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# Multiscale Simulation Study on Residual Trapping in Subsurface Rocks with Clay Minerals: Implications for Geological Carbon Storage

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Geological carbon storage is a promising and feasible technique for greenhouse gas mitigation. To improve CO<sub>2</sub> storage efficiency and develop monitoring techniques, it is important to know the CO<sub>2</sub> flow behavior and capillary trapping mechanisms in subsurface rocks. Clay minerals, often found in sandstone, may exert a vital impact on the displacement process. However, the diversity of rock components, notably clay minerals, has been consistently overlooked in previous studies. In this study, we presented a new concept, namely, digital rock physical chemistry, by integrating molecular-scale and pore-scale simulations to investigate CO<sub>2</sub> residual trapping mechanisms in porous systems, for high-efficiency geological carbon storage. A digital rock with kaolinite clay minerals is used for the porous media. The decane, CO<sub>2</sub>, and their mixtures are used as the fluid to be displaced. The intrinsic physicochemical properties, including the fluid viscosity, the fluid-water interfacial tension, and the fluid-water-mineral wettability at varying CO<sub>2</sub> concentrations, are investigated using molecular dynamics simulation. These molecular-scale properties are then upscaled into a core/pore-scale system with the help of lattice Boltzmann simulation. The results are summarized into a 3D phase diagram, which reveals the non-monotonic variations of the initial-residual (I-R) curves across different CO<sub>2</sub> concentrations. Although the obtained I-R curves in oil and CO<sub>2</sub> displacement exhibit similar trends, the trapping characteristics, including residual saturation and fluid distributions, differ. These findings underscore the critical roles of molecular scale interfacial phenomena and rock surfaces, particularly those related to kaolinite clay minerals, in subsurface multiphase seepage and geological carbon storage, highlighting the importance of digital rock physical chemistry.

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## Porous Media & Biology Focused Abstracts

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## References

## Conference Proceedings

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