Influence of Silica Nanopore Size on the Transport of Confined Hydrocarbons and CO_2

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Scientific Achievement

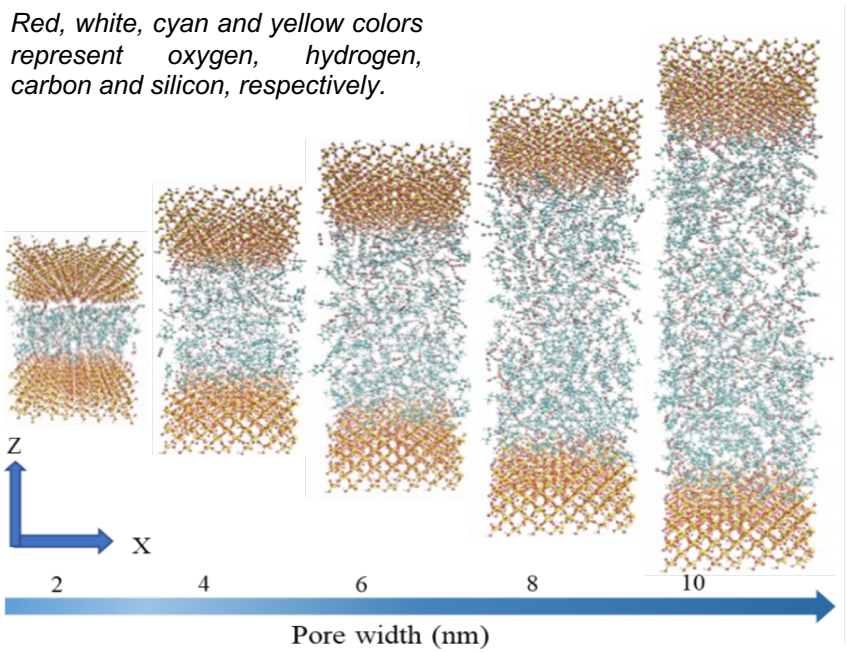
Facilitating fundamental understanding of principles supporting energy applications, lighter molecules, such as propane, were preferentially displaced by CO_2 in silica nanopores compared to heavier liquids, such as toluene, which also diffused more slowly in confinement.

Significance and Impact

Enhanced affinity of molecules for surfaces influences how different compounds move and are absorbed in confined fluids, as in natural rock, and these phenomena are not accounted for in bulk fluid transport relationships, such as Darcy's Law.

Research Details

- Molecular simulations for trajectories in different size Si nanopores
- Periodic array of 2-10 nm slit shaped pores
- Fluid density in each pore was set to 0.8 g/cm^3, representative of subsurface fluids



Snapshot of the simulation cells containing silica surfaces with CO_2, toluene and propane molecules in confinement.

Mohammed, S. and Gadikota, G., 2019. CO_2-Induced displacement and diffusive transport of shale geofluids in silica nanopores of varying sizes. *Journal of CO_2 Utilization*, *32*, pp.37-45.

Work was performed at University of Wisconsin Madison and Cornell University

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