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Perspective

Characterization and simulation of underground hydrogen storage across scales

Qingqi Zhao[1], Zhenkai Bo[2], Bin Pan[3], Yuhang Wang[4]*

[1]*Stuttgart Center for Simulation Science, University of Stuttgart, Stuttgart 70569, Germany*

[2]*Institute of GeoEnergy Engineering, Heriot-Watt University, Edinburgh EH144AS, United Kingdom*

[3]*State Key Laboratory of Petroleum Resources and Engineering, China University of Petroleum, Beijing 102249, P. R. China*

[4]*School of Environmental Studies, China University of Geosciences, Wuhan 430074, P. R. China*

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Abstract:
Underground hydrogen storage has emerged as a pivotal component of the low-carbon energy transition, providing a viable solution to the intermittency of renewable energy sources. The distinctive physical and chemical properties of hydrogen, together with its interactions with surrounding rocks and fluids, introduce unique challenges for subsurface storage. This perspective presents recent advances in experimental and modeling efforts of underground hydrogen storage from a multi-scale perspective, highlighting that established methods from hydrocarbon recovery and carbon dioxide storage remain valuable for studying hydrogen systems, yet effectively translating and scaling the relevant physical processes requires renewed attention. Improving the purity and recovery efficiency of stored hydrogen will be central to guiding future reseach on hydrogen storage in geological porous media.

1. Introduction

In recent years, substantial progress has been made in both experimental and numerical simulations to assess the feasibility, integrity, and performance of underground hydrogen storage (UHS) systems. Advances in site-specific geological characterization, pore-scale imaging, and laboratory-based flow tests have improved our understanding of hydrogen-rock-fluid interactions. Simultaneously, numerical studies, ranging from pore-scale models to field-scale ones, have become increasingly comprehensive, enabling more accurate predictions of hydrogen migration, mixing, and potential trapping. This paper aims to synthesize recent developments in the characterization and modeling of UHS, and to identify research directions needed to support safe and efficient operations of UHS at scale.

2. Experimental characterization of adsorption and diffusion dynamics

Experimental data on H_2 adsorption and diffusion, two processes central to storage efficiency, remain limited but are beginning to reveal key trends. Adsorption measurements on coals show relatively low capacities, generally below 1.2 mmol/g, with adsorption increasing steeply at low pressures and plateauing at higher pressures, while temperature exerts only a minor effect. Diffusion experiments indicate that H_2 moves significantly faster through coal than CH_4 under comparable conditions, suggesting that coal formations may offer favorable injectivity for underground storage (Iglauer et al., 2021; Liu and Liu et al., 2023). Similar experiments on kerogen samples further highlight the distinctive behavior of H_2 relative to other gases. Compared with CH_4 and CO_2, H_2 exhibits the lowest adsorption capacity, implying

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*Corresponding author.
E-mail address: qingqi.zhao@itlr.uni-stuttgart.de (Q. Zhao); z.bo@hw.ac.uk (Z. Bo); binpan@cug.edu.cn (B. Pan); wangyuhang17@cug.edu.cn (Y. Wang).

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minimal storage loss due to adsorption, while the high CO_2 adsorption capacity underscores the complementary potential of co-located CO_2 sequestration. Wettability measurements add another layer of complexity: kerogen surfaces can range from weakly water-wet to gas-wet, with a stronger affinity toward CH_4 and H_2 than helium (Pan et al., 2025). In gas-wet systems, capillary forces may promote gas penetration into the caprock, raising concerns over leakage risks.

H_2 diffusion also occurs through its mixing with cushion gases in the pore space (Hematpur et al., 2023). Commonly used cushion gases such as CO_2, CH_4, and N_2 play important roles in stabilizing reservoir pressure and isolating formation water, but their interaction with hydrogen inevitably leads to reduced purity upon recovery (Heinemann et al., 2021; Saeed and Jadhawar et al., 2024). Quantifying this diffusive mixing under reservoir conditions is therefore essential for assessing storage performance. Experimental studies have provided valuable insights into the pressure and temperature dependence of hydrogen-cushion gas diffusion, using techniques such as infrared spectroscopy and steady-flow measurements. More recently, Raman spectroscopy has enabled measurements under reservoir pressure and temperature conditions. The resulting correlation provides a solid basis for assessing the mixing in field-scale operations (Wang et al., 2025). It is worth mentioning that the diffusion of H_2 in the cushion gas involves not only molecular diffusion driven by concentration gradients, but also thermal diffusion induced by temperature gradients. In a recent work which investigated the thermal diffusion between H_2 and CO_2 (Wang et al., 2024c), H_2 prefers accumulating in the warmer region, enhancing the diffusive mixing during H_2 injection phase. This indicates that the Soret effect plays a role when the temperature difference between the wellbore and reservoir is pronounced.

Collectively, these advances provide fundamental parameters for quantifying H_2 interactions with rocks and cushion gases, yet challenges remain in translating laboratory measurements to real storage sites. For instance, diffusion measurements are often reported as bulk averages, leaving the role of pore-scale structure and connectivity relatively unexplored. Pore-scale models provide a pathway to connect microscopic processes with macroscopic behaviors.

3. Pore-scale multiphase flow modeling in porous media

Pore-scale modeling has enhanced our understanding of hydrogen-brine displacement, trapping, and remobilization under UHS conditions (Purswani et al., 2024; Foroughi et al., 2025). Two primary approaches dominate: Lattice Boltzmann methods (LBM) conduct direct numerical simulations on micro-CT-derived geometries, effectively capturing complex interfaces and boundaries (Wang et al., 2024a). Recent LBM studies have validated capillary entry, interface curvature, and phase connectivity against experimental data, demonstrating their fidelity in modeling complex pore-scale phenomena (Wang et al., 2024b). Additionally, LBM has quantified how spatially heterogeneous wettability fields influence displacement pathways, relative permeability, capillary pressure, and residual trapping (Guo et al., 2022). Generally, more water-wet conditions increase capillary pressure, reduce hydrogen relative permeability during imbibition, and lower residual hydrogen saturation compared to less water-wet scenarios (Zhao et al., 2024). Future work may focus on how variations in wettability correlation length further influence gas-phase connectivity and trapping.

Pore network modeling (PNM) complements LBM by efficiently representing pore spaces as interconnected pores and throats, facilitating rapid parametric exploration of capillary-dominated flows (Blunt et al., 2001; Zhao et al., 2023). Cross-comparisons with LBM demonstrate that PNM effectively captures the primary trends at significantly reduced computational costs. PNM simulations have identified two key geometric predictors of residual trapping: a high pore-to-throat size ratio, promoting snap-off and trapping, and high pore connectivity, enhancing hydrogen continuity and reducing residual saturation (Hashemi et al., 2021). Additionally, PNM generates high-dimensional datasets, including detailed pore and throat properties, making it particularly suitable for machine learning applications (Baychev et al., 2019). Recent studies have leveraged advanced neural network architectures trained on unstructured pore-network grids to predict and optimize porous media properties, highlighting a promising research direction for future UHS pore-scale studies (Zhao et al., 2025). Overall, integrating detailed pore-scale findings, including wettability variations and structural sensitivities, into robust models remains essential for accurate predictions and effective design of UHS operations (Boon et al., 2024).

4. Field-scale numerical simulation and techno-economic assessment

Field-scale numerical simulation of UHS operations in various reservoir types has received intensive research attentions since some of the very early works (Feldmann et al., 2016; Luboń et al., 2020). After a surface check, many later works focus on different operational aspects of UHS through numerical simulations (Delshad et al., 2023), and have started to incorporate the key parameters, e.g., binary diffusion coefficients and relative permeability curves, that were measured or predicted at the pore-scale, into field-scale models (Bo et al., 2023). Results indicate that the multi-component, multi-phase system involving hydrogen exhibits distinct behaviors compared to more established systems such as CO_2 storage, further highlighting the essence of identifying and accurately characterizing these key parameters. It should be noted that the microbial activities, particularly methanogenesis and sulfate reduction, may lead to the loss of stored hydrogen, which is undesirable for long-term UHS operations (Dopffel et al., 2021). Modeling the biotic physics at reservoir-scale, to the best of our knowledge, has not gone beyond the realm established by the previous studies and deserves further investigation.

One of the most important aims of field-scale UHS simulation is feasibility investigation, which usually refers to techno-economic assessment. There have been many techno-economic models for analyzing the feasibility of UHS in

various operational settings, e.g., in a salt cavern, depleted hydrocarbon reservoirs, and saline aquifers. These models typically calculate the levelized cost of hydrogen storage (LCHS), defined as the total cost of the UHS projects divided by the net present value of total working gas content over the project life. The smaller the LCHS, the easier to reach a breakeven with a real hydrogen gas price spread, the more profitable the UHS project. Here, the real hydrogen gas price spread is defined as the net present value of gas buy-in and sell-out prices difference. Such LCHS is also usually compared with the levelized cost of energy storage of an underground gas storage project, investigating the potential to transform an underground gas storage into an UHS project. Under constant working gas to cushion gas ratio with the same capital, operational, and decommissioning costs, UHS inherently has higher LCHS than underground gas storage due to hydrogen's lower volumetric energy density and potential purification costs from gas mixing (Chen et al., 2023). Note that the LCHS should not be the only feasibility indicator for UHS projects. Depending on the business model of hydrogen storage, e.g., hydrogen stored as a product or a form of energy carrier, the real hydrogen gas price spread would be distinct in different cases (Lin et al., 2024). The conclusions made regarding UHS projects vary accordingly. Most of the previous studies define cost and revenue parameters with assumptions based on the local market (Lord et al., 2014). Meanwhile, only a few cases derive these values from actual UHS injection/production profiles obtained through reservoir simulations (Bo et al., 2024). Therefore, it is recommended considering realistic gas price spread, project net present value (NPV), and injection/production profiles into any future techno-economic models for UHS feasibility assessment. This can be achieved by coupling reservoir simulation outputs (daily or monthly injection/production rates) with NPV models that incorporate dynamic hydrogen price spreads based on regional supply-demand forecasts or local wholesale gas price history.

5. Summary

As the global shift toward renewable energy accelerates, the demand for large-scale, long-duration energy storage solutions is becoming increasingly urgent. UHS offers a promising pathway to ensure a stable and resilient energy supply by buffering seasonal fluctuations in generation and demand. Looking forward, research efforts will increasingly focus on improving both the purity and recovery rate of stored hydrogen, as these parameters are critical for the economic viability and operational reliability of UHS. Achieving this goal will require the development of advanced characterization methods capable of monitoring hydrogen losses due to trapping or diffusion, as well as identifying and quantifying impurity generation pathways, such as microbial conversion, geochemical reactions, and physical mixing with formation gases.

In addition, bridging the gap between pore-scale physics and continuum-scale models will be crucial for informing engineering controls. This scale translation will allow detailed insights from laboratory experiments and high-resolution simulations to be embedded into reservoir-scale models, improving their ability to forecast storage performance under varying geological and operational conditions. Coupled with long-term field monitoring and integrated modeling frameworks, these advancements will provide the technical foundation necessary for its large-scale commercial deployment in the evolving low-carbon energy landscape.

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Conflict of interest

The authors declare no competing interest.

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