Hydrogen solubility in NaCl brine under subsurface storage conditions: molecular simulations and thermodynamic modeling.

Halla Kerkache [a], Hai Hoang [c,d], Pierre Cézac [b], Salaheddine Chabab [a,b], Guillaume Galliero [a]

[a] Universite de Pau et des Pays de l'Adour, E2S UPPA, CNRS, TOTALENERGIES, LFCR, UMR5150, Pau, France

[b] Universite de Pau et des Pays de l'Adour, Laboratoire de Thermique, Energetique et Procédés (LaTEP), Rue Jules Ferry BP 7511, 64075 Pau Cedex, France

[c] Institute of Fundamental and Applied Sciences, Duy Tan University, Tran Nhat Duat Street, District 1, Ho Chi Minh City, Vietnam

[d] Faculty of Environmental and Natural Sciences, Duy Tan University, 03 Quang Trung Street, Da Nang, Vietnam

Abstract

Deep saline aquifers have emerged as a promising option for large-scale energy storage through hydrogen storage after the Power-to-Gas process. The availability of these porous geological reservoirs and their high capacity make them an attractive solution [1, 2]. However, the interaction between gas, brine, and rock in this environment can lead to physico-chemical and biochemical phenomena that can directly impact the mobility and stability of hydrogen.

Unfortunately, due to the complexity, cost, and hazardous nature of these systems, there are limited studies on phase equilibria of H_2/brine systems [3-6]. This work aims to address these gaps by generating new equilibrium data for H_2/brine systems using Monte Carlo simulation. The new generated data are validated against laboratory experiments and used to adjust thermodynamic models for implementation in large-scale simulation tools.

References

1. Tarkowski, R., *Underground hydrogen storage: Characteristics and prospects.* Renewable and Sustainable Energy Reviews, 2019. **105**: p. 86-94.
2. Raad, S.M.J., Y. Leonenko, and H. Hassanzadeh, *Hydrogen storage in saline aquifers: Opportunities and challenges.* Renewable and Sustainable Energy Reviews, 2022. **168**: p. 112846.
3. Lopez-Lazaro, C., et al., *Predicting the phase behavior of hydrogen in NaCl brines by molecular simulation for geological applications.* BSGF-Earth Sciences Bulletin, 2019. **190**(1): p. 7.
4. Chabab, S., et al., *Measurements and predictive models of high-pressure H2 solubility in brine (H2O+ NaCl) for underground hydrogen storage application.* International Journal of Hydrogen Energy, 2020. **45**(56): p. 32206-32220.
5. Torín-Ollarves, G.A. and J.M. Trusler, *Solubility of hydrogen in sodium chloride brine at high pressures.* Fluid Phase Equilibria, 2021. **539**: p. 113025.
6. van Rooijen, W., et al., *Interfacial Tensions, Solubilities, and Transport Properties of the H2/H2O/NaCl System: A Molecular Simulation Study.* Journal of Chemical & Engineering Data, 2023.