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

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Introduction

◆ Scientific Issues

- ➢ The influence of physicochemical properties on transport behavior of $CaCO_3$ in saturated homogeneous porous media.
- ➢ The interdependency of structural heterogeneity and reactive transport process in saturated porous media.

◆ Challenges

- ➢ Visualize as well as record pore-scale processes and properties in both experiments and numerical simulations.
- ➢ Understand the mechanism of structural heterogeneity.

Objectives

- ✓ Determine the influence of salinity, acidity, flow rate and particle size on transport behavior of $CaCO_3$.
- ✓ Examine the effect of physical heterogeneities on carbonate reactive transport in saturated porous media.
- ✓ Investigate the impact of reactive transport on structure formation via XCT visualization.

Methods

◆ Flow Cell Construction

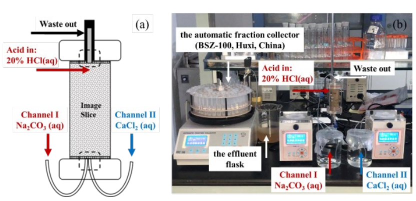

Fig. 1. (a) Schematic diagram of the flow cell illustrating Channel I of Na2CO3 (aq) and Channel II CaCl2 (aq). (b) Column experimental device and setups.

◆ Column experiments

- ➢ Column 1-3: medium particle size quartz sand for different environmental conditions;
- ➢ Column 4-8: different setups and levels of heterogeneity.

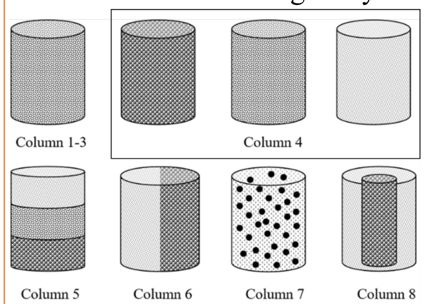

Fig. 2. Schematics of packing structures of the columns.

◆ HP1 simulations

- ➢ Richards equation

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

- ➢ Convection-diffusion equation

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

$$R = kC_{CaCl_2}C_{Na_2CO_3}$$

- ➢ Reaction

$$Ca^{2+} + CO_3^{2-} = CaCO_3$$

◆ XCT image processing

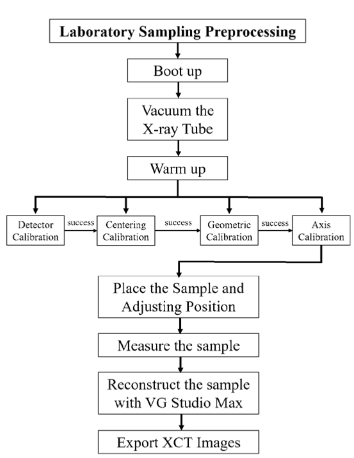

Fig. 3. Workflow of the XCT scanning experiment.

◆ Morphological calculation

- ➢ Minkowski functionals
- ➢ Porosity distribution

Results

◆ Transport behavior under different physicochemical conditions

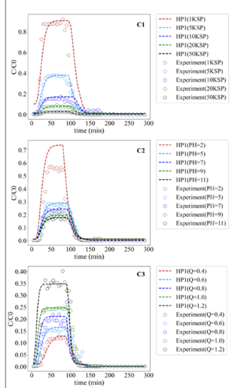

Fig. 4. Breakthrough curves of different salinity conditions(C1), different acidity conditions(C2) and different flow rate conditions(C3).

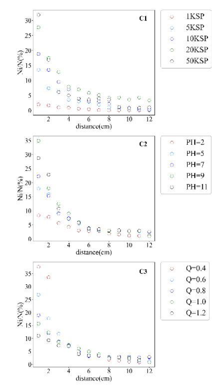

Fig. 5. Retention curves of Ca^{2+} reactive transport with (a) salinity variation; (b) acidity variation; (c) flow rate variation.

◆ Effects of structural heterogeneity

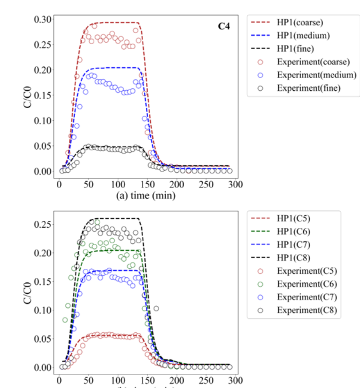

Fig. 6. Observed breakthrough curves in saturated heterogeneous porous media under different medium particles (a) and different structure (b).

◆ Downscaling from XCT perspective

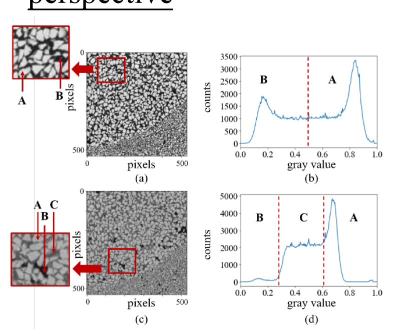

Fig. 7. The sliced images of different components and the profiles of grayscale value.

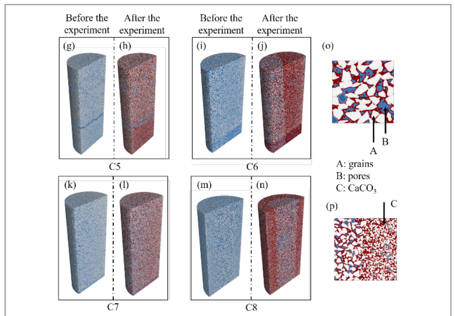

Fig. 8. XCT 3D structures of Ca^{2+} reactive transport process of C5-C8.

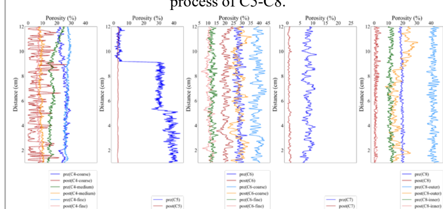

Fig. 9. Porosity distribution of C4-C8 (a-g) along the z direction. The PD process of $CaCO_3$ reduced the pore space significantly.

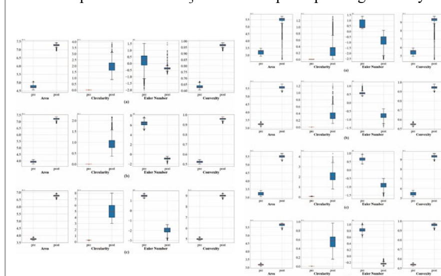

Fig. 10. Morphological calculation of C4-C8.

Conclusion

- ◆ Salinity increase causes precipitation enrichment in porous medium, resulting weak breakthroughs. The increase of acidity and flow rate promote early breakthroughs.
- ◆ The microporosity generated by calcium precipitates strongly affects the evaluation of morphological parameters.
- ◆ Structural heterogeneity and the increase of particle size promote the reactive transport of calcium carbonate.
- ◆ The HP1 simulation results agree with the column experimental results, providing essential parameter information.