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Computing Fick diffusion coefficients using equilibrium molecular dynamics for binary mixtures of hydrogen relevant for underground hydrogen storage

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Scaling up renewable energy production needs to be accompanied by a concomitant scaling of storage technologies. In this regard, hydrogen (H₂) is an attractive energy carrier due to its large specific energy capacity and its clean combustion products. However, its low mass density requires gigantic volumes (billion m³) to store energy in the order of TWh. Geological formations such as depleted gas reservoirs conveniently provide these large volumes. To maintain a safe operational pressure range, a cushion gas is introduced into the reservoir, which expands and compresses during the storage cycles of H₂. A large compressibility of this gas maximizes the storage capacity of H₂ during injection, and minimal mixing facilitates an efficient recovery of pure H₂ during production. Among many options such as nitrogen, methane and H₂ itself, carbon dioxide is also considered a suitable cushion gas due to its large compressibility at supercritical conditions^[1].

On timescales relevant to storage (weeks to years), the cushion gas will mix with H₂ through molecular diffusion and flow-induced mechanical dispersion. This work focuses on molecular diffusion, as the first step towards quantifying mixing of the stored H₂ and the cushion gas. According to Fick's law, the diffusing mass flux is a product of gradient in mole-fraction and the (molecular) diffusion coefficient D. Fick diffusion coefficients exhibit strong dependencies on thermodynamic variables such as the mixture composition, temperature T, and pressure P. In this work, we compute D at various mixture compositions using equilibrium molecular dynamics^[2] for $P \in [20,300]$ bar and $T \in [250,350]$ K for various binary gas mixtures. The analytic expression for diffusion coefficients based on kinetic theory of gases deviates significantly from our predictions - thus emphasizing the need to account for molecular interactions. Furthermore, we provide fit functions to enable fast and accurate prediction of diffusion coefficients at reservoir conditions, which are beneficial for reservoir flow simulators. Finally, the phase equilibria of these gas mixtures are also predicted using molecular simulations.

Participation

In-Person

References

[1] Curtis M. Oldenburg, Energy & Fuels 2003 17 (1), 240-246
[2] Seyed Hossein Jamali, Ludger Wolff, Tim M. Becker, Mariëtte de Groen, Mahinder Ramdin, Remco Hartkamp, André Bardow, Thijs J. H. Vlugt, and Othonas A. Moultos, Journal of Chemical Information and Modeling 2019 59 (4), 1290-1294

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