

Invited review

Interfacial dynamics and mass transfer in underground hydrogen storage applications: A review of H₂ flow, stability and storage performance

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Abstract:

Hydrogen is emerging as a clean energy carrier in the global transition toward decarbonized energy systems. Leveraging established subsurface engineering expertise, underground hydrogen storage can be realized in salt caverns, depleted hydrocarbon reservoirs, and deep saline aquifers. However, the physicochemical characteristics of hydrogen including low viscosity, high diffusivity and strong chemical reactivity create unique challenges for its containment, transport and recovery from porous media. This review systematically analyzes the known interfacial and pore-scale mechanisms governing hydrogen migration, trapping and loss in heterogeneous reservoirs. The key processes comprise capillary trapping, molecular diffusion, interfacial reactions, and microbial activity. Interactions among hydrogen, brine and mineral surfaces are evaluated in terms of wettability, interfacial tension and pore connectivity, all of which directly influence storage efficiency and recovery performance. Advanced experimental methods such as nuclear magnetic resonance, microfluidics models, and X-ray computed tomography, combined with pore-scale simulations, are assessed for their ability to characterize multiphase flow and reactive transport behavior. Furthermore, the impact of operational factors like cushion gas composition, pressure cycling and injection-production strategies on storage integrity is discussed. Addressing these multi-physics and multi-scale challenges is essential for the safe and efficient implementation of underground hydrogen storage. Finally, this review identifies priority research directions aimed at improving mechanistic predictions and optimizing the operational management of hydrogen behavior in subsurface environments.

1. Introduction

According to the International Energy Agency, the global energy share of fossil fuels is projected to decline from 80% to 73% by 2030 (IEA, 2023). While fossil fuel demand remains robust, emerging indicators suggest a shifting trajectory. Although the accelerated deployment of decarbonized energy

alternatives has slowed the integration of new fossil fuel assets, reducing oil and gas investment alone is insufficient to meet the Net Zero Emissions by 2050 scenario (Tanaka and O'Neill, 2018; Raimi and Newell, 2024). As climate concerns intensify, hydrogen (H₂) has emerged as a critical clean energy vector. Produced via water electrolysis using

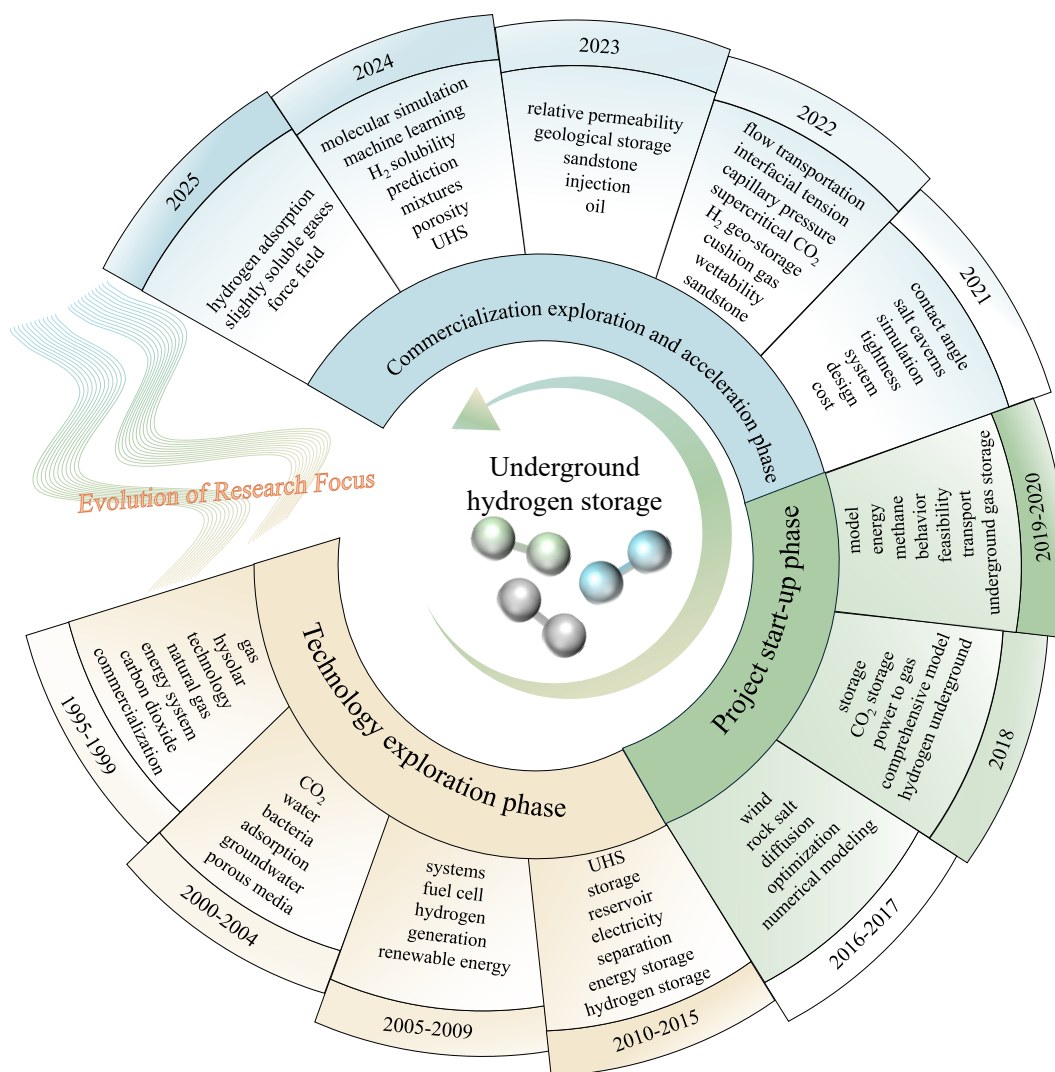


Fig. 1. UHS keyword analysis over the past three decades.

renewable electricity, H₂ enables the effective management of seasonal and meteorological variability in solar and wind power generation (Schäppi et al., 2022; de Kleijne et al., 2024).

The expanding role of H₂ as an energy source necessitates large-scale storage solutions. Current options, including high-pressure gaseous storage, cryogenic liquid H₂, metal hydrides, and organic liquid carriers, face constraints in terms of cost, energy density and technological maturity (Lao et al., 2024). While the U.S. Department of Energy targets 7.5 wt% gravimetric capacity and 70 g/L volumetric capacity at \$266/kg (Zhang et al., 2016), the low density of H₂ requires heavy pressure vessels (e.g., 700 bar), challenging aboveground storage implementation (Klymyshyn et al., 2024). Extensive carbon capture and storage experience has demonstrated subsurface storage feasibility, positioning underground hydrogen storage (UHS) as a promising alternative (Wang et al., 2023b). Unlike aboveground storage (MWh scale), UHS offers TWh-scale capacity at approximately \$1.23/kg in depleted reservoirs (Tarkowski, 2019), with minimal environmental impact and

enhanced safety through isolation from atmospheric oxygen.

Suitable geological formations, including depleted oil/gas fields, salt caverns, and deep saline aquifers, provide vast storage capacity from seasonal to monthly scales, supported by customized leakage prevention measures (Matos et al., 2019). As shown in Fig. 1, research output and impact in this field have grown steadily since 1995, reflecting the accelerated technological progress. Although advances in reservoir screening, injection-production optimization, safety monitoring, and risk management have established foundations for H₂ economy development, addressing reservoir stability, leakage risks and economic viability remains essential for UHS commercialization.

While some previous reviews have focused on UHS (summarized in Table 1) and established valuable foundations, knowledge gaps persist in H₂ flow mechanisms, mass transfer indicators, and systematic leakage analysis. To address this gap, this review synthesizes the recent advances to provide a comprehensive understanding of UHS, emphasizing sub-

Table 1. Literature review summary on underground hydrogen storage

Reference	Focus Areas	Conclusions
Tarkowski (2019); Jafari Raad et al. (2022)	-Reservoir site selection & cost -Technical limits & social regulations	-Well integrity is the key cost and leakage risk. -Widespread UHS faces technical and regulatory barriers, requiring dynamic aquifer models.
Heinemann et al. (2021); Muhammed et al. (2022); Raza et al. (2022)	-Multi-physical coupling processes -H ₂ loss pathways & mechanisms	-Hydrodynamic, geochemical and microbial processes collectively govern subsurface H ₂ loss. -Geological and mineral reactions cause substantial H ₂ loss, while predictive modeling remains constrained by insufficient long-term data.
Thiyagarajan et al. (2022); Sadkhan and Al-Mudhafar (2024); Davoodi et al. (2025)	-Reservoir geologic properties & integrity -Fluid properties & cyclic effects	-Dynamic reservoir properties control H ₂ capacity. -H ₂ mobility and wettability govern efficiency and leakage.
Muhammed et al. (2022); Kalam et al. (2023)	-Reservoir selection & optimization -Geochemical interactions	-Depleted gas reservoirs are currently the most viable storage choice. -Gas adsorption/desorption plays a vital role, and integration with steam methane reforming must include carbon capture and storage.

surface flow mechanisms (permeability, capillary pressure, interfacial tension), reservoir instability causes, and mitigation strategies (Fig. 2). Unlike CO₂ geological storage, UHS involves cyclic injection/withdrawal, requiring enhanced recovery strategies including reservoir optimization, injection-production refinement, and cushion gas adaptation from natural gas storage. Through a systematic analysis of technical challenges and research advances, this work provides a valuable reference for policymakers, researchers and industry professionals, supporting innovative breakthroughs in UHS technology and accelerating the global transition toward a sustainable, low-carbon energy future.

2. Mechanisms of hydrogen flow and mass transfer in porous media

The flow and mass transfer of H₂ underground are critically influenced by its low viscosity, high diffusivity, and high reactivity (Raza et al., 2022). This section provides an in-depth discussion of how the unique properties of H₂ govern the efficiency and safety of high-pressure underground storage.

2.1 Physical properties of hydrogen under subsurface storage conditions

The viability of UHS is governed by the unique physicochemical properties of H₂ (Table 2). Its minimal molecular size enables high diffusion coefficients in geological media (Thiyagarajan et al., 2022; Al-Shafi et al., 2023), while its exceptional low density and viscosity enhance fluid mobility and gravitational segregation (Cachadiña et al., 2022). Although favorable for recovery efficiency, these characteristics increase leakage risks. Storage security depends on balancing H₂ buoyancy against caprock capillary entry pressure, defining maximum storage depths (Iglauer, 2022).

H₂ exhibits contrasting energy density characteristics: high gravimetric but low volumetric density necessitates larger storage volumes than methane. Solubility in formation fluids presents another loss pathway, being temperature-, pressure-, and salinity-dependent (Muhammed et al., 2022), with significantly higher solubility in residual hydrocarbons than brine. This characteristic is particularly relevant for depleted hydrocarbon reservoirs. To manage rapid pressure depletion during withdrawal, CH₄ or CO₂ cushion gases maintain reservoir stability (Saeed and Jadhawar, 2024). Predicting complex multiphase flow requires advanced equations of state specific to UHS conditions (Hassannayebi et al., 2019; Lao et al., 2024). Future work should refine dynamic storage capacity and safety thresholds through integrated numerical simulations coupling H₂S unique properties with site-specific geology.

2.2 Reservoir characteristics influencing hydrogen flow

The macroscopic flow of H₂ follows pressure gradients and Darcy's law, while the flow dynamics are also controlled by reservoir structure, petrophysical properties and in-situ conditions. Understanding these factors is essential for assessing the feasibility and safety of high-pressure H₂ storage.

2.2.1 Key governing factors and interplay

The efficiency and security of UHS are governed by a complex interplay of geochemical and physicochemical factors. These include geochemical parameters (pH, pE), salinity and ionic composition, and the coupled effects of pressure and temperature, which collectively control the migration, trapping and potential losses of H₂ within subsurface formations, as shown in Fig. 3(a). The dominant mechanisms and their impacts across different reservoir types are synthetically summarized

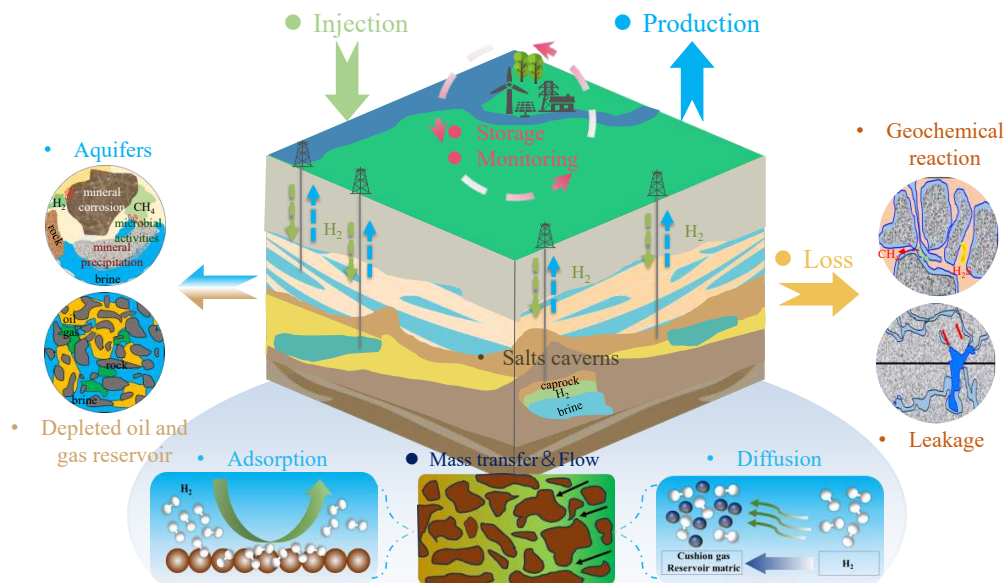


Fig. 2. Flowchart of UHS and analysis of key challenges and processes.

Table 2. Comparison of physical properties of H₂, CO₂ and CH₄ (Al-Yaseri et al., 2022; Muhammed et al., 2022; Rezk and Adebayo, 2024).

Parameter	H ₂	CO ₂	CH ₄
Molecular weight (g/mol)	2.016	44.01	16.043
Density (kg/m ³)	0.082	1.98	0.657
Volumetric energy density (MJ/m ³)	10.8-12.7	/	35.8-39.8
Gravimetric energy density (MJ/kg)	120-141.7	/	50-55.5
Diffusion coefficient in air (cm ² /s)	0.756	0.16	0.21
Solubility in water (g/100g)	0.00016	0.169	0.0023
Viscosity (Pa·s)	8.76×10^{-6}	1.46×10^{-5}	1.10×10^{-5}

The default conditions for all parameters are 298.15 K and 0.1 MPa.

in Table S1.

Salinity and ionic composition are vital influential factors of geochemical and multiphase behavior in subsurface H₂ systems. Elevated salinity increases formation water density and viscosity, thereby reducing reservoir permeability and impeding H₂ flow (Rezaei, 2022). Meanwhile, ionic characteristics further modulate H₂ behavior. Cl⁻ demonstrates stronger adsorption than Na⁺, while variations in K⁺, Mg²⁺, and Ca²⁺ alter mineral dissolution equilibria (Figs. 3(b) and 3(d)). These geochemical processes are fundamental controls of UHS performance, as they govern the spatial distribution of H₂ saturation and critically impact the final recovery factor (Fig. 3(c)). Quantifying the relationships between these controlling factors and H₂ flow dynamics is essential for optimizing storage efficiency in aqueous reservoirs.

The coupled effects of pressure and temperature are fundamental, with interfacial tension (IFT) serving as a key property linking these variables to H₂ behavior (Fig. 4(a)). IFT, which controls H₂ distribution and capillary trapping, decreases with

increasing temperature and pressure, with temperature exerting a more pronounced effect (Fig. 4(b)) (Young, 1805; Esfandiyari et al., 2022). While rising pressure and temperature promote favorable wetting conditions and can enhance H₂ adsorption in organic-rich reservoirs, lower reservoir pressures significantly increase leakage risk (Arif et al., 2022; Esfandiyari et al., 2022). Consequently, most UHS systems are optimally operated within specific pressure-temperature ranges to balance storage density and reservoir integrity, necessitating the site-specific consideration of geothermal gradients and rock mechanics.

2.2.2 Rock types and mineral composition

The physicochemical properties of different rock types govern the behavior of H₂ in terms of storage, migration and retention within subsurface reservoirs (Perera, 2023). Sandstone typically exhibits high porosity and permeability, facilitating H₂ transport and recovery; however, CT scans reveal that H₂ predominantly occupies larger pores, while smaller pore throats remain brine-saturated, limiting the ef-

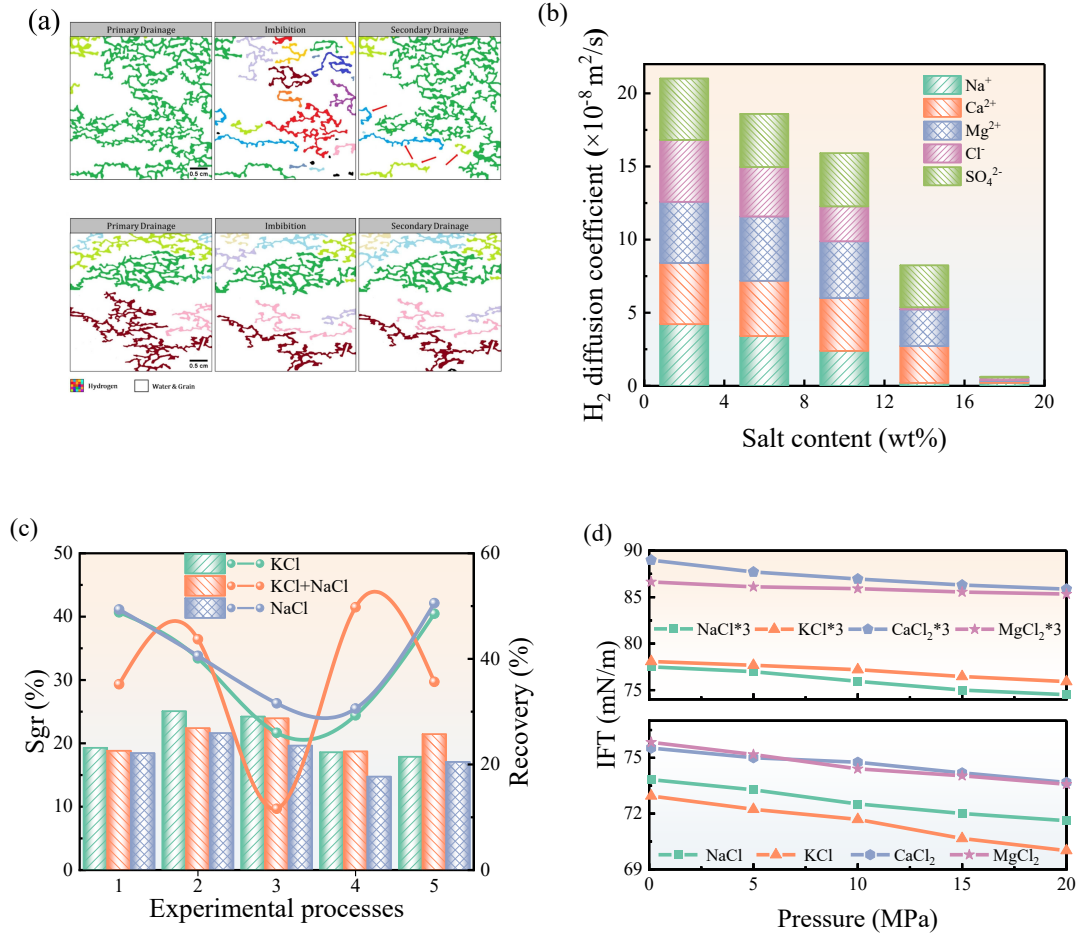


Fig. 3. Multiscale effects of salinity and ion type on H₂ behavior in porous media. (a) Capillary trapping of H₂ (Bahrami et al., 2024) (adapted from Bagheri et al. (2023), with permission); (b) H₂ diffusion coefficient under different ion contents (Li et al., 2024b); (c) Residual H₂ saturations and recovery for subsequent cycles (Bhimineni et al., 2023; Medina et al., 2024); (d) Relationship between ion and interfacial tension (IFT) (Chow et al., 2018; Hosseini et al., 2022b; Janjua et al., 2024).

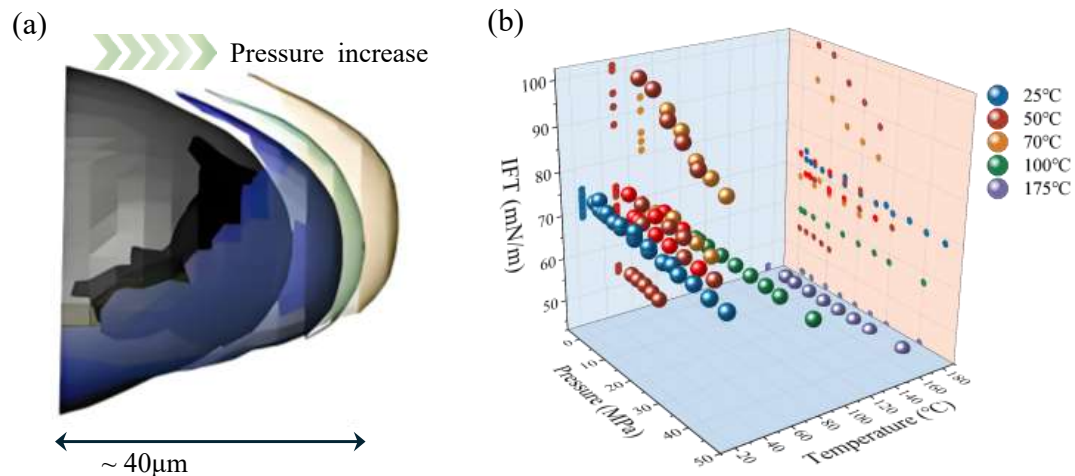


Fig. 4. Effect of temperature and pressure on the UHS process. (a) Interface progression at different pressures (Dokhon et al., 2024); (b) Relationship between pressure/temperature and IFT (Chow et al., 2018; Alanazi et al., 2023).

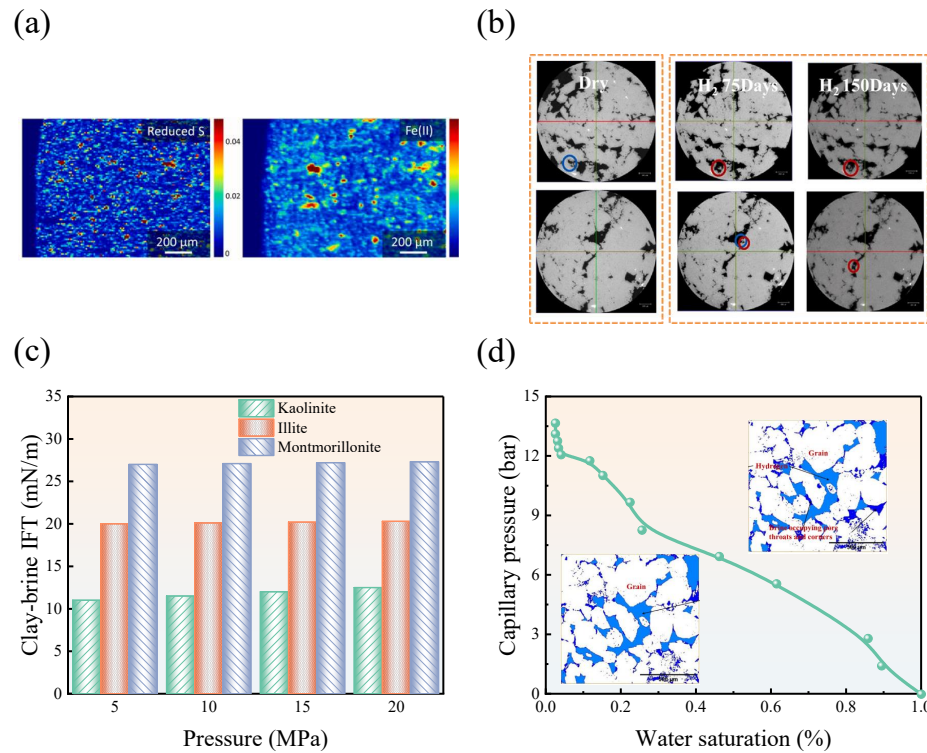


Fig. 5. Characterization of different rock types. (a) Insignificant shale alteration (Rooney et al., 2024); (b) Possible mineral dissolution/precipitation within the dolomite matrix (Al-Yaseri et al., 2024b); (c) Different clay-brine IFT as a function of H₂ pressure (Yekeen et al., 2022); (d) Schematic of sandstone capillary pressure distribution curve and H₂ saturation variation (Jha et al., 2021; Al-Yaseri et al., 2024a).

fective gas mobility (Fig. 5(a)) (Kumar et al., 2021; Zeng et al., 2023a). Meanwhile, carbonate rocks generally have lower porosity and permeability, though fracture networks can provide viable storage space. High temperatures inhibit calcite-H₂ interactions, whereas elevated pressures promote reactions between the rock and gas phases (Figs. 5(b) and 5(c)) (Aslannezhad et al., 2023). Clay minerals, as common cementing materials, significantly influence reservoir mechanical behavior, with their impact intensity following the order of montmorillonite > illite > kaolinite, as shown in Fig. 5(c) (Li et al., 2023). The strong hydrophilicity of these minerals also affects H₂ adsorption and flow efficiency. In terms of wettability, sandstone is typically strongly water-wet (Fig. 5(d)) (Zhao et al., 2011), which favors H₂ capillary trapping. As water saturation increases, the relative permeability of H₂ decreases, suppressing viscous fingering but also increasing residual gas saturation (Fig. 5(d)) (Rezaei, 2022).

In summary, sandstone and carbonate rocks as potential reservoirs exhibit complementary characteristics: sandstone possesses excellent storage and transport capacity but low microscopic pore utilization efficiency, while carbonate rocks rely on fracture systems where temperature and pressure conditions significantly regulate their interaction with hydrogen. Reservoir selection requires comprehensive consideration of macroscopic storage-permeability performance, microscopic pore-throat structure, fluid dynamics, and rock-gas interaction

mechanisms.

2.3 Mass transfer mechanisms of hydrogen

In UHS, mass transfer encompasses the microscale distribution and migration of H₂ via diffusion, adsorption and desorption. These processes govern the spatial distribution of H₂ and determine the storage capacity and transport efficiency of the system, particularly in formations with high specific surface area (Perera, 2023). A thorough understanding of these mechanisms and their controlling factors is essential for optimizing UHS performance.

2.3.1 Diffusion and penetration in porous media

Subsurface rock formations exhibit heterogeneous pore structures, including micropores, fractures and larger interconnected voids (Fig. 6(a)). After injection stops, H₂ plume migration and mixing are governed by molecular diffusion, concentration-driven mutual diffusion and mechanical dispersion due to subsurface heterogeneity. The H₂ diffusion coefficient is primarily controlled by porosity, pore connectivity, and the effective molecular diffusion coefficient (Figs. 6(c) and 6(d)).

Molecular dynamics simulations show that H₂ diffusion in water-saturated clay minerals, which are common components of caprocks, is significantly influenced by the type of exchangeable cations and the distribution of layer charges

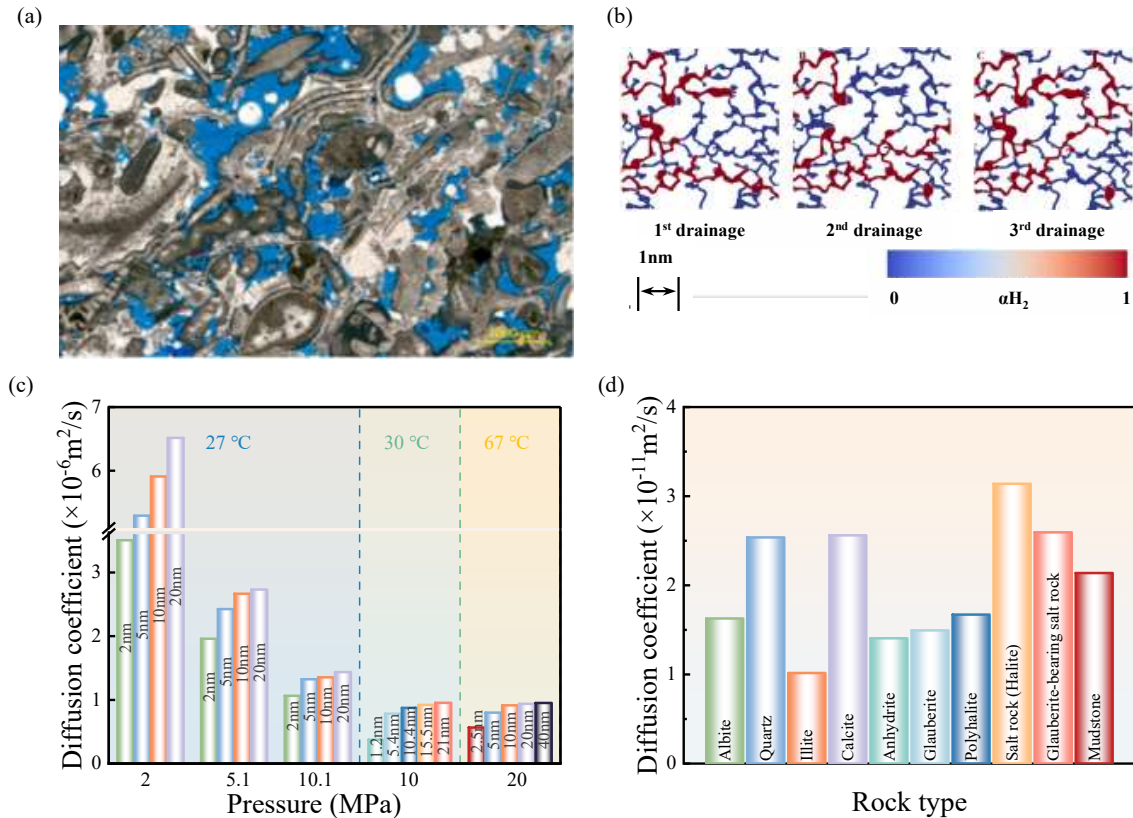


Fig. 6. Micro-scale motion images of H₂ porous media. (a) Pore cross-section of carbonate sample (Rezk and Adebayo, 2024); (b) H₂ diffusion pathway (Bagheri et al., 2023) (adapted from Bagheri et al. (2023), with permission); (c) Diffusion coefficient of H₂ in different pore sizes (A et al., 2024; Oliver et al., 2024; Shang et al., 2024); (d) Diffusion coefficients in different rocks (Song et al., 2024).

(Heinemann et al., 2021). Diffusion pathways are also affected by the capillary number, as shown in Fig. 6(b). In highly permeable samples under low flow rates, the wetting phase moves through smaller pores, bypassing larger H₂ clusters. Trapped H₂ ganglia can obstruct flow paths, isolating gas bubbles and preventing reconnection with the continuous gas phase (Bagheri et al., 2023). Consequently, highly permeable rocks facilitate more efficient H₂ diffusion and migration (Jangda et al., 2023). Future research should focus on refining existing experimental and numerical methods to accurately predict H₂ diffusion dynamics in confined media. Optimizing injection strategies, such as permeability-based rate adjustment and diffusion coefficient calibration, to closely match aqueous-phase values can significantly improve storage efficiency.

2.3.2 Adsorption kinetics and surface interactions

H₂ adsorption during UHS significantly influences both storage capacity and transport dynamics. This process is particularly critical in reservoirs with high specific surface area and is strongly dependent on pressure and the composition of cementing materials (Perera, 2023; Feng et al., 2024) (Fig. 7(a)). Molecular-scale studies revealed that in pores larger than 5 nm, most H₂ remains in the bulk phase, resulting in negligible adsorption loss (Shang et al., 2024); thus, formations

with dominant pore sizes exceeding 5 nm are considered more suitable for UHS, as depicted in Figs. 7(b) and 7(d). However, competitive adsorption with cushion gases like CH₄ or CO₂ occurs in confined nanopores. While pure H₂ exhibits higher adsorption capacity, pore surfaces often have a preferential affinity for CO₂ or CH₄, which can enhance H₂ desorption and reduce the overall H₂ storage capacity (Fig. 7(c)) (Oliver et al., 2024; Zhang et al., 2024). For most mineral surfaces, adsorption capacity is primarily governed by pressure, which significantly enhances H₂ uptake, whereas temperature exerts an opposite effect, reducing adsorption and thus storage efficiency. Therefore, a precise evaluation of H₂ adsorption behavior under specific reservoir conditions is essential for optimizing storage formation design and improving UHS performance.

3. Stability in UHS

The long-term stability of UHS systems is critical to their viability as large-scale energy storage solutions. This encompasses a range of factors, including material durability under prolonged exposure, adaptability to dynamic reservoir conditions, risks of H₂ leakage and biogeochemical consumption, as well as challenges related to H₂ cycling efficiency and recovery.

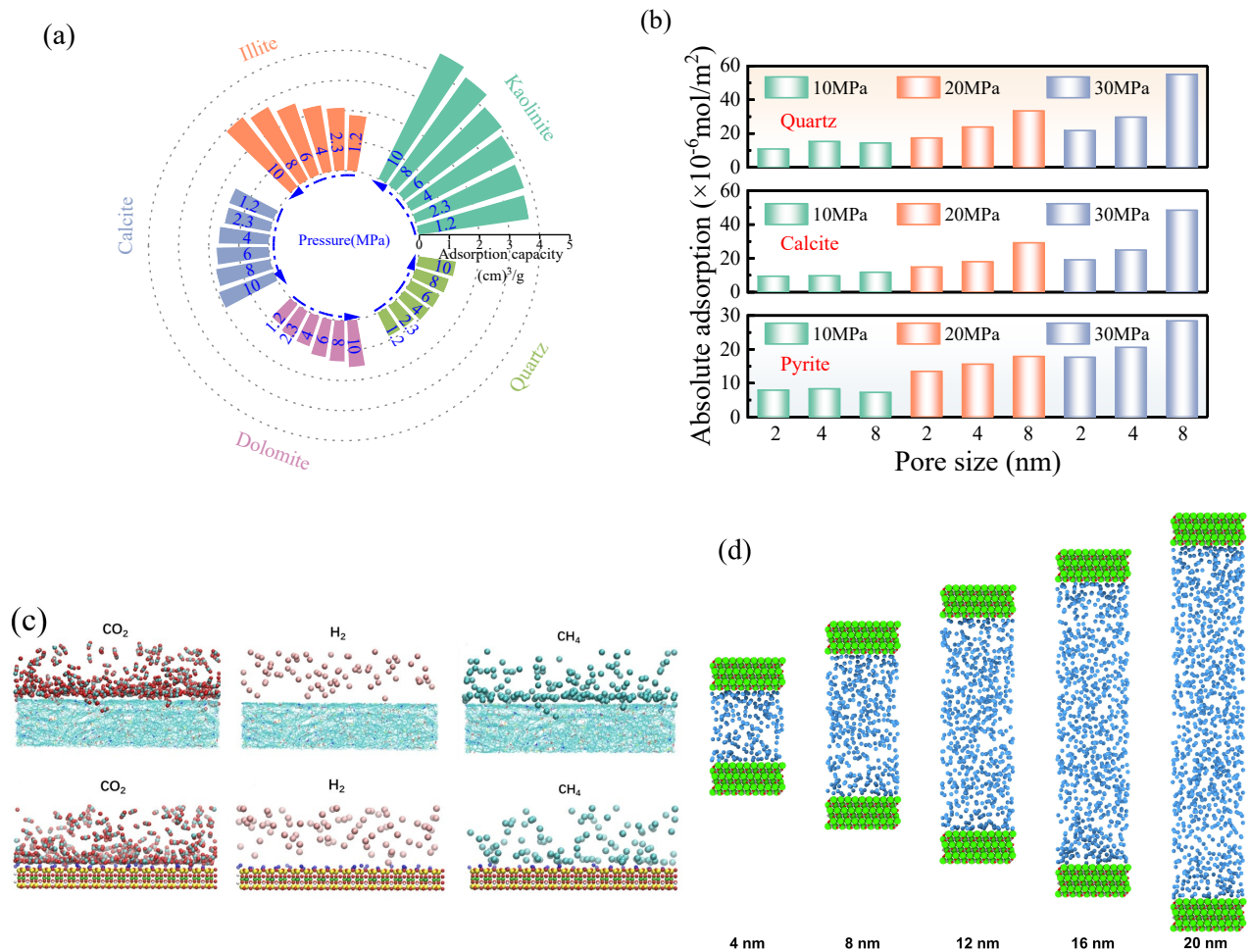


Fig. 7. Comparison of competitive adsorption of different gases. (a) Adsorption capacity of H_2 under different rocks (Zhao et al., 2025); (b) Adsorption capacity of H_2 at different rock pore sizes (Oliver et al., 2024; Lee et al., 2025); (c) Molecular distribution on the surfaces of casein and MMT (Zhang et al., 2024); (d) H_2 diffusion through carbonate slits of different pore sizes (Li et al., 2024b).

3.1 Wellbore integrity and near-wellbore sensitivity

Underground hydrogen storage operations cyclically impact wellbore integrity through H_2 embrittlement of metals and cement degradation. Repeated injection and extraction weaken well systems, potentially causing crack propagation and zonal isolation failure (Bo et al., 2021; Ramesh Kumar et al., 2023).

Nanoparticle additives like SiO_2 and Al_2O_3 improve cement crack resistance, though TiO_2 agglomeration at high concentrations reduces strength (McElroy et al., 2021). H_2 's high diffusivity enables microdefect penetration, accelerated when mixed with CH_4 cushion gas (Bo et al., 2021). Long-term H_2 exposure induces bubble accumulation and cement weakening, while redox-sensitive minerals like hematite undergo reductive dissolution (Hussain et al., 2022). Sulfate-reducing bacteria near the wellbore promote sulfide precipitation, enhancing corrosion and reducing permeability (Amirthan and Perera, 2023). External factors such as 5%-25% salt concentrations enhance cement properties, whereas oil-based mud causes strength

degradation (Arbad and Teodoriu, 2020; Arbad et al., 2021). While short-term high-pressure H_2 exposure shows minimal steel degradation (Boersheim et al., 2019), long-term blistering and embrittlement risks persist. Defective cement poses greater immediate concern, with estimated annual leakage rates of 0.1%-10% potentially forming flammable H_2 -air mixtures (4%-75% vol) and creating explosion hazards (Abohamzeh et al., 2021; Hematpur et al., 2023).

Near-wellbore redox reactions involving H_2/H_2O impair cement sealing, influenced by solubility, water saturation, mineralogy, and environmental parameters. Although microbial activity accelerates degradation, minerals like manganese carbonate and calcite can mitigate damage (McElroy et al., 2021). Reactive minerals including carbonates, sulfides, and pH-sensitive clays adversely affect formation stability (Hussain et al., 2022). Such instability may cause downhole failures, fluid release, and reduced storage efficiency (Tarkowski, 2019). Future research should focus on alternative cement formulations, slurry properties, and chemical admixtures for long-term integrity enhancement.

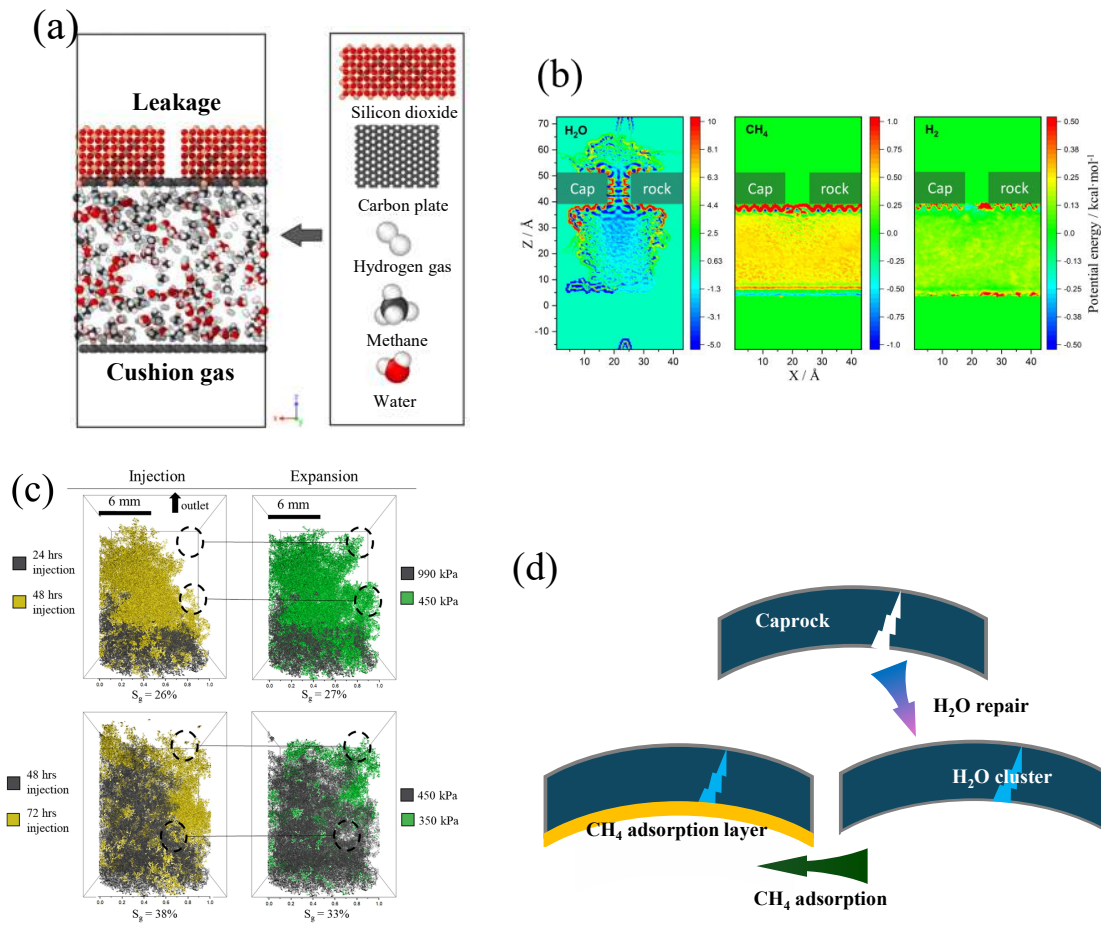


Fig. 8. Molecular diffusion of H_2 in a porous medium. (a) Molecular model of the H_2 leakage system (Liu et al., 2024a); (b) Potential energy contour plots (Liu et al., 2024a); (c) H_2 diffusion expansion (Dokhon et al., 2024); (d) Schematic of H_2O and CH_4 sealing mechanism for inhibiting H_2 leakage (Liu et al., 2024a).

3.2 Stability during hydrogen storage

Reservoir-stored H_2 can be depleted via two main pathways: physical leakage and geochemical interactions with in-situ gases and minerals. Both processes can alter critical reservoir characteristics, potentially compromising formation integrity and overall storage performance.

3.2.1 Chemical reactions and H_2 consumption

Under typical underground hydrogen storage conditions, abiotic reactions require extreme environments including temperatures exceeding 100°C , pressures above 15 MPa, and salinities beyond 288 g/L to proceed measurably over extended durations, particularly in pyrite-rich formations (Amirthan and Perera, 2023). The chemical behavior of H_2 in porous media is mainly governed by mineral dissolution processes within the H_2 -brine-mineral system.

Geochemical interactions trigger redox and dissolution-precipitation reactions that promote H_2 dissociation, leading to substantial hydrogen loss and mineral alteration (Hassanayebi et al., 2019). Although mineral dissolution improves rock porosity and permeability, it undermines granular cementation, which reactivates microfractures and jeopardizes

both formation integrity and long-term containment security (Jacquemet, 2021). Such alterations often create dissolution channels that serve as preferential leakage pathways, accelerating further dissolution-precipitation cycles and ultimately degrading reservoir mechanical strength (Zeng et al., 2023b).

Simulations demonstrate that quartz and silicate minerals exhibit minimal reactivity with H_2 , maintaining high stability in brine environments. Clay minerals (kaolinite, montmorillonite, illite) show negligible dissolution over 30-year periods, suggesting limited impact on caprock integrity (Zeng et al., 2023a).

In calcareous shales, calcite reductive dissolution by aqueous H_2 weakens grain structure and increases sand production risk (Sekar et al., 2023). Although only 0.003% calcite dissolves over 30 years, its high volumetric proportion (up to 82.16%) raises concerns for long-term caprock stability in large-scale UHS (Bo et al., 2021). Minor precipitation of secondary minerals (calcium feldspar, pyrrhotite, schistose zeolite) exerts negligible influence on overall integrity due to low abundance and solubility (Gholami, 2023). While chemical consumption of H_2 through microbial or mineral reactions is not the primary loss mechanism in UHS, it can significantly impact storage efficiency and safety under specific reservoir

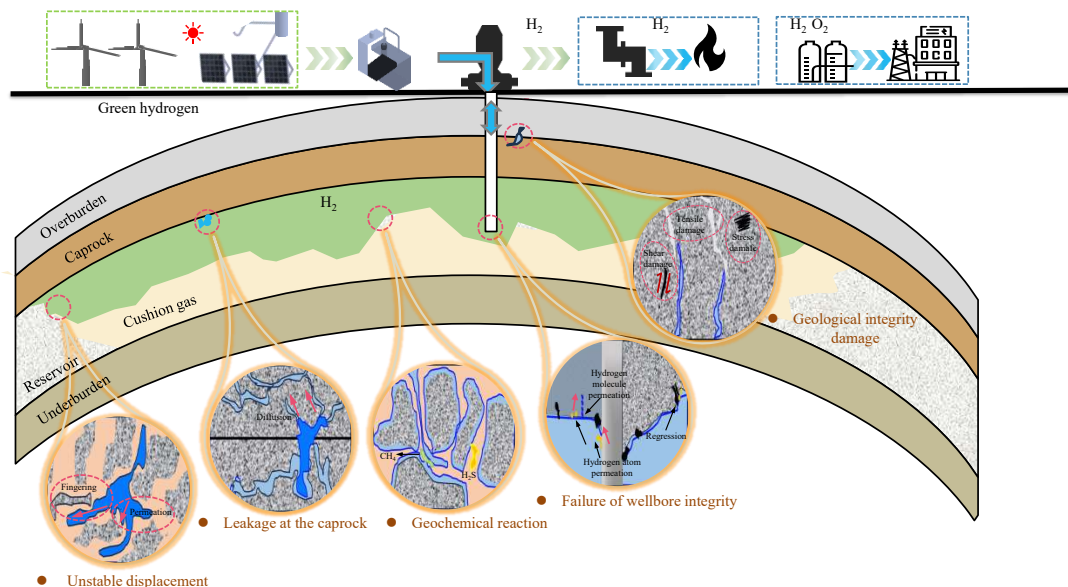


Fig. 9. Geologic uncertainty of H₂ storage in porous media (Zeng et al., 2023b).

conditions. Optimization of temperature, pressure, and pH parameters can effectively minimize these chemical losses and enhance overall storage performance.

3.2.2 Physical leakage pathways

Compared to chemical reactions, H₂ is more prone to physical leakage during UHS, which primarily occurs through diffusion, permeation or seal failure, posing significant environmental and safety risks (Heinemann et al., 2021). Owing to its low molecular weight, H₂ exhibits high diffusivity (Figs. 8(a) and 8(c)). Molecular diffusion, though slower than advection, becomes dominant during idle periods, with an effective diffusion coefficient influenced by porosity, saturation and pore structure (Feldmann et al., 2016). In depleted reservoirs, H₂ interphase diffusion leads to mixing with cushion gases (e.g., CO₂, CH₄), reducing recovery purity. One field test recorded 84.3% H₂ recovery after 285 days using CO₂ as cushion gas, with traces of CH₄ suggesting microbial activity consuming H₂ (Hellerschmied et al., 2024). Future studies should clarify the feasibility of H₂ co-storage and biogeochemical boundaries. Caprock integrity is critical in preventing upward leakage. Under reservoir conditions, most caprock minerals are water-wet, enhancing residual trapping. The coexistence of CH₄ and H₂O can form a mixed barrier that effectively suppresses H₂ migration through nanoscale defects (Figs. 8(b) and 8(d)). However, pressure cycling during UHS can induce damage in the caprock and reservoir, especially in shallow (tensile) or deep (shear) settings, potentially reactivating fractures or faults (Fig. 9) (Zeng et al., 2023b).

3.3 Safety of H₂ recovery

In UHS operations, the primary focus remains on injected H₂ volume and recovery efficiency. Certain key factors such as reservoir capacity, injection-production strategies, and cushion gas selection critically govern both the safety and economic

viability of H₂ storage.

3.3.1 Criteria for storage site suitability

Geologic complexity often leads to H₂ retention and lower recovery, whereas highly permeable formations with strong pore connectivity enhance H₂ productivity and reduce extraction costs (Zhao et al., 2024). Salt caverns, aquifers, and depleted oil and gas reservoirs represent the main UHS options. As shown in Fig. 10(a), salt caverns under medium-to-low pressure conditions facilitate rapid withdrawal and achieve high recovery rates of 80%-95%. Meanwhile, aquifers, though lower in pressure, are more influenced by cushion gas and typically yield 60%-80% recovery. Depleted oil and gas reservoirs, which host 74% of global UHS projects, offer recovery rates of 70%-90% and are well-suited for large-scale, long-term storage (Fig. 10(b)) (Zamehrian and Sadaee, 2022; Wang et al., 2024a; Leng et al., 2025). Therefore, an optimal storage site should combine high porosity for capacity with high permeability for flow efficiency while ensuring a well-balanced fracture network to minimize leakage and maximize overall storage performance.

3.3.2 Flexibility in injection and extraction strategies

A portion of injected H₂ becomes irreversibly trapped through pore-scale mechanisms and fluid interactions. Injection strategy strongly influences distribution and recovery: top-layer injection creates higher gas saturation in upper zones but underutilizes deeper regions, reducing overall recovery compared to fully perforated well schemes (Fig. 11(a)). Grid-based modeling reveals substantial pore-space underutilization, with approximately 10% of pores maintaining H₂ concentrations below 1% during injection, while about 5% of pore volume retains over 1.5% H₂ during production (Wang et al., 2024b). Cyclic operations are affected by permeability hysteresis and pressure effects. Ignoring relative permeability

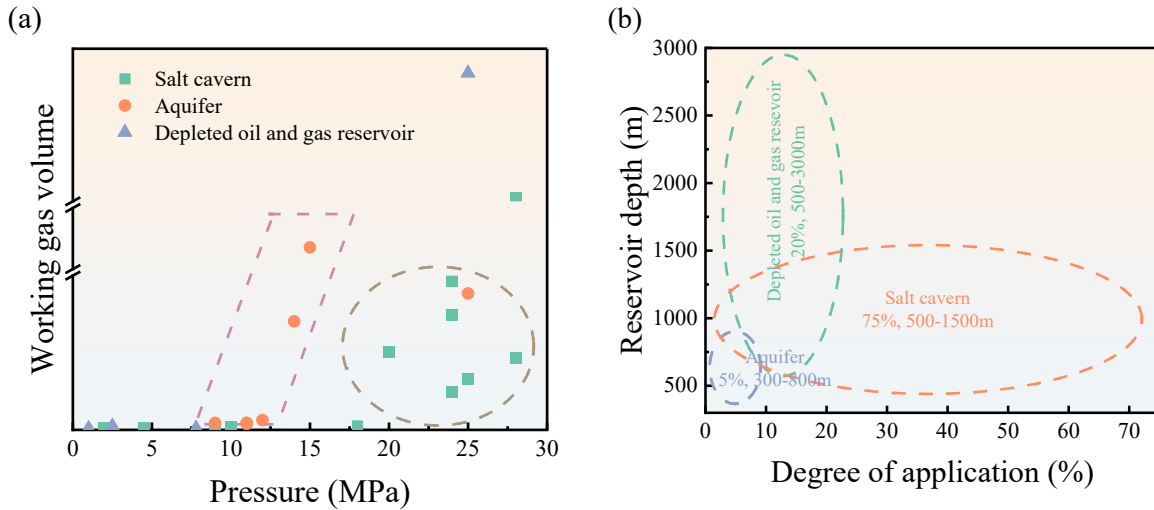


Fig. 10. UHS different reservoir types (Sekar et al., 2023; Zhu et al., 2023; Li et al., 2024a; Sadkhan and Al-Mudhafar, 2024; Jia et al., 2025; Leng et al., 2025). (a) Reserves of reservoir types under different working pressures; (b) Percentage and depth of application of the three reservoir types.

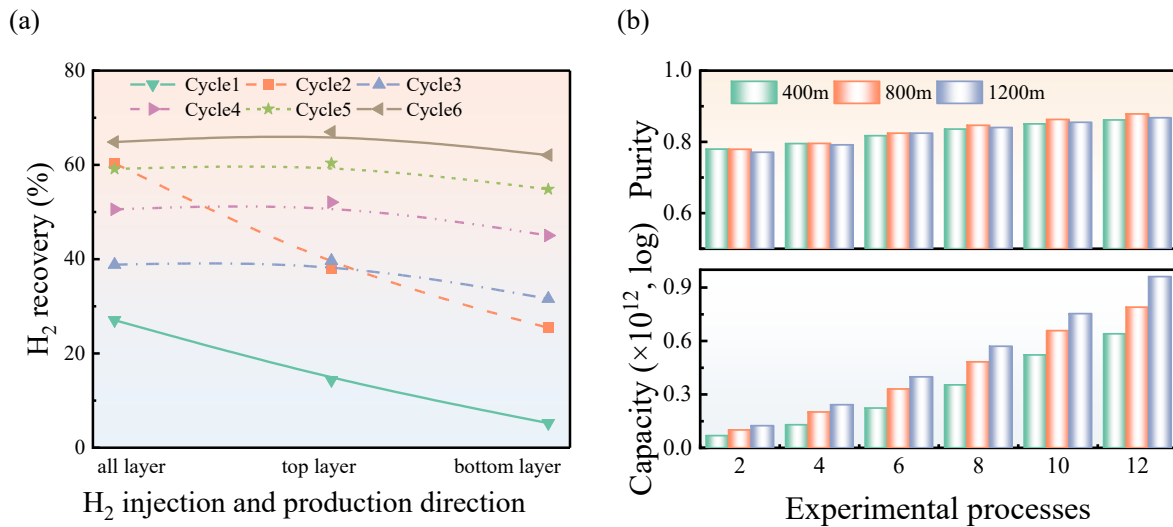


Fig. 11. UHS performance curves for different injection and extraction cycles. (a) H₂ recovery of different programs under different cycles (Zamehrian et al., 2024); (b) Performance predictions for different well spacing distances (Indro et al., 2025).

hysteresis leads to uniform recovery distribution, while higher pressure at depth increases H₂ viscosity, moderately slowing injection and production rates (Rezaei, 2022). Extended injection-production cycles enhance H₂ retention in aquifers while improving recovery efficiency over multiple cycles (Fig. 11(a)), with optimized production durations further boosting output.

Following repeated cycles, residual H₂ persists as cushion gas due to rock-fluid interactions. Although later cycles achieve improved purity and capacity with wider well spacing (Fig. 11(b)), inter-well trapping constrains efficiency. For long-term UHS operation, recovery rates should be dynamically adjusted according to residual gas concentrations, with shorter cyclic phases recommended to maximize overall recovery

performance.

3.3.3 Optimization of cushion gas distribution

Cushion gas (CG) is essential for maintaining reservoir pressure, stabilizing H₂ distribution and ensuring operational safety during H₂ storage cycles. It mitigates rapid pressure drops during extraction and moderate temperature fluctuations, thereby protecting storage integrity (Bahrami et al., 2023). The required CG volume varies significantly across reservoir type: approximately 30% in salt caverns, 40%-50% in porous rocks, 50%-60% in depleted hydrocarbon reservoirs, and up to 80% in aquifers (Bünger et al., 2016; Muhammed et al., 2022; Muhammed et al., 2023). The choice of CG significantly affects H₂ recovery and purity. While pure H₂

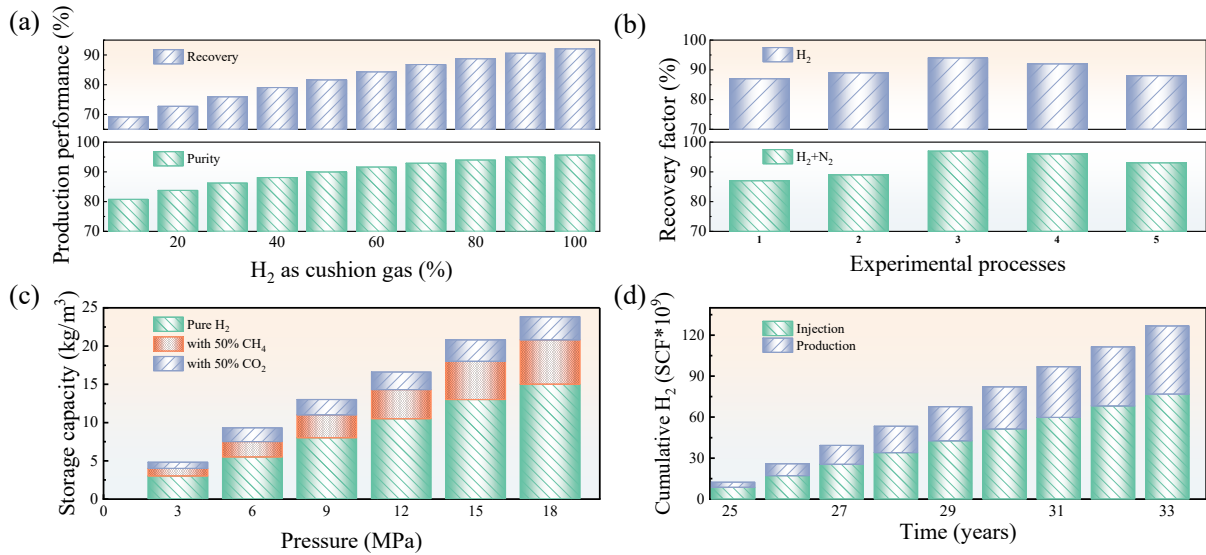


Fig. 12. Effect of cushion gas on H₂ recovery. (a) Effect of H₂ cushion gas injection on the production performance (Ramsari et al., 2025); (b) H₂ recovery factor in different cycles (Bahrami et al., 2023); (c) H₂ storage capacity at various pressure conditions (Zhang et al., 2024); (d) Basic case of H₂ injection/production during UHS (Zamehrian and Sedaei, 2022).

as CG maximizes output purity, it is less economical (Fig. 12(a)). Alternative gases including N₂, CH₄ and CO₂ offer cost advantages, with CO₂ also providing carbon sequestration benefits (Jahanbakhsh et al., 2024; Zhang et al., 2024). As shown in Figs. 12(b) and 12(c), molecular simulations indicate that CO₂ may perform better than CH₄ in terms of storage capacity under varying pressure and compositions. Multi-cycle studies revealed that N₂ yields the highest H₂ recovery, whereas CO₂ results in the lowest recovery but supports carbon reduction goals. Over multiple cycles, H₂ recovery and purity generally improve; however, progressive mixing with CG reduces the volumetric energy density of the produced gas (Fig. 12(d)). In practice, selecting the optimal cushion gas requires balancing technical, economic and environmental factors to maximize the overall performance of the UHS project in question.

4. Challenges and future development trend

4.1 Current challenges and research gaps

UHS represents a promising technology for supporting the hydrogen economy and clean energy transition. However, several critical challenges must be addressed before its widespread deployment:

Long-term storage stability remains a primary concern, as repeated injection-production cycles induce pressure and temperature fluctuations that can cause rock fatigue, fault reactivation, and microfracture development in caprocks and wellbores, potentially compromising containment integrity (Ramesh Kumar et al., 2023; Ren et al., 2025).

At the microscale, insufficient understanding of H₂ flow mechanisms and biogeochemical interactions poses significant limitations. Subsurface microorganisms can metabolize H₂, producing methane or hydrogen sulfide, which not only reduces gas recovery but also degrades gas quality (Tarkowski

, 2019; Jacquemet, 2021).

Containment security is further challenged by H₂'s high diffusivity and low viscosity, increasing leakage risks through caprocks and faults. Additionally, hydrogen embrittlement threatens the mechanical integrity of metal well components, raising long-term reliability concerns.

4.2 Promising research directions and future outlook

Future research should be guided by addressing the aforementioned challenges through interdisciplinary collaboration. The following prioritized directions are recommended to advance UHS toward maturity and scalability:

Advanced modeling and monitoring: Developing integrated monitoring and modeling tools to predict reservoir behavior in real time and assess long-term stability.

In-situ experimental validation: Conducting in-situ experiments under realistic formation conditions to validate models and clarify biogeochemical pathways.

Cushion gas and additive engineering: Engineering advanced cushion gas systems and functional additives (e.g., nanoparticles) to control H₂ mobility and improve recovery efficiency.

Pore-scale simulation: Applying pore-scale simulations, such as molecular dynamics, to elucidate H₂ transport and trapping mechanisms in confined porous media.

5. Summary

UHS represents a crucial enabling technology for large scale renewable energy integration, with demonstration projects already implemented in multiple countries. However, most UHS approaches remain in early development phases, with significant knowledge gaps regarding long term impacts

on reservoir integrity, microbial ecology, and hydrogen loss pathways. Addressing these challenges requires fundamental research and comprehensive feasibility studies to optimize operational parameters and ensure storage security in complex geological environments.

This review systematically analyzes UHS challenges through integration of subsurface engineering data, experimental findings, and computational modeling results. Multiscale assessment reveals distinctive hydrogen behavior in porous media, where exceptional diffusivity and permeability create unique transport dynamics compared to conventional gases. Phase behavior under reservoir conditions significantly influences storage performance, while geochemical interactions with formation minerals and fluids present potential threats to seal integrity. These factors collectively elevate containment risks, particularly in heterogeneous formations.

Recovery efficiency emerges as a key performance indicator, governed by geological constraints, operational parameters, and management protocols. Comparative analysis of hydrogen properties against conventional gases provides essential insights for storage design optimization and cushion gas selection. Priority research directions should focus on integrating advanced monitoring technologies with high fidelity numerical simulations, while developing robust risk assessment methodologies. Significant understanding gaps persist regarding abiotic hydrogen reactions under actual storage conditions, as current knowledge derives largely from non UHS contexts. Elucidating hydrogen transport mechanisms in subsurface environments remains fundamental to technology advancement and sustainable energy transition support.

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Supplementary file

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Conflict of interest

The authors declare that they do not have any conflict of interest or personal relationships that could have influenced the work reported in this paper.

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