Effects of physicochemical properties and structural heterogeneity on mineral precipitation and dissolution in saturated porous media

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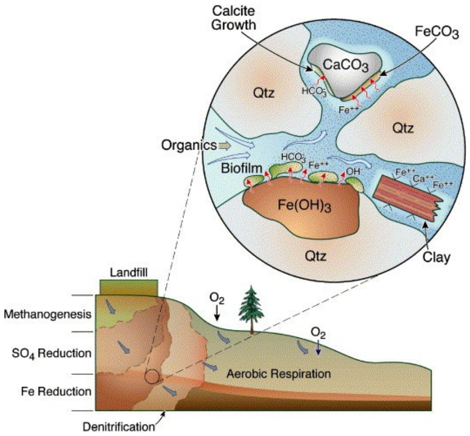
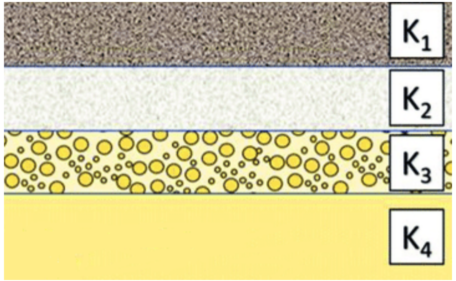
Scientific questions

I. Effects of physicochemical properties on the transport behavior of $CaCO_3$

II. The interplay between structural heterogeneity and reactive transport processes



Steefel et al., 2005



van Lopik et al., 2020

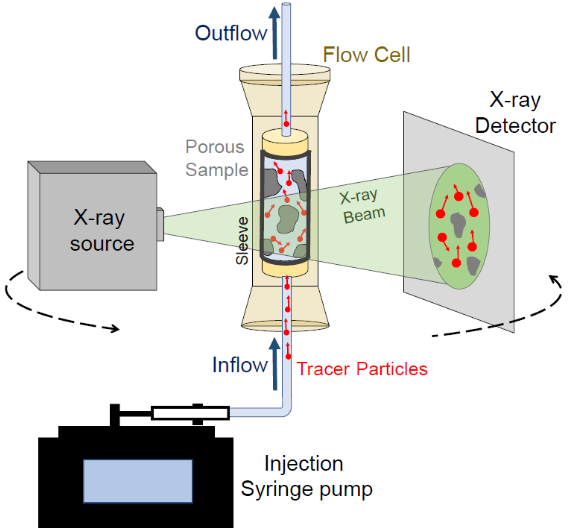
physicochemical properties

structural heterogeneity

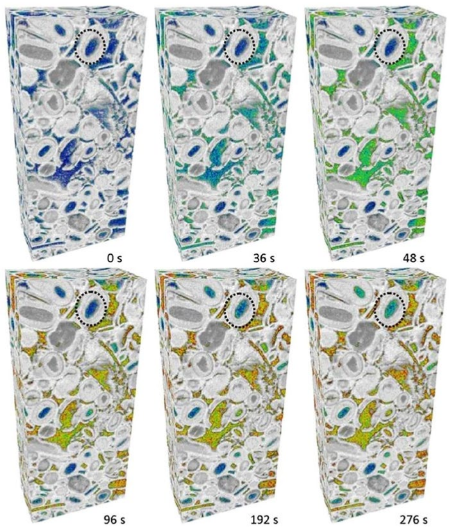
Challenges

I. How to visualize pore-scale processes during experiments?

II. How to quantify the effects of structural heterogeneity?

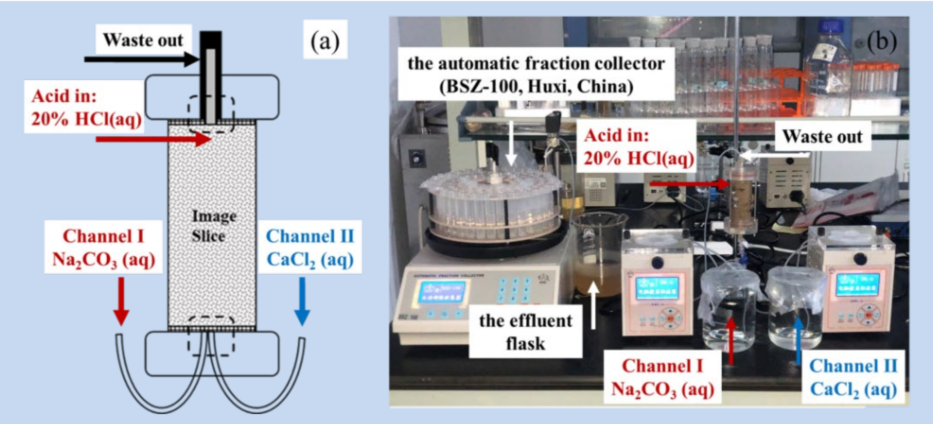


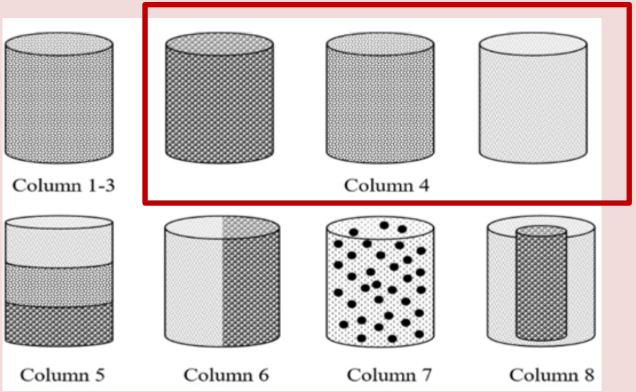
Bultreys et al., 2022



Ferreira et al., 2022

Methods: Column experiments





	S1 mmol	S2 mmol		A1	A2		Q1 ml/min	Q2 ml/min
C1	1.2	1.2	C2	PH=2	PH=11.2	C3	0.4	0.4
	6	6		PH=5			0.6	0.6
	12	12		PH=7			0.8	0.8
	24	24		PH=9			1	1
	60	60		PH=11			1.2	1.2
C4 - C8	12	12		PH=6.5	PH=11.2		0.6	0.6

Column 1-3:
medium particle size quartz sand under different environmental conditions;

Column 4-8:
different setups and levels of heterogeneity.

Methods: HYDRUS – PHREEQC simulations

Governing equations

- Richards equation:

$$C(h)\frac{\partial h}{\partial t} - \nabla \cdot K(h)\nabla h - \frac{\partial K}{\partial z} = 0 \quad (1)$$

- Convection – diffusion equation:

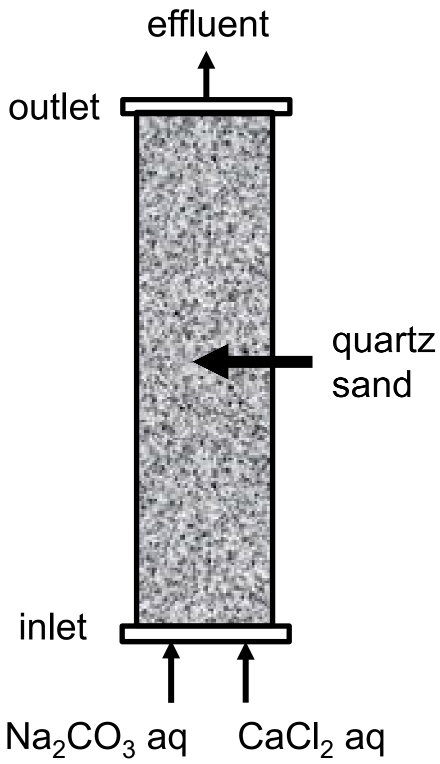
$$\frac{\partial C_i}{\partial t} + \vec{u} \cdot \nabla C_i = D\nabla^2 C_i + R \quad (2)$$

$$R = kC_{CaCl_2}C_{Na_2CO_3} \quad (3)$$

- Reaction:

$$Ca^{2+} + CO_3^{2-} \rightarrow CaCO_3 \quad (4)$$

Simulation processes



Basic information

Water flow

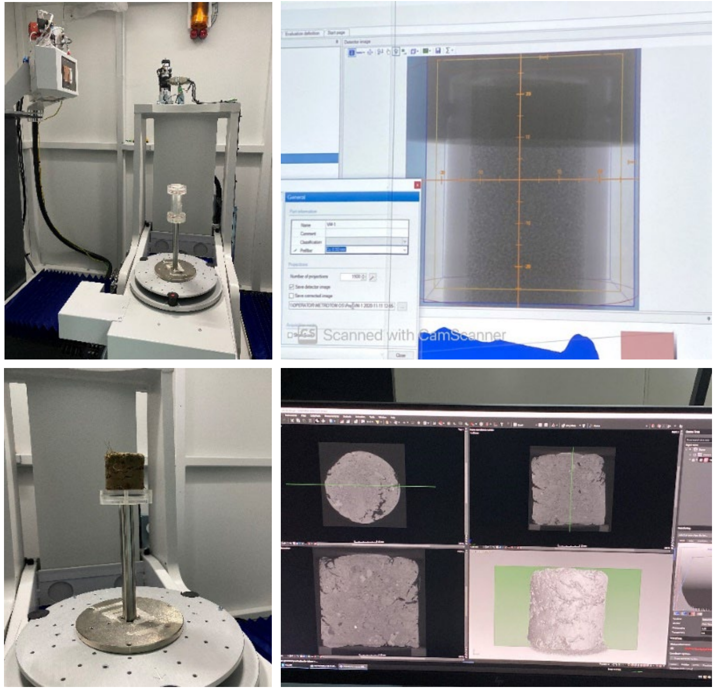
Solute transport

Boundary condition

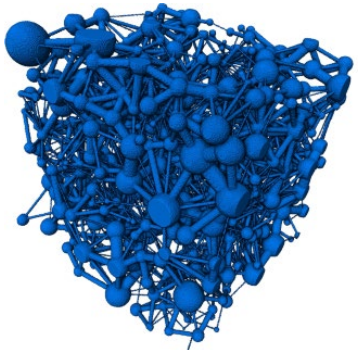
Initial condition

Methods: XCT visualization and post-processing

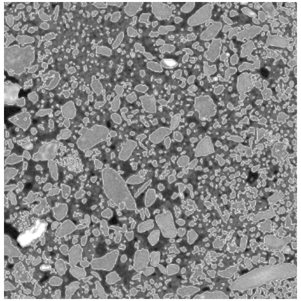
XCT image processing



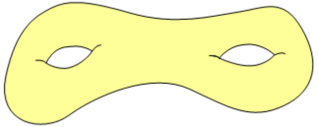
Morphological calculation



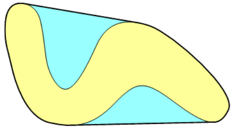
pore volume



surface area



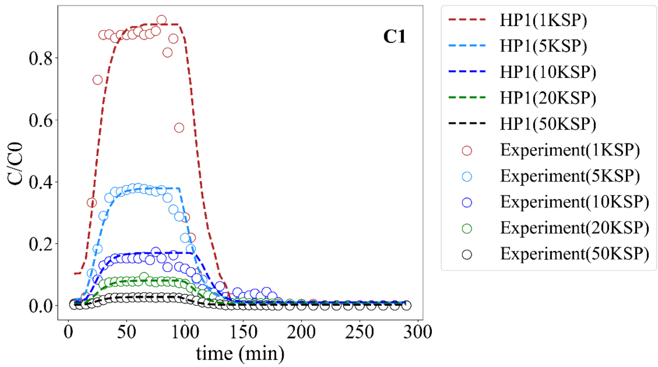
Euler number

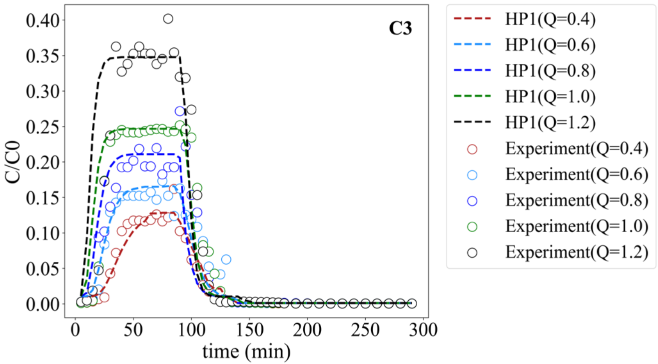


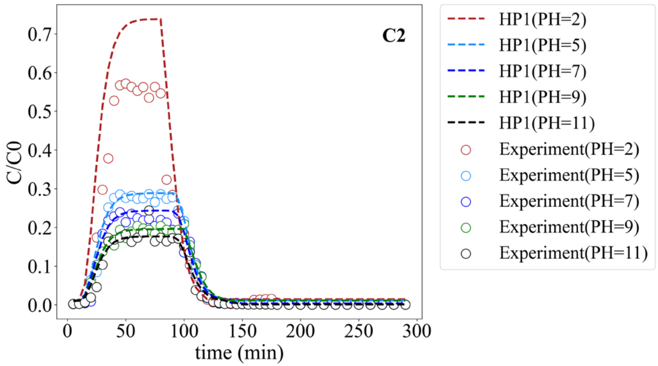
convexity

Blunt et al., 2017; Legland & Carreras, 2018

Results: Transport behavior under different physicochemical conditions







C1: the effects of salinity

Salinity increase → precipitation enrichment → weak Ca^{2+} breakthroughs

C2: the effects of acidity

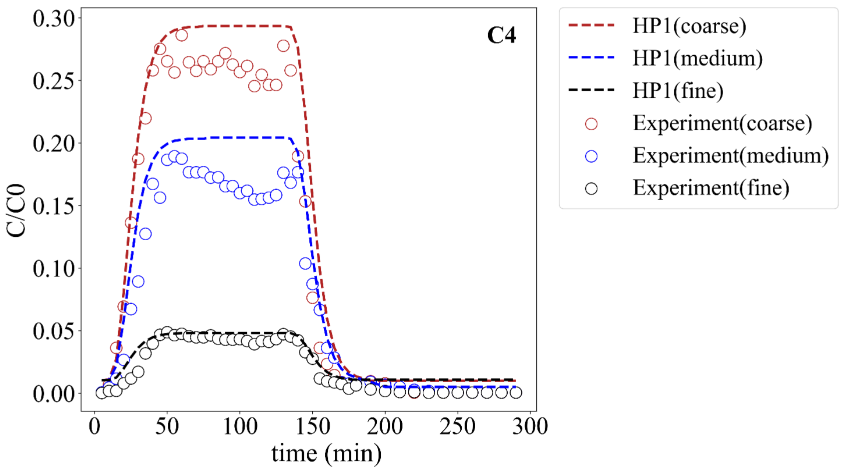
Acidity increase → precipitation shrink → strong Ca^{2+} breakthroughs

C3: the effects of flow rate

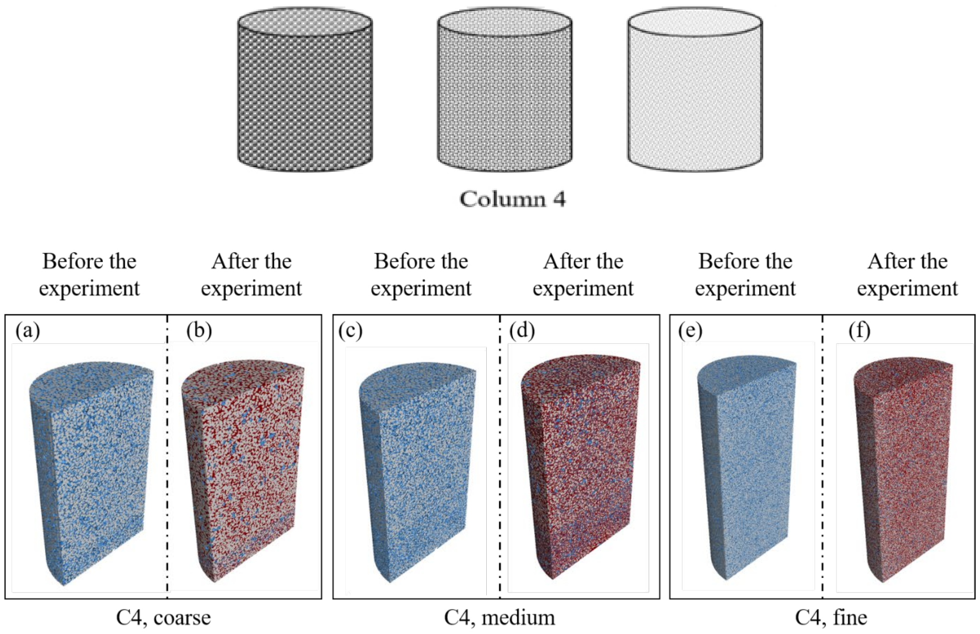
Flow rate increase → precipitation shrink → strong Ca^{2+} breakthroughs

Results: Effects of structural heterogeneity

Breakthrough curves of C4



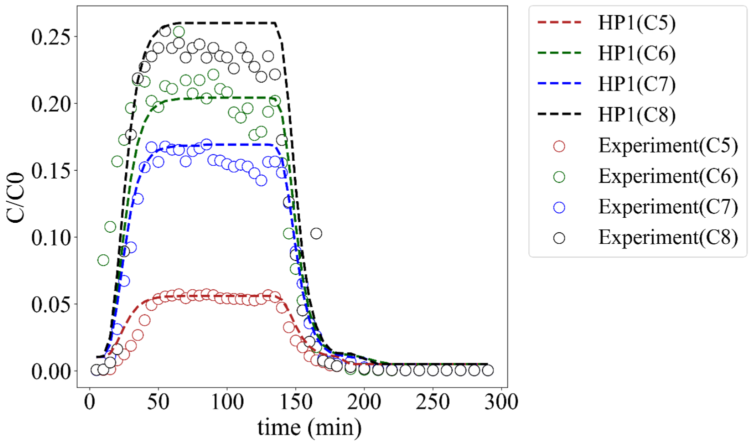
3D visualization of C4

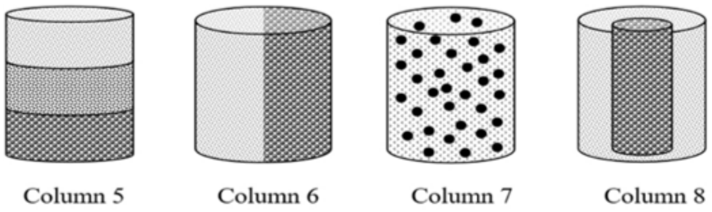


- ❖ Low porosity promotes precipitation; while precipitation decrease pore connectivity.
- ❖ The increase of particle size leads to early breakthrough and higher peak concentration.

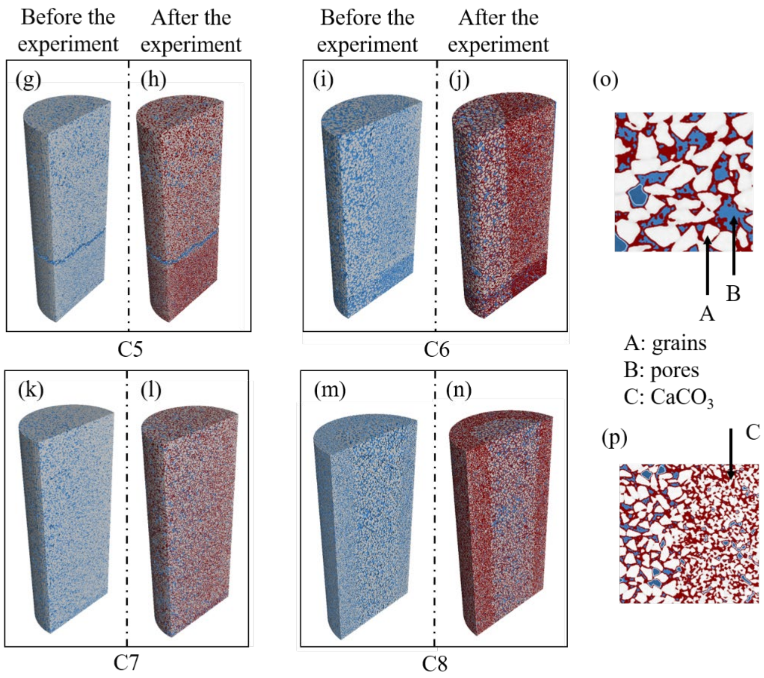
Results: Effects of structural heterogeneity

Breakthrough curves of C5~8





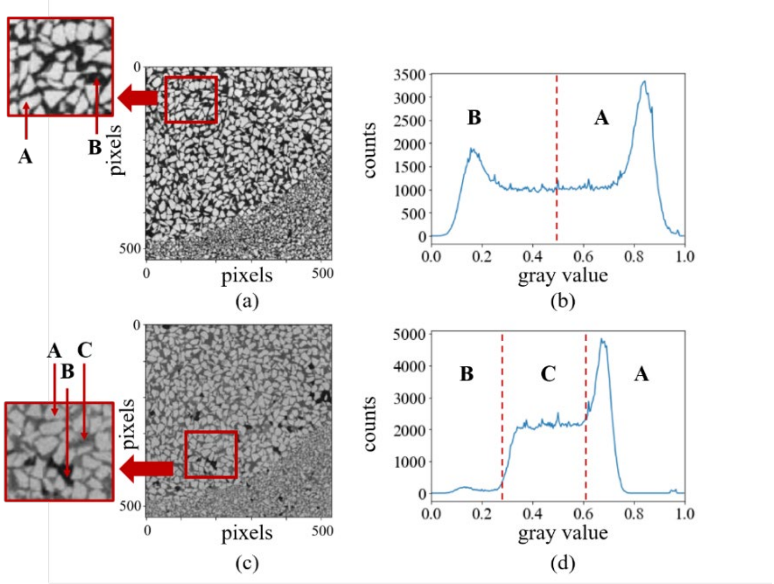
3D visualization of C5~8



❖ Vertical layering causes more $CaCO_3$ precipitation accumulated in the columns.

Results: Downscaling from XCT perspective

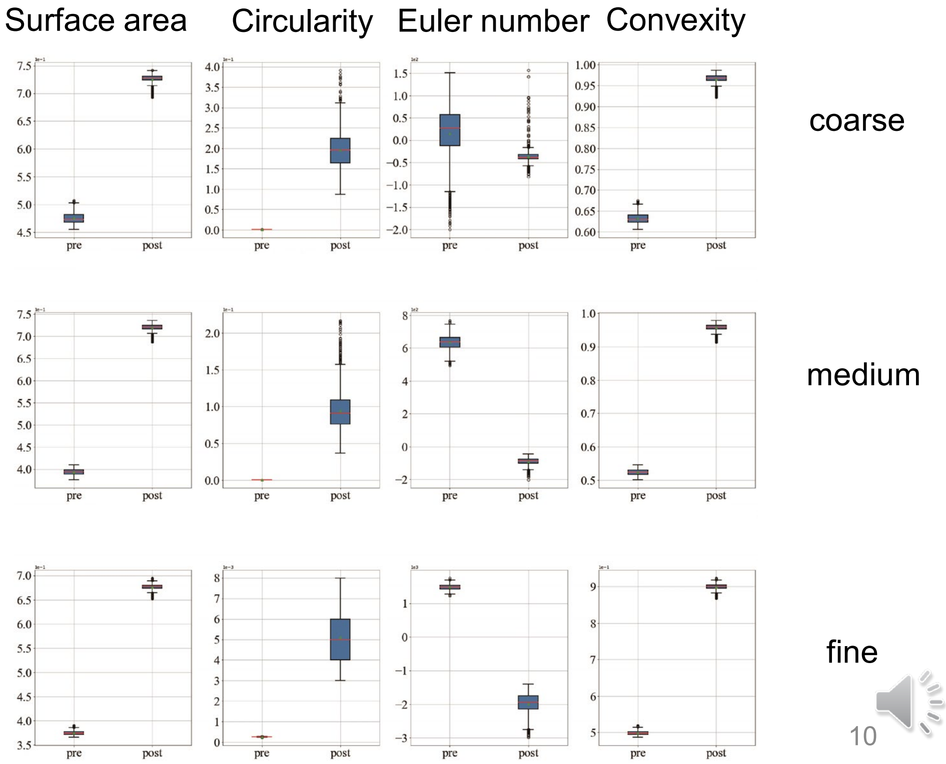
Sliced images and histograms



A: sand, B: pore, and C: carbonate

- ❖ $CaCO_3$ is often precipitated in narrower pores and accumulated first on concave surface.

- ❖ Significant decrease of pore connectivity and increased level of heterogeneity on grain surface after the PD process.



Conclusion

I. The traditional breakthrough curves were able to demonstrate the macroscopic behavior of reactive transport and reveal the effect of physiochemical properties on precipitation – dissolution process.

II. XCT visualization and morphological calculation provide microscopic information that help explain the macroscopic transport phenomenon in heterogeneous porous media under various conditions.

III. High-quality data from XCT images could serve as an input for further pore-scale modelling and simulations.

Thanks for listening!

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