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Molecular simulations and experiments for the diffusion of hydrogen in brine

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The global shift towards carbon-neutral energy systems has heightened the need for efficient and secure storage solutions for renewable energies, with hydrogen (H_2) storage in deep saline aquifers emerging as a viable option for large-scale storage with high flexibility in terms of the number of annual storage cycles and the stored gas volume. This study aims to advance our understanding of hydrogen storage by investigating the diffusion coefficient of pure hydrogen and its mixtures with carbon dioxide in brine. This study uses experimental conditions similar to the Ketzin site in Brandenburg, Germany.

Molecular dynamics (MD) simulations were employed to predict the diffusion coefficients of hydrogen in chloride brine containing various cations (Na^+, K^+, Ca^{2+}) under a range of conditions (pressures from 1 to 218 atm and temperatures from 298 to 648 K). These simulations demonstrated that hydrogen diffusivity is significantly influenced by temperature, pressure, and ionic composition. The Arrhenius behavior observed for temperature dependence showed limitations at higher temperatures (≥ 400 K), indicating the need for more complex modeling approaches. The study utilized the TIP4P/2005 model for water, a two-site model for hydrogen, and the OPLS model for chloride ions, with simulations performed in the LAMMPS software. Experimental investigations complemented the simulations, employing a dual-chamber system to measure hydrogen diffusion through various rock samples, including Bentheimer sandstone, Werra rock salt, and Opalinus clay. The measured diffusion coefficients ranged from 10^{-8} to 10^{-9} m^2/s, with wetted samples showing greater hydrogen retention due to pore water saturation and microcrack closure from recrystallization in rock salt.

Our finding highlights the essential role of MD simulations in providing detailed insights into hydrogen diffusion in brine for a wide range of operating conditions, significantly contributing to the understanding and development of hydrogen storage mechanisms in geological formations. Integrating molecular simulations with experimental data offers a robust validation of the computational models in predicting hydrogen diffusion in saline aquifers.

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