Improved Understanding of CO_2/Brine/Mineral Interactions

Scientific Achievement

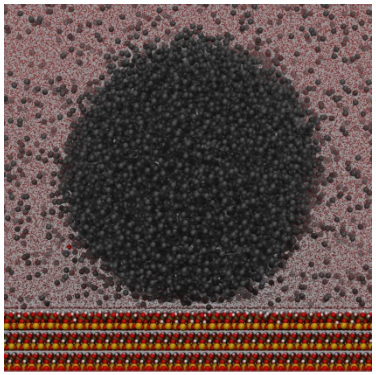
Derived contact angles for supercricital CO_2, in water and brine, on the basal surfaces of kaolinite clay. This research provides an accurate molecular description of CO_2 for evaluating surface tension, contact angles, capillary flow, snap-off, and related phenomena associated with CO_2 trapping.

Significance and Impact

Knowledge of molecular interactions at each interface in fluid/fluid/mineral system inform larger scale conceptual models for two-phase surface wetting, hence transport and distribution of supercritical CO_2 in the reservoir.

Publications

Tenney, C., and R. T. Cygan (2014 (In Press)), Molecular simulation of carbon dioxide, brine, and clay mineral interactions and determination of contact angles, *Environmental Science & Technology*.



Snapshot of an infinitely long CO_2 "droplet" on the gibbsite surface of kaolinite in the presence of water containing dissolved CO_2 after 10 ns at 330 K and 20 MPa. The system contains 15,000 CO_2 molecules and 130,000 H_2O molecules. Aluminum, silicon, oxygen, and hydrogen atoms within the kaolinite slab are represented as brown, yellow, red, and white spheres, respectively. Above the kaolinite slab, black spheres are CO_2 carbon atoms and red dots are H_2O oxygen atoms. Atoms represented as spheres are rendered at 60% of their van der Waals radius.

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