

Molecular dynamics simulations of the capillary properties of water, CO₂, and organics in a quartz nanopore

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The wettability of mineral surfaces by water is an important property influencing multiphase flow in soils and sedimentary rocks. In particular, for technologies that rely on trapping supercritical CO₂ in sedimentary formations, wettability is a fundamental property influencing stratigraphic and residual trapping. Atomistic simulations have shown promise in elucidating wettability data discrepancies such as those potentially caused by organic contamination or by the transition from the continuum-scale droplet to the nano-scale adsorbed water film. This study uses Molecular Dynamics (MD) simulations to model equilibrated water and CO₂ at various pressures and with various organic molecules in a quartz nanopore. We use non-equilibrium MD to simulate flow to observe dynamic properties. We are able to analyze the adsorbed water film and the fluid-fluid interface, and we compare our observations to theoretical values using thermodynamic equations. We show that the augmented Young–Laplace equation accurately captures the relationship between the observed radius of curvature, the capillary pressure between the bulk fluid phases, and the disjoining pressure in the adsorbed water film. We examine the thermodynamics of thin water films in novel depth, and present new methodologies for characterizing curvature approaching a mineral interface and for comparing continuum and nanoscale manifestations of wettability. We find that discrepancies in both the experimental and MD database may be influenced by proximity to solid surfaces and adsorbed wetting films. We further examine these behaviors by incorporating organic molecules into the system, which we find tend to collect at the water-CO₂ interface without significantly altering wetting.