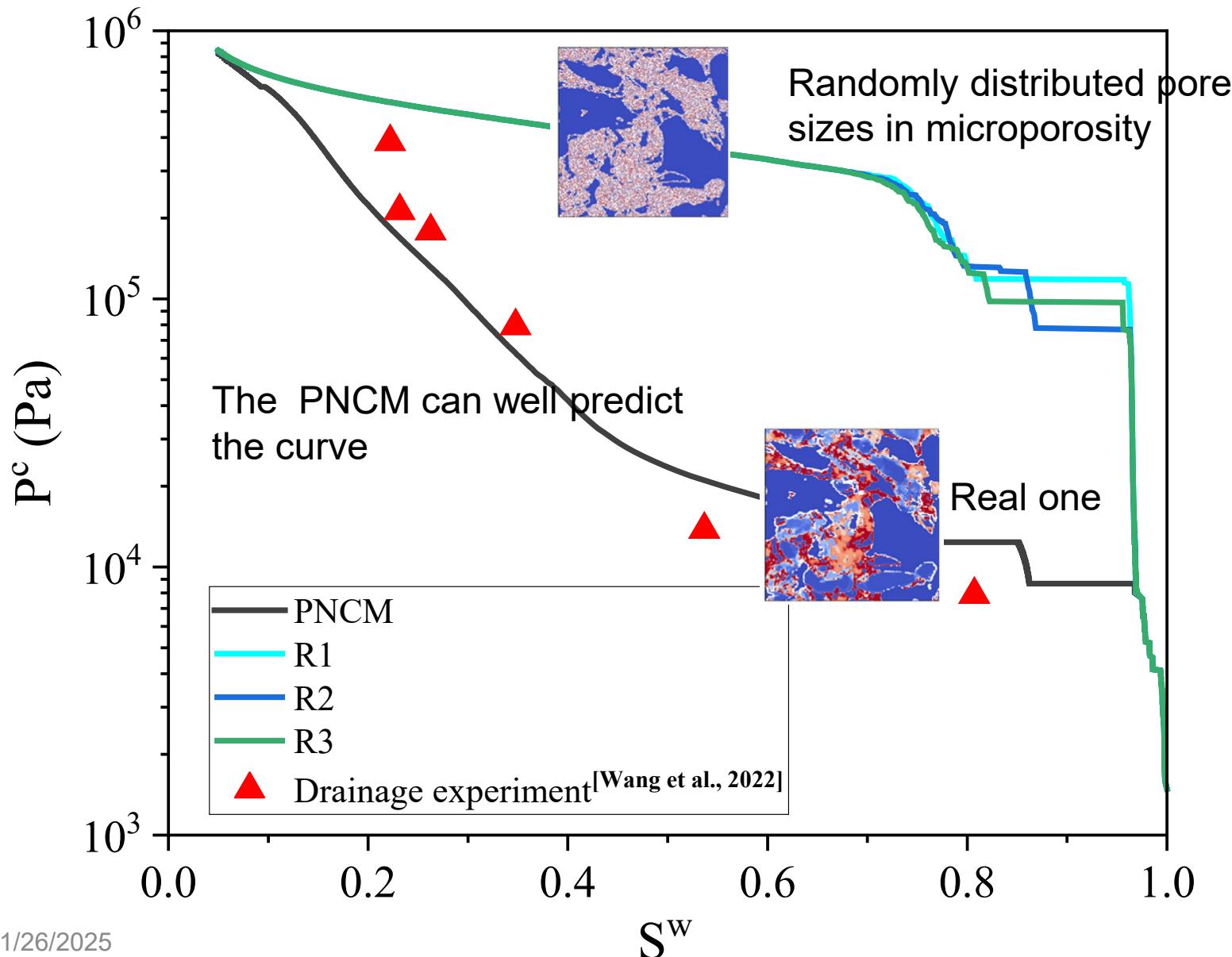
Digital rock	By the multiscale pore-network model (-)	By the pore-network-continuum model (-)	By the reference model (-)
ES3.1	17.24	19.61	19.23
ES3.6	23.81	23.81	23.26
ES6.5	18.52	20.41	19.23

The prediction of electrical formation factor is satisfied

Verification of MPNM: capillary pressure curve

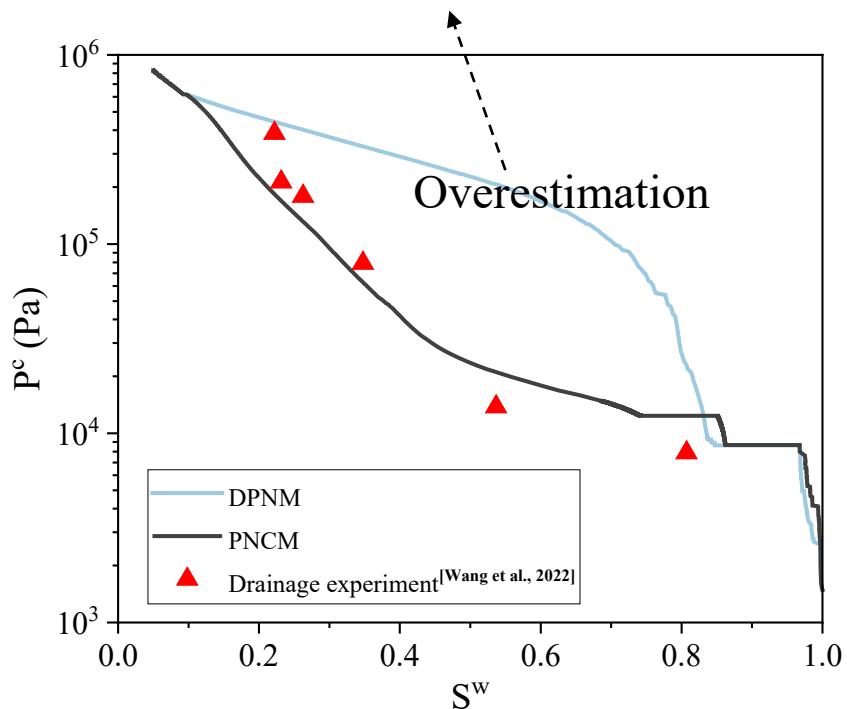


Verification of MPNM: capillary pressure curve

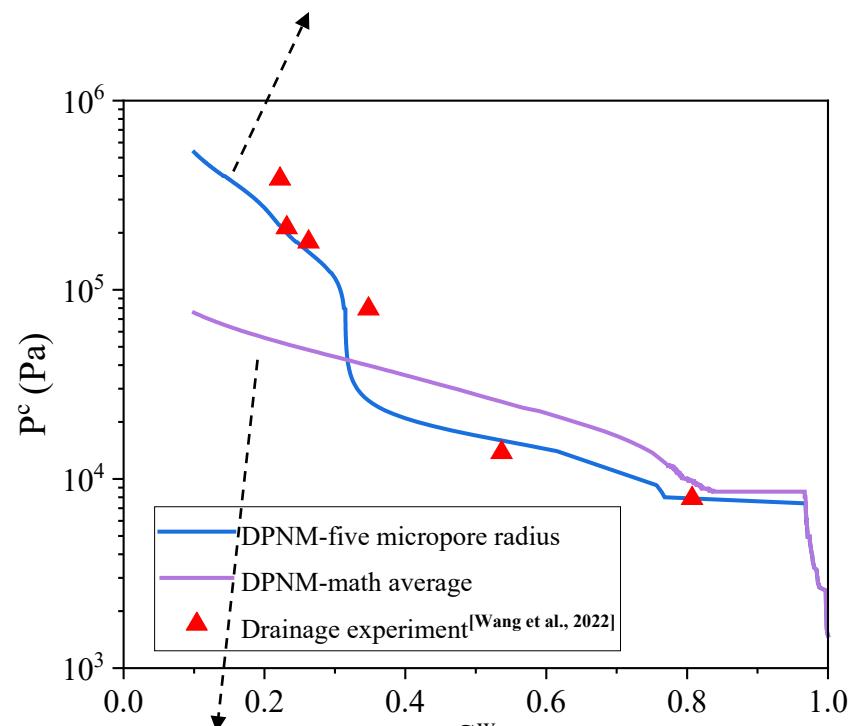


Verification of MPNM: capillary pressure curve

① Average based on sphere-assumption



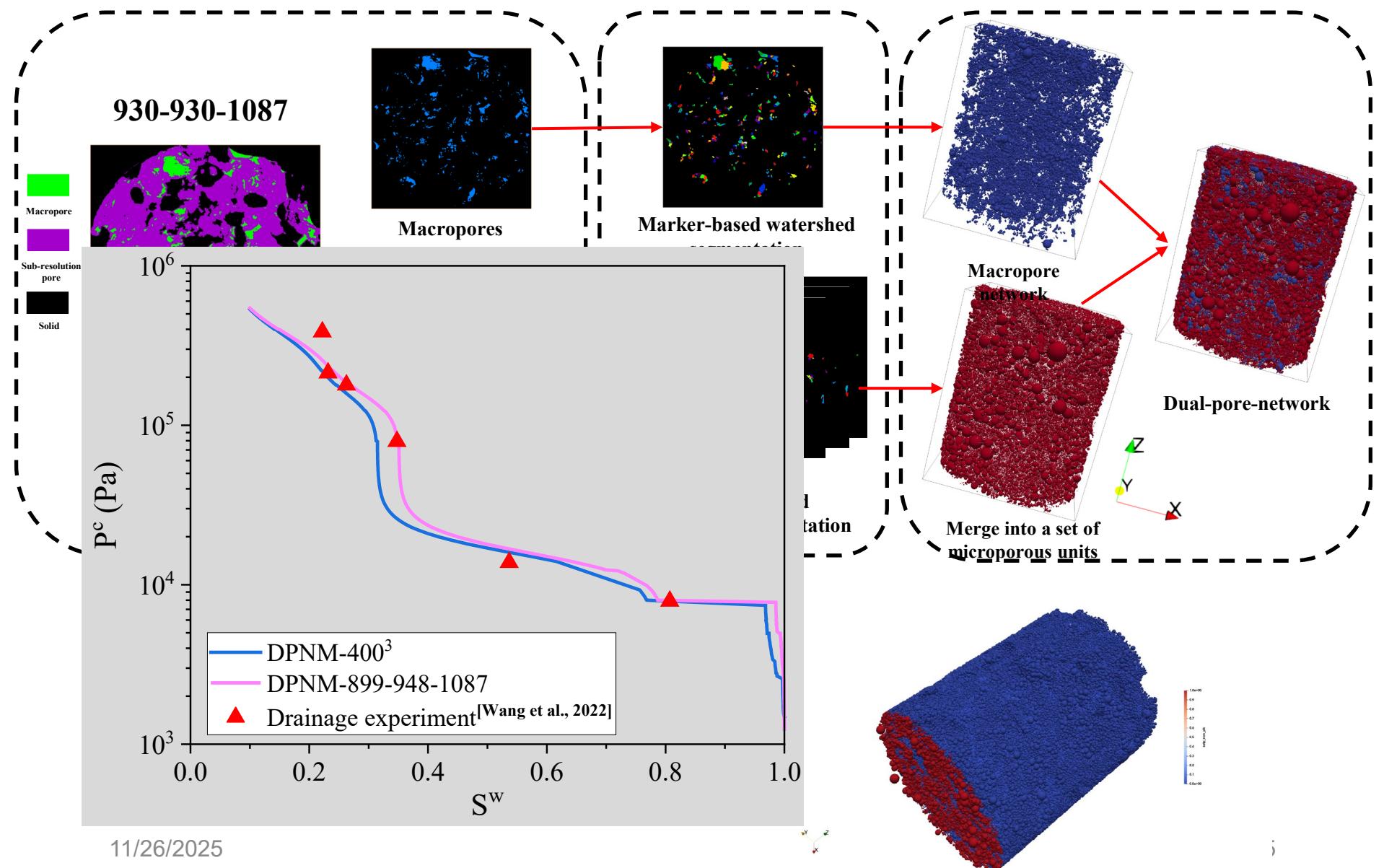
③ Entry-pressure-based sub-rock typing (Wang et al., 2022)



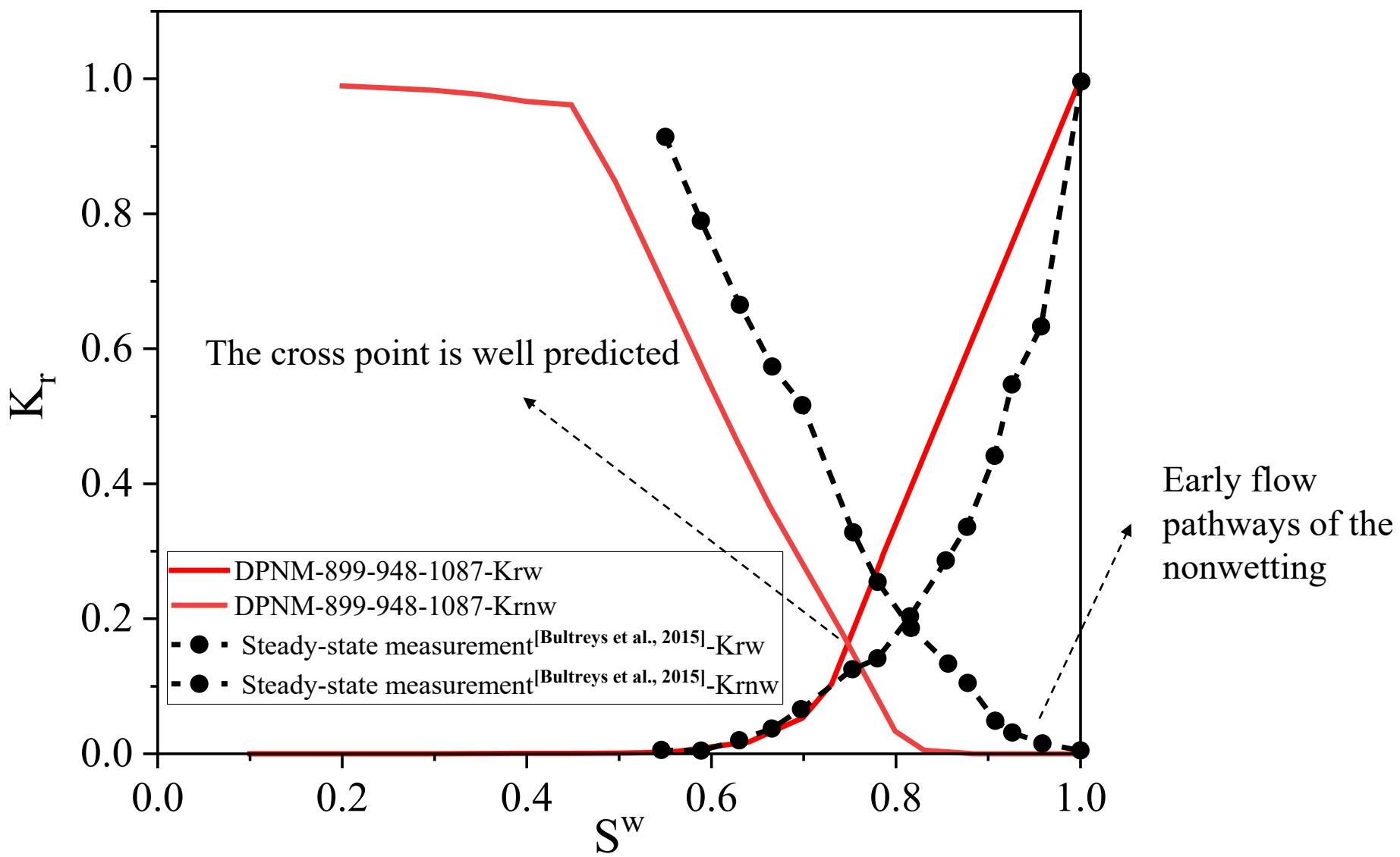
② Average based on voxel-counting

- The **sub-rock typing** is essential to the efficient multiscale pore-network model.
- 400^3 size **is adequate to** the prediction of capillary pressure curve.

Capillary pressure (the full image of ES6.5)



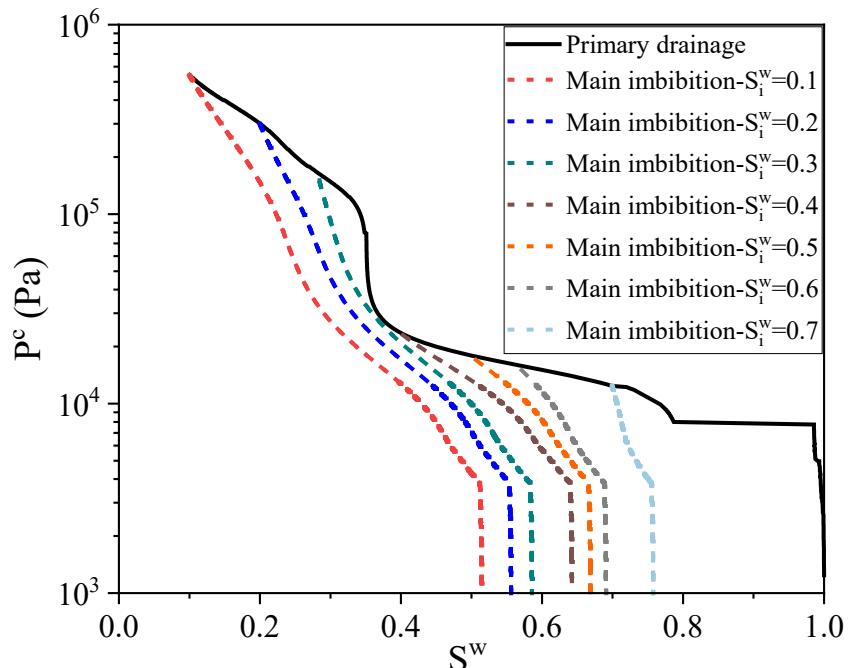
Relative permeability (the full image of ES6.5)



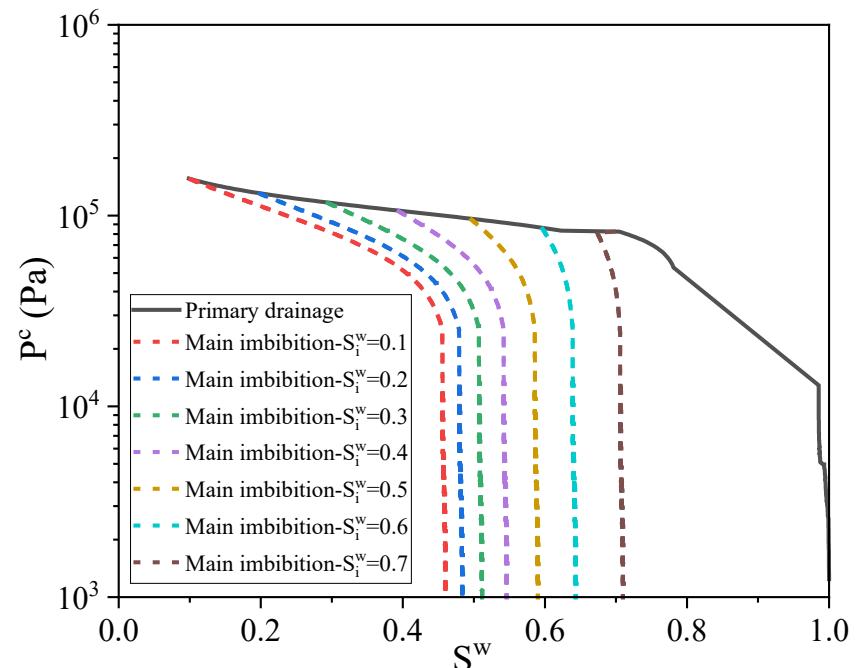
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Capillary trapping

Do not consider Ostwald ripening and remobilization



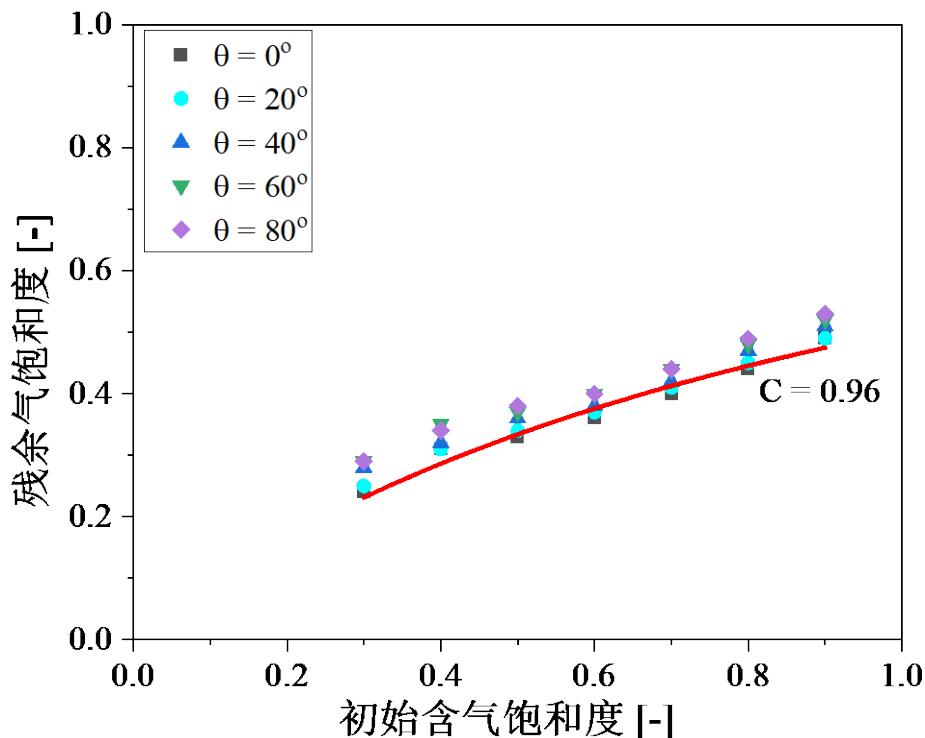
ES6.5: heterogeneous microporosity



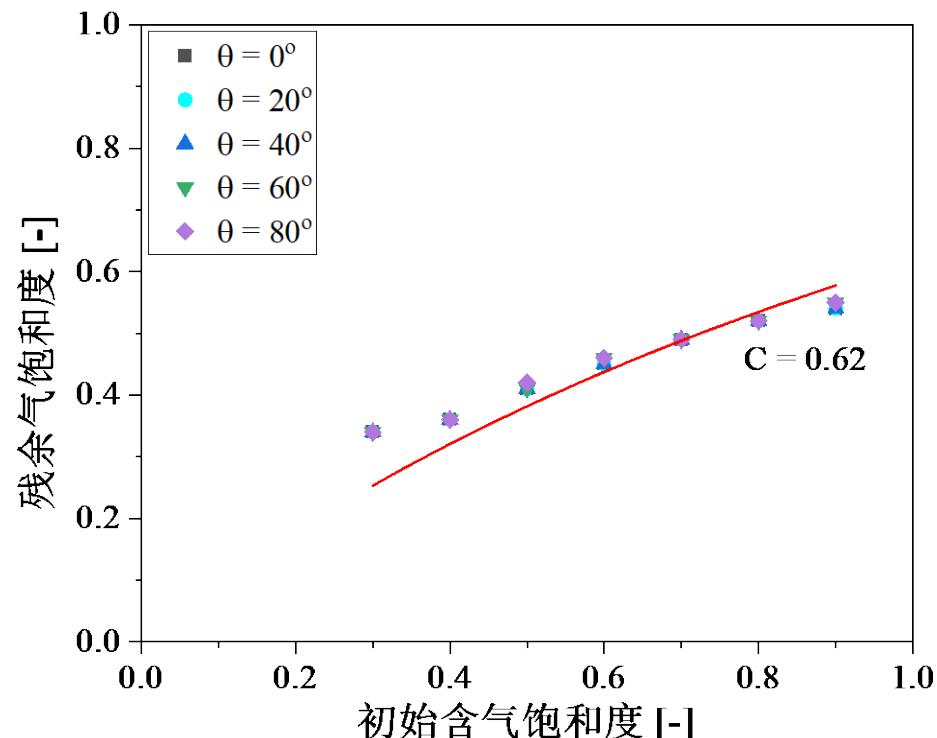
Assuming constant mean pore size of microporosity

Capillary trapping

$$S_{nw,r} = \frac{S_{nw,i}}{1 + CS_{nw,i}}$$



Tune the wettability of macropores



(b)

<https://czqin.github.io/publication/zhao-master-2022>



Conclusions and outlook

Conclusions

- ❑ A **high-efficient** multiscale pore-network model (MPNM) is developed, and verified against the **high-resolution** pore-network-continuum model (PNCM).
- ❑ Microporosity of ES rocks has strong heterogeneity of mean pore sizes.
- ❑ Three types of averaging microporosity voxels are tested. It is found that **the sub-rock typing** is necessary to guarantee the reliable predictions of both single-phase and two-phase flow parameters.
- ❑ We can **predict** absolute permeability, formation factor, capillary pressure and relative permeability.
- ❑ Heterogeneity of pore structures enhances capillary trapping?

Outlook

- ❑ Advance the modeling framework to **two-phase flow dynamics**.
- ❑ Understand how microporosity influences material properties, and extend capillary pressure and relative permeability **empirical models**.



Thank you for
your attention!

Chao-Zhong Qin (秦朝中)

<https://czqin.github.io/>

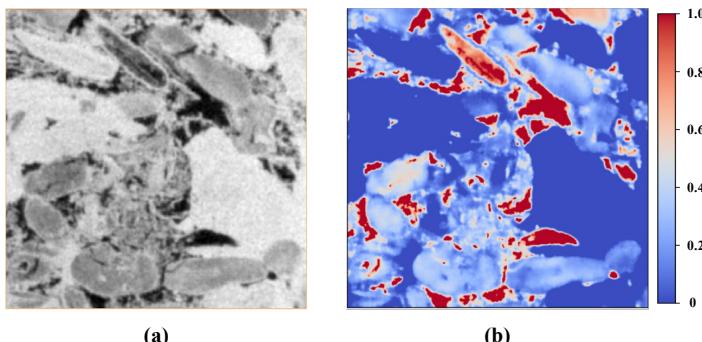
Test samples of carbonate digital rocks

<https://www.digitalrocksportal.org/>

Digital rock	Voxel size (μm)	Microporosity	Image size (voxels)	Total Porosity (%)	Absolute permeability (mD)
					Experimental
ES3.1	3.1	Uniform mean pore size	2000×2000×1725	25	260 ± 60
ES3.6	3.6	Uniform mean pore size	1000×1000×1000	29	/
ES6.5	6.5	Heterogeneous	1316×1316×1087	25	202.4 ± 86.9

ES3.1 and ES3.6 have the MICP curves; ES6.5 has **the porosity map and the entry-pressure map** of subresolution microporosity.

The porosity map of ES6.5





Predictions of absolute permeability and formation factor

Subvolume of digital rock	Pore regions	Original voxels	Volume fraction	In the MPNM	In the PNCM
ES3.1	Macropores	6332318	9.9%	3569	3569
	Microporosity	21562493	33.7%	8375	3929815
ES3.6	Macropores	5040267	7.9%	2172	2172
	Microporosity	32676964	51.1%	13228	4494989
ES6.5	Macropores	3694907	5.8%	3827	3827
	Microporosity	40618405	63.5%	7930	4147069

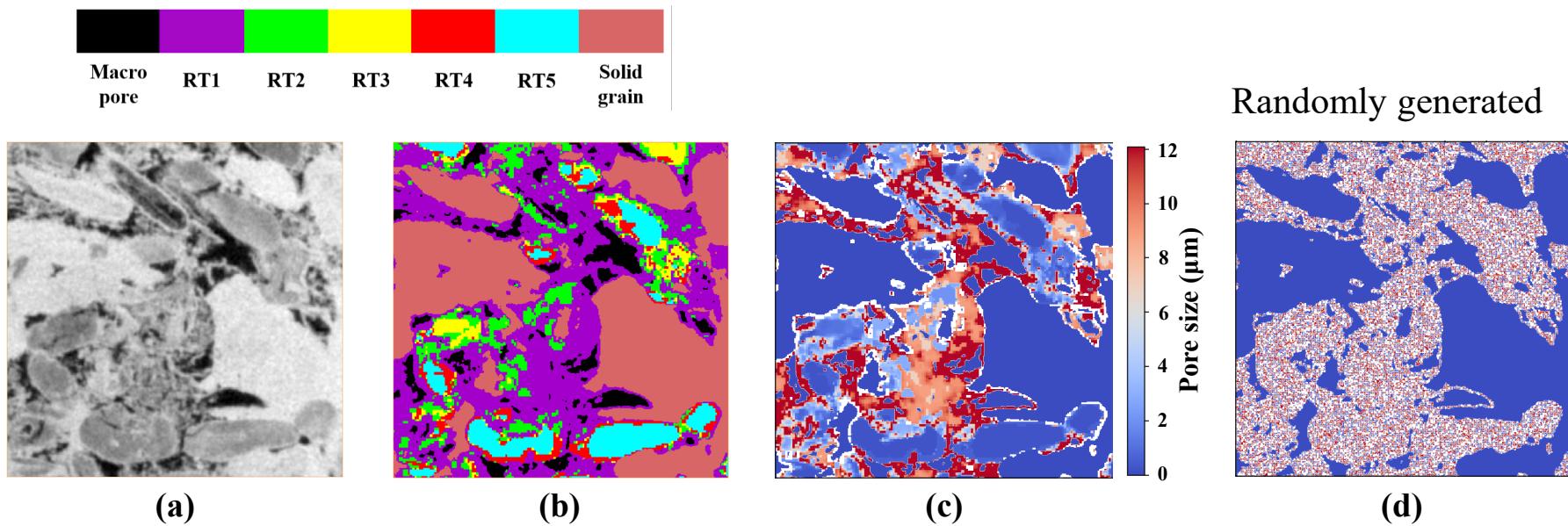
90% reduction in computational grids

Why does the MPNM underestimate the absolute permeability?

Digital rock	Mean pore size (μm)	By the MPNM (mD)	By the PNCM (mD)	By the reference model (mD)
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ES3.6	0.74	34	37	37
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ES3.6	23.81	23.81	23.26
ES6.5	18.52	20.41	19.23

The prediction of formation factor is satisfied



- The sub-rock typing helps with the prediction, but the CT-based characterization is **costly and time-consuming** !
- If only the MICP data is used, **the correlation of pore sizes** should be taken into account.

