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Advancing Underground Hydrogen Storage: Insights from Molecular Simulations of Wettability and Interfacial Tension

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The intermittency in energy supply and demand from renewable resources, which is often caused by seasonal variations, necessitates the development of long-term energy storage solutions. One promising approach is Underground Hydrogen Storage (UHS), a scheme in which hydrogen is strategically stored in subsurface formations to maintain market equilibrium. Depleted oil and gas reservoirs and saline aquifers present an attractive option for UHS. The appeal of these reservoirs lies in their existing infrastructure and the presence of subsurface traps, which are essential for sealing reservoir fluids. To fully leverage these reservoirs for UHS, it's crucial to understand the wettability and interfacial tension (IFT) of the gas, brine, and rock systems. These properties play a significant role in determining capillary pressure, fluid migration, and drainage in porous media. We used molecular dynamics simulations to study the impact of temperature (300 and 323 K) and pressure (5, 10, 15, and 20 MPa) on the IFT between hydrogen and formation brine. We also investigated the effects of two carrier gases, methane and carbon dioxide, on the system. Our findings revealed that the IFT of pure hydrogen/brine did not change significantly (less than 1 mN/m) with pressure. However, the addition of methane and carbon dioxide to the system lowered the IFT, with carbon dioxide having a more pronounced impact. In addition to IFT, we studied the contact angle between a gas phase (comprising hydrogen and its mixtures with methane and carbon dioxide), the brine and rock (calcite and silica) at a pressure of 20 MPa and a temperature of 300 K. With the exception of the H2-CO2/brine/silica, all systems exhibited complete water-wetting with a zero-contact angle. The exception can be attributed to the complete protonation of silanol groups, which is caused by the dissolution and hydration of CO2 to form carbonic acid, resulting in a low pH of 3. This research contributes to our understanding of UHS and provides valuable insights that could aid in the optimization of energy storage strategies. It underscores the importance of considering the effects of temperature, pressure, and carrier gases on the IFT and wettability of the system, which are critical for the efficient storage and retrieval of hydrogen in subsurface formations.

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