

## Original article

# Subsurface storage of CO<sub>2</sub>, H<sub>2</sub>, and natural gas: A review of site-selection criteria and decision-support approaches

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### Keywords:

Multi-criteria decision-making  
geographic information system  
machine learning  
energy storage systems  
geologic gas storage  
underground gas storage

### Cited as:

Duah, P., Johnson, M. B., Aryana, S.  
A. Subsurface storage of CO<sub>2</sub>, H<sub>2</sub>, and  
natural gas: A review of site-selection  
criteria and decision-support approaches.  
*Advances in Geo-Energy Research*, 2026,  
20(3): 277-293.  
<https://doi.org/10.46690/ager.2026.06.08>

### Abstract:

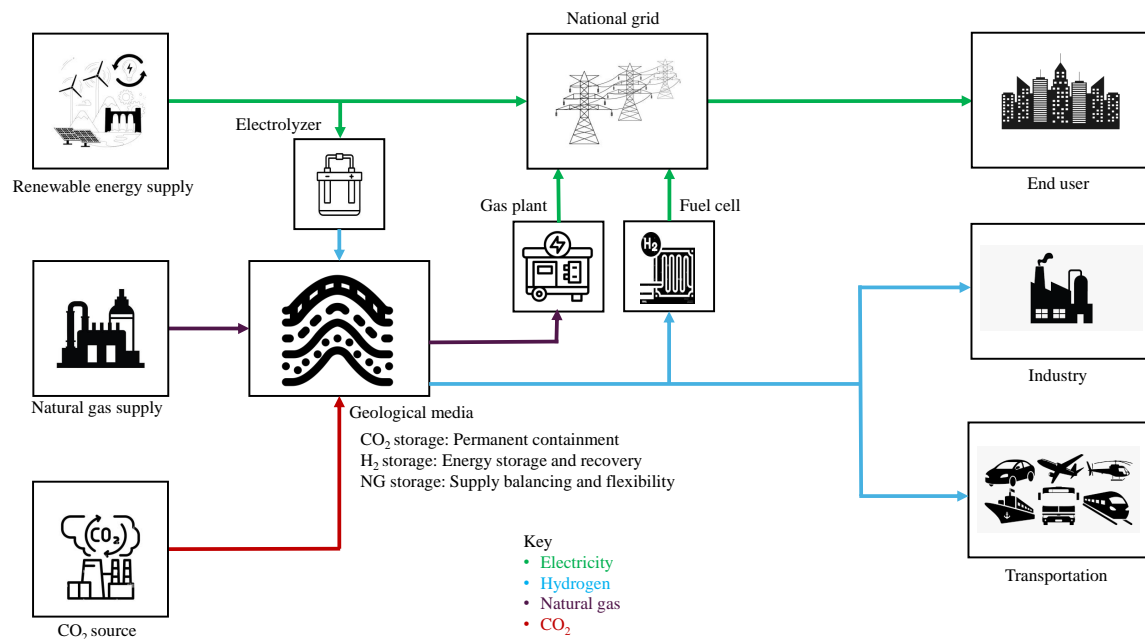
The transition to a low-carbon energy system and the emergence of a hydrogen economy have increased the need for large-scale, reliable subsurface storage of carbon dioxide, hydrogen, and natural gas. Selecting suitable storage sites requires balancing geological, technical, environmental, economic, and social criteria, while accounting for the distinct physical and chemical behaviors of each gas and the intended service. This paper adopts a unified, gas-aware framework to synthesize site-selection criteria and decision-support methods for subsurface gas storage across the principal geological options: deep saline aquifers, depleted hydrocarbon reservoirs, and salt caverns. The study examines decision-making approaches ranging from conventional multi-criteria decision-making and fuzzy extensions to Geographic Information System-based spatial analysis, reservoir simulation, and emerging machine-learning techniques for large-scale screening and uncertainty quantification and mitigation. Drawing on global case studies, it identifies methodological limitations, gas-specific knowledge gaps, and data challenges that constrain confident site selection, particularly for hydrogen storage in deep saline aquifers and depleted reservoirs, including reactivity and microbial consumption risks, purity and mixing constraints, and cushion-gas economics. Future directions emphasize the need for integrated, explainable, and adaptive decision frameworks tailored to gas-specific behaviors and storage contexts; expanded large-scale H<sub>2</sub> demonstrations in saline aquifers and depleted reservoirs; tighter coupling of monitoring, modeling, and decision tools throughout the project lifecycle; and regulatory frameworks that clarify long-term liability and strengthen public engagement and trust. Collectively, these insights provide a structured basis for developing robust and transparent decision pathways for strategic subsurface storage in support of energy-transition objectives.

## 1. Introduction

As the global energy sector shifts towards low-carbon and hydrogen-based energy systems, the need for reliable, large-scale subsurface storage of gases such as carbon dioxide (CO<sub>2</sub>), hydrogen (H<sub>2</sub>), and natural gas (NG) has increased significantly. These gases play different roles in the energy transition as summarized in Fig. 1.

Selecting an appropriate storage site requires integrating

geological, techno-economic, environmental, and regulatory factors (Van Rooijen and Hajibeygi, 2025). Geological formations, such as deep saline aquifers (DSA), depleted hydrocarbon reservoirs, and salt caverns, are the primary candidates for large-scale gas storage, each with distinct operational characteristics and associated uncertainties (Sadkhan and Al-Mudhafar, 2024). Gas-specific behavior further complicates site selection process, as storage performance and risks vary across the gas systems. Therefore, site selection approaches



**Fig. 1.** Integrated pathways for CO<sub>2</sub>, H<sub>2</sub>, and NG within the energy system.

must be flexible and explicitly account for gas-specific behavior within a unified evaluation framework. Traditional site screening methods must be complemented by advanced decision-support tools which can manage uncertainty and improve the transparency and consistency of site selection.

Recent reviews have advanced the field by proposing CO<sub>2</sub>-specific site selection workflows (Rashidi et al., 2025), criteria-based screening frameworks for underground hydrogen storage in porous media (Van Rooijen and Hajibeygi, 2025), and broader assessments of hydrogen storage technologies and challenges (Davoodi et al., 2025). However, these studies are primarily developed within single-gas contexts or specific storage settings, and while they incorporate multiple criteria or methods, they do not explicitly provide a unified structure for cross-gas comparison and integrated decision-making across gas systems.

This review adopts a cross-gas, gas-aware perspective and proposes a unified site-selection and decision-support framework that integrates CO<sub>2</sub>, H<sub>2</sub>, and NG storage across DSA, depleted reservoirs, and salt caverns. The framework brings together gas-specific behavior, geological setting, evaluation criteria, decision scale, and supporting methods, including GIS, MCDM, reservoir simulation, and ML, within a unified decision structure. This integration enables systematic comparison of similarities, differences, and trade-offs across storage systems, rather than treating each gas or method in isolation. The synthesis and conclusions in this review are also informed by lessons from representative CO<sub>2</sub>, H<sub>2</sub>, and NG underground storage projects across different geological settings. A summary of these projects is provided in Supplementary file (Appendix A; Appendix B Table S1).

The term “subsurface storage” is used broadly to refer to the storage of gases below Earth’s surface in geological environments, while “geological storage” is used more specifically

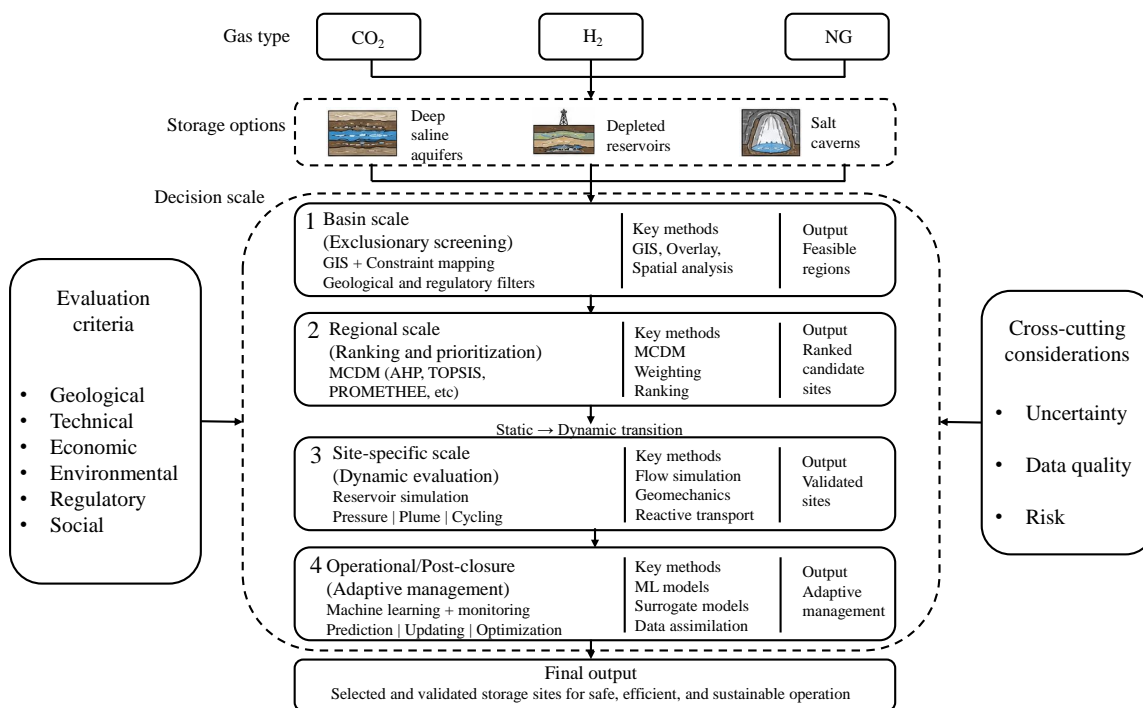
to denote storage within natural geological formations such as DSA, depleted reservoirs, and salt caverns. Unless otherwise stated, the terms are used consistently within these respective contexts. The structure of the paper is as follows: Section 2 presents the unified gas-aware decision framework; Section 3 describes geological storage options; Section 4 outlines site-selection criteria; Section 5 reviews decision-support methods; Section 6 discusses challenges, research gaps, and future directions; and Section 7 concludes.

## 2. Unified decision framework

A schematic overview of the framework is presented in Fig. 2. The framework is organized around three primary decision scales. At the basin scale (Stage 1: Exclusionary screening), the objective is to identify broadly feasible regions (basins and fairways) by applying exclusionary constraints based on geological, environmental, and regulatory criteria. Sites that do not meet essential criteria are eliminated. The evaluation relies on available data and spatial analysis tools, commonly implemented using GIS, to filter unsuitable formations and highlight candidate basins.

At the regional scale (Stage 2: Ranking), the focus shifts from “is it possible?” to “which sites are optimal?”. Candidate structures within the basin are compared using MCDM approaches that integrate geological, operational, economic, and socio-regulatory indicators. Each site is evaluated against a set of criteria with assigned weights, enabling transparent ranking under uncertainty and conflicting objectives.

At the site-specific scale (Stage 3: detailed characterization and risk analysis), assessment becomes dynamic and model-driven. Physics-based reservoir simulation is used to evaluate pressure propagation, plume migration, injectivity, containment integrity, and, where relevant, cyclic injection-



**Fig. 2.** Schematic representation of the unified, gas-aware decision framework for subsurface storage site selection.

withdrawal performance. These dynamic processes are critical for confirming storage feasibility and operational performance beyond static screening.

The framework also extends to a fourth stage focused on operational and post-closure management. Here, monitoring data and model predictions are integrated to support adaptive decision-making over the project lifecycle. ML, surrogate modeling, and data assimilation are used to update system understanding, reduce uncertainty, and optimize operations. This stage links prediction with real-time system performance and emphasizes continuous evaluation beyond initial site selection.

Across all stages, uncertainty, data quality, and risk are central considerations. They influence both method selection and result interpretation, and must be consistently addressed throughout screening, ranking, detailed evaluation, and operation. The unified framework introduced here provides the organizational structure for the remainder of the review, while the detailed storage options, selection criteria, and decision-support methods associated with each stage are discussed in Sections 3-5.

### 3. Geological storage options

Subsurface gas storage depends on the ability of geological formations to contain fluids at elevated pressures over relevant timeframes. Suitable formations require adequate porosity and permeability with low-permeability seals. Formations lacking these properties, such as crystalline or metamorphic rocks, are generally unsuitable (Bachu, 2003), although some volcanic basalts may support CO<sub>2</sub> geological storage through mineralization under favorable conditions (Kelemen et al., 2019). Tectonically active zones and critically stressed faults can

increase leakage and induced seismicity risk (Rutqvist et al., 2016).

DSA are widespread sedimentary formations saturated with brine, typically located at depths of several hundred to a few thousand meters, that offer large capacity but involve higher uncertainty and require extensive characterization (Mim et al., 2023). Depleted reservoirs are former hydrocarbon accumulations with proven containment, detailed subsurface data, and existing infrastructure, although risks associated with legacy wells, leakage pathways, and gas mixing must still be managed (Sadkhan and Al-Mudhafar, 2024). Salt caverns are solution-mined voids in thick halite formations that provide excellent containment due to the low permeability and favorable mechanical behavior of halite, require smaller cushion-gas volumes, and support high injection-withdrawal rates, but they are geographically limited (Williams et al., 2022).

Table 1 summarizes key performance indicators across storage options, including cushion-gas requirements, storage-only levelized cost of storage (LCOS) ranges, containment considerations, technology maturity (TRL), and deliverability metrics. The LCOS values are indicative ranges compiled from multiple literature sources and should be interpreted cautiously. Reported values vary substantially because of differences in system boundaries, modeling assumptions, and project conditions, including working and cushion gas volumes, compression and dehydration energy, injection-withdrawal strategies, cycling frequency, infrastructure reuse, discount rates, project lifetime, and geographic context. These values are intended for relative comparison among storage options rather than direct project-specific economic assessment. TRL values follow the standard 1-9 Technology Readiness

**Table 1.** Comparative metrics for underground hydrogen storage by formation.

Format	Capacity	Cushion gas*	LCOS (H <sub>2</sub> )	Containment and risks	Maturity (TRL)	Cycling and deliverability	Representative sources
Salt caverns	High-per cavern; modular	20%-30%	\$0.5-1.0/kg-H <sub>2</sub>	Very low-perm salt; risks: well integrity; roof stability; salt creep; needs pressure maintenance	High (7-9); commercial H <sub>2</sub> /NG	Ramp in minutes; intra-day to weekly; full discharge days-weeks; 10-20+ cycles/yr	Chen et al., 2023; Talukdar et al., 2024
Depleted reservoir	Very-high at-field scale	40%-70% (H <sub>2</sub> ); (NG often 50%)	\$1.0-1.6/kg-H <sub>2</sub>	Porous-media risks: microbial H <sub>2</sub> loss, gas mixing, geochemical reactions; legacy wells	Emerging (4-6); pilots/field trials	Ramp in hours; seasonal to multi-week; full discharge weeks-months; 1-3 cycles/yr	Muhammed et al., 2023; Talukdar et al., 2024
DSA	Very high; least characterized for H <sub>2</sub>	80% (H <sub>2</sub> )	\$2.0-3.0/kg-H <sub>2</sub>	Similar porous-media risks; greater uncertainty in recovery; high-monitoring need	Early (1-3); no commercial pure-H <sub>2</sub>	Lower deliverability; slow pressure propagation; ≤ 1 cycle/yr (seasonal)	Chen et al., 2023; Heinemann et al., 2021

Notes: \* Cushion gas relevant to H<sub>2</sub>/NG cyclic storage; not applicable to CO<sub>2</sub> geological storage.

ness Level framework defined by the U.S. Department of Energy. TRL 1-3 represent early-stage research and concept development, TRL 4-6 correspond to laboratory validation and pilot-scale demonstration in relevant environments, and TRL 7-9 indicate system demonstration, field deployment, and commercial operation.

The suitability of these formations depends on the stored gas. Table 2 provides a qualitative comparison of suitability and associated trade-offs for each gas-formation pairing. The ratings (L = limited, M = conditional, H = generally suitable) are based on literature synthesis considering technical feasibility, operational maturity, containment reliability, deliverability, and key geological and operational constraints, and are intended for comparative interpretation rather than formal quantitative scoring.

Beyond static geology, storage formations differ in how they respond to injection and withdrawal, including pressure changes, cycling effects, fluid-rock interactions, and long-term containment and deliverability. These processes are especially important for H<sub>2</sub> and NG under repeated cycling and for CO<sub>2</sub> under sustained pressure buildup, supporting the need for dynamic and multiphysics simulations in later-stage evaluation. The differences among storage formations influence how site-selection criteria are defined and evaluated, as well as the choice of decision-support methods applied throughout the unified framework, as discussed in subsequent sections.

#### 4. Selection criteria for subsurface gas storage

Selecting subsurface storage sites has evolved from simple geological screening to integrated, risk-aware evaluation. Early approaches focused on physical suitability, including trap integrity, reservoir quality, and capacity (Bennion et al., 2000). Over time, criteria expanded to include operational feasibility, economics, regulation, environmental protection, and social

acceptance, with gas-specific behavior influencing both screening thresholds and project design.

While these criteria are essential for identifying suitable storage formations, they are largely based on static properties and initial conditions. Subsurface storage systems are dynamic, and performance evolves during injection, storage, and withdrawal. Key processes include pressure propagation, plume migration, fluid displacement, gas mixing, and well-to-well interactions, all of which influence injectivity, containment, recovery, and pressure distribution (Sadkhan and Al-Mudhafar, 2024). Therefore, favorable static properties do not necessarily guarantee favorable operational performance. These considerations highlight the importance of incorporating dynamic criteria into subsurface storage evaluation.

Capturing these processes requires dynamic, time-dependent modeling approaches. Early-stage screening often relies on static criteria, whereas later-stage evaluation increasingly incorporates dynamic criteria linked to operational behavior. Criteria are adapted to gas type, formation, and project objectives, with explicit treatment of uncertainty and sensitivity to key assumptions. Table 3 summarizes the multi-scale structure of site selection, associated criteria, methods, and gas-specific considerations.

#### 4.1 Geological and petrophysical criteria

Geological and petrophysical properties govern storage capacity, containment, injectivity, and long-term stability. Basin-scale screening prioritizes sedimentary formations with laterally continuous reservoirs and competent seals capable of sustaining pressure without exceeding geomechanical limits. Tectonic setting is critical, with stable basins generally preferred over active regions due to lower leakage and seismicity risks.

At regional and site-specific scales, key parameters include

**Table 2.** Indicative suitability of formations for CO<sub>2</sub>, H<sub>2</sub>, and NG with condensed advantages/limitations.

Formation	CO <sub>2</sub>	H <sub>2</sub>	NG	Key advantages	Key limitations
DSA	H	L	M	Largest capacity; multiple trapping (structural, residual, solubility, mineral); wide on/offshore distribution	Higher uncertainty; demanding monitoring; high cushion for H <sub>2</sub> ; slow deliverability
Depleted reservoirs	H	M	H	Proven traps; rich subsurface data; existing wells and pipelines; lower new CAPEX	Legacy well integrity; gas mixing and microbial/geochemical losses (H <sub>2</sub> ); pressure window constraints
Salt caverns	L	H	H	Excellent seal; fastest cycling and high deliverability; small footprint; modular	Limited volume per cavern; geographic constraints; brine disposal during leaching; high CAPEX

**Table 3.** Multi-scale structure of subsurface storage site selection and evaluation.

Scale	Objective	Key criteria	Rationale	Gas-specific interpretation
Basin scale (screening)	Identify feasible regions and exclude unsuitable areas	Structural/stratigraphic closure, seal integrity, preliminary pressure-constrained capacity, preliminary geochemical stability, infrastructure access, regulatory constraints	Ensures fundamental geological suitability and eliminates high-risk or impractical regions early in the workflow using static and readily available indicators	CO <sub>2</sub> : containment integrity and pressure limits dominate; H <sub>2</sub> : sensitivity to reactivity, microbial activity, and losses; NG: basic feasibility of deliverability and infrastructure access
Regional scale (ranking)	Compare and prioritize candidate structures	Reservoir quality, seal integrity, fault architecture, storage capacity, deliverability potential, infrastructure proximity	Differentiates viable candidates based on relative performance potential and development feasibility under multiple criteria	CO <sub>2</sub> : trapping mechanisms and monitoring feasibility; H <sub>2</sub> /NG: cushion gas requirements and cyclic performance
Site-specific scale (detailed analysis)	Validate performance, safety, and operational limits	Injection behavior, pressure evolution, plume migration, storage performance, well interactions, geomechanics	Confirms whether selected sites can operate safely and efficiently under realistic, dynamic conditions	CO <sub>2</sub> : plume evolution, pressure management, long-term containment; H <sub>2</sub> : mobility, mixing, reactivity, recovery losses; NG: deliverability and cyclic performance stability

reservoir thickness, porosity, permeability, and connectivity. Porosity on the order of 10% or higher and permeability around 10-100 mD (order of magnitude screening values) are commonly cited as lower bounds, although acceptable thresholds depend on heterogeneity, relative permeability behavior, well architecture, and pressure-management strategy (Tarkowski et al., 2021; Oni et al., 2025).

Adsorption and adsorption-induced deformation can change permeability, injectivity, and storage performance, especially in organic-rich and clay-bearing formations. Adsorption strength generally follows CO<sub>2</sub> > CH<sub>4</sub> > H<sub>2</sub>, so CO<sub>2</sub> tends to cause stronger swelling and permeability changes, CH<sub>4</sub> has moderate effects, and H<sub>2</sub> is weaker but still relevant in clay- or kerogen-rich systems (Raza et al., 2022; Babaei et al., 2025). These effects may influence gas trapping, recovery, cyclic performance, and storage efficiency, but are minimal in clean sandstones and largely absent in salt caverns. Site

screening should therefore consider mineralogy, total organic carbon, clay content, adsorption capacity, swelling potential, and stress-dependent permeability where relevant.

For H<sub>2</sub> storage, microbial and geochemical risks should be included as measurable screening criteria rather than treated as general hazards. Microbial activity can consume H<sub>2</sub> and produce CH<sub>4</sub> or H<sub>2</sub>S, affecting gas quality, corrosion, and permeability (Dopffel et al., 2021; Safari et al., 2025). Site screening should therefore consider brine chemistry, salinity, pH, sulfate, redox conditions, temperature, mineralogy, and microbial activity, using core analysis, brine sampling, microbial assays, and reactive-transport modeling where needed. These factors are especially important in depleted reservoirs and saline aquifers, while salt caverns generally have lower microbial risk because of limited water and hypersaline conditions (Dopffel et al., 2021).

Seal effectiveness depends on caprock permeability, thick-

ness, lateral continuity, pore-throat structure, and capillary entry/breakthrough pressure (Zhang et al., 2024). Faults and fractures are evaluated carefully, as transmissive or critically stressed features may compromise containment unless demonstrated to be stable (Yang et al., 2024). Hydrogeological conditions influence pressure dissipation and storage capacity, particularly for CO<sub>2</sub>, where large connected systems reduce pressure buildup (Ringrose et al., 2021).

Criteria for salt formations include thickness, homogeneity, and depth to ensure cavern stability, economically viable operating pressures, and controlled leaching. Mechanical behavior and long-term creep are also important considerations (Williams et al., 2022). Cavern development typically requires salt thicknesses on the order of ~100 m or more (site-dependent) (Qian et al., 2025). Highly soluble or mechanically weak evaporite layers (e.g., carnallite, kieserite) are avoided due to their impact on leaching control and cavern integrity (Sheikheh et al., 2025). At the project scale, salt body geometry, internal complexity, and the density and quality of available subsurface data influence confidence in cavern spacing, total cavern count, and long-term performance (Li et al., 2022).

Although the same geological criteria apply across storage systems, their functional role differs by gas depending on storage objectives and fluid behavior. This cross-gas variation is summarized in Supplementary file (Appendix B Table S2). For CO<sub>2</sub>, these properties primarily control pressure buildup, plume migration, and long-term trapping. For H<sub>2</sub>, they additionally influence mixing, fingering, and potential losses, making heterogeneity and connectivity more critical. For NG, geological properties are evaluated mainly in terms of their impact on deliverability and cyclic performance. This highlights that identical geological parameters must be interpreted differently depending on the gas stored.

## 4.2 Technical (operational) and economic criteria

Technical and economic criteria determine whether geological suitability translates into operational performance and project value. Key technical indicators include injectivity, deliverability, pressure limits, cycling capability, and gas quality maintenance (Davoodi et al., 2025). Additional cross-cutting indicators include cavern stability, containment and well integrity under the planned operating envelope, and the ability to maintain gas quality at required specifications. These indicators depend on the interaction between working gas, cushion gas, and resident fluids, which collectively control pressure build-up, flow efficiency, and withdrawal performance through multiphase flow effects (Heinemann et al., 2022).

Gas-specific behavior modifies technical thresholds. For CO<sub>2</sub> storage, operational criteria prioritize sustained injectivity under pressure-management constraints, plume control, and compatibility with monitoring and verification requirements. For H<sub>2</sub> storage, operational feasibility depends on controlling mobility-driven losses, maintaining recovery efficiency, and managing gas purity under repeated cycling, which increases the importance of flow-rate control, cushion gas management,

pressure management, and gas treatment requirements. H<sub>2</sub> systems may require explicit accounting for mixing/dispersion and potential consumption mechanisms that affect both hydrogen recovery and quality, where in porous media, gas mixing, reservoir heterogeneity, and repeated cycling can lower withdrawn H<sub>2</sub> purity, while microbial and geochemical processes may cause additional losses (Heinemann et al., 2022; Ghaedi et al., 2024). For NG storage, long-established practice emphasizes seasonal or multi-cycle deliverability, pressure-dependent withdrawal performance, and efficient reservoir re-pressurization between cycles, with cushion-gas sizing, reservoir pressure management, and water-bearing boundaries playing key roles in operational planning (Plaat, 2009).

Economic criteria integrate these technical characteristics with infrastructure, logistics, and market context. Capital expenditure includes site development, wells, cavern leaching where applicable, compression and dehydration facilities, and monitoring systems while operating expenditure is dominated by compression power, surface processing, monitoring, maintenance, and insurance. Beyond aggregate cost metrics, project value also depends on operational flexibility and market function. These costs are often summarized through LCOS or equivalent unit-cost metrics, allowing comparison across storage options under comparable working-capacity assumptions (Talukdar et al., 2024).

Cushion gas represents a major economic and operational constraint in H<sub>2</sub> and NG geologic storage because it is required to maintain reservoir pressure and deliverability but is not routinely recoverable as working inventory. This creates a significant upfront capital commitment because the gas must be procured and may remain tied up over long operational periods. In H<sub>2</sub> storage, mixing and compositional changes between cushion and working gas can reduce effective recovery and increase surface-processing requirements, making cushion-gas management both an economic and reservoir-performance consideration (Heinemann et al., 2022). Cushion gas selection (e.g., CH<sub>4</sub>, N<sub>2</sub>, CO<sub>2</sub>, or H<sub>2</sub>) involves trade-offs between cost, recovery efficiency, purity, and long-term operation (Prigmore et al., 2024). Site screening should therefore consider cushion gas, reservoir heterogeneity, residual gas composition, microbial activity, expected purity, and surface treatment needs alongside standard geological criteria. Consequently, cushion gas should be evaluated not only as a cost parameter but also as a key operational and design criterion in techno-economic screening and storage optimization.

NG storage economics are mainly driven by seasonal price differences, with additional value from short-term arbitrage when frequent cycling is possible (Löhndorf and Wozabal, 2021). Salt caverns are well suited for capturing short-term value, where limited mixing supports higher purity and recovery, whereas porous-media storage is typically used for seasonal balancing and long-duration storage (Małachowska et al., 2022). For CO<sub>2</sub> storage, economic viability is driven more by policy incentives, infrastructure sharing, transport-network optimization, and economies of scale (Gunawan et al., 2024). For H<sub>2</sub> storage, economic value is linked to providing firm supply, balance variable production, and meet end-use purity specifications (Wickham et al., 2022). Generally, hub-and-

cluster development, shared pipeline networks, and centralized compression or capture systems can significantly reduce costs at scales, while simplifying permitting and monitoring making transport distance to sources and sinks and source-sink proximity an important consideration in regional screening (Gunawan et al., 2024).

Practical constraints further shape techno-economic screening. Water depth, drilling complexity, and formation depth influence well costs and feasibility, while extreme depths often reduce porosity and increase cementation-related risks, motivating early exclusion thresholds in basin-scale screening. Offshore development introduces additional constraints related to installation windows, platform access, and subsea infrastructure. At later stages, integrated techno-economic models combine subsurface performance with surface facility design and financial assumptions to test sensitivity to gas prices, utilization rates, policy incentives, and operating strategies.

Techno-economic assessment increasingly considers whole-system effects (upstream and downstream value chains) beyond subsurface performance. For H<sub>2</sub>, economics depends on production, compression, purification, transport, and end-use requirements, while CO<sub>2</sub> storage is strongly influenced by capture costs and source-sink matching. NG storage remains closely tied to existing infrastructure and markets. As a result, integrated techno-economic assessment and life cycle assessment approaches are increasingly used to assess energy use, emissions, infrastructure needs, and environmental trade-offs across the full system (Wang et al., 2024; Tayyib et al., 2025). These analyses are especially important when comparing storage options with different cycling behavior, purification needs, and cushion-gas requirements. For example, porous H<sub>2</sub> storage in depleted reservoir may need extra purification and compression due to gas mixing, whereas salt caverns can reduce these downstream requirements despite higher initial costs.

Technical and economic criteria therefore represent a convergence point where gas behavior, operational strategy, and market context interact. While injectivity, pressure limits, and infrastructure are relevant across all gases, CO<sub>2</sub> projects are primarily driven by policy-supported cost structures and large-scale injection efficiency, whereas H<sub>2</sub> and NG storage depend more strongly on cycling performance, inventory management, and market flexibility. Early-stage screening relies on simplified indicators and conservative thresholds, while regional and site-specific evaluations increasingly depend on dynamic modeling, scenario analysis, and uncertainty quantification. This staged approach ensures that only candidates capable of meeting both operational and economic objectives progress to detailed characterization and investment decision under explicit performance and risk tolerances. This reinforces the need to evaluate techno-economic feasibility within a gas-specific operational context, even when using a shared framework.

### 4.3 Environmental and safety criteria

Environmental protection and safety are critical for project feasibility and public acceptance. Environmental and safety risks are similarly cross-cutting but gas-dependent: leakage,

induced seismicity, and groundwater protection are universal concerns. Therefore, risk assessment approaches must be adapted to reflect both shared geomechanical processes and gas-specific hazard profiles. Leakage risk is assessed through caprock integrity, fault reactivation potential, and wellbore condition, particularly legacy wells (Hajiyev et al., 2025). Accordingly, well-integrity screening typically involves identifying existing wells from records, testing selected wells where possible, and maintaining safe distances from poorly documented or high-risk wells.

Induced seismicity is a critical geomechanical risk in subsurface gas storage, particularly where injection increases reservoir pressure near pre-existing faults, and therefore, induced seismicity assessment should be integrated into both site selection and operational planning rather than treated only as a generic safety constraint (Schultz et al., 2023). It is assessed through geomechanical modeling and operational pressure limits, with conservative thresholds typically applied in tectonically stressed regions, often coupled with monitoring-based operating protocols. Pressure buildup can reduce effective normal stress and promote fault slip if critically stressed conditions are reached. The risk depends on the in-situ stress state, fault orientation, fault permeability, pressure propagation, injection rate, and operating pressure limits. Quantitative assessment typically requires coupled reservoir-geomechanical modeling to evaluate pressure evolution and fault stability, often using failure criteria such as Mohr-Coulomb analysis (Rutqvist, 2012). Operationally, this risk is managed through conservative pressure limits, traffic-light monitoring systems, microseismic surveillance, and adaptive injection control (Verdon and Bommer, 2021).

For H<sub>2</sub> and NG storage, cyclic operations cause repeated pressure and temperature changes that may lead to stress redistribution, fault reactivation, well integrity issues, and caprock deformation, while for CO<sub>2</sub> storage, long-term pressure buildup and plume migration can influence fault stability over extended periods (Schultz et al., 2023). In porous formations, these effects build up through pressure diffusion, while in salt caverns they mainly affect salt creep, cavern convergence, and thermal damage (Coarita-Tintaya et al., 2025). As a result, evaluating cyclic storage should include geomechanical limits and operating pressure windows, not just static geological criteria. Maximum pressures must stay below fracture or caprock failure limits, while minimum pressures help reduce compaction in porous formations and excessive creep in salt caverns (Bérest et al., 2020). These limits vary by gas and storage type.

Protection of overlying groundwater requires showing that pressure change, buoyant gas migration, and brine displacement will not contaminate protected aquifers (Hussain et al., 2016). Achieving this depends on a well-planned monitoring program that includes baseline characterization, operational surveillance, and clear response plan that is credible to regulators and communities and integrated into regular operations.

Local environmental conditions impose practical constraints. Complex terrain can increase construction costs and impacts, while ecologically sensitive or remote settings may

create additional permitting and logistical challenges. Reliable access to water and power is essential: salt caverns require substantial water volumes for leaching, and surface facilities depend on continuous power for compression and dehydration (Warren, 2016). Locating sites far from these utilities raises costs and introduces delays. Safety setbacks from population centers mitigate noise, vibration, and hazard exposure, and most siting frameworks exclude protected lands, critical habitats, and source-water protection zones during early screening (Irfan et al., 2014).

Process safety considerations also differ by gas: CO<sub>2</sub> leakage may pose localized asphyxiation and can contribute to corrosion and materials-compatibility issues in wells and surface facilities. H<sub>2</sub> leakage introduces additional concerns related to flammability and subsurface reactivity. These hazards are typically addressed through quantitative risk assessment, emergency response planning, and the design of safety systems and exclusion zones appropriate to the inventory and operating pressures (Schultz et al., 2023).

Managing responsibility after closure and ensuring long-term oversight are essential. Projects must demonstrate durable containment through credible measurement, monitoring, and verification plans and clearly assigned responsibilities after operations end, especially for CO<sub>2</sub> storage, where containment performance must be ensured over decades to centuries. Clear criteria for site closure, post-closure monitoring duration, and liability transfer, where applicable, can improve regulatory certainty and help strengthen public trust (Wilson et al., 2007).

#### 4.4 Regulatory and social criteria

Regulatory frameworks and social acceptance strongly influence project development and vary significantly across jurisdictions. Appendix B Table S3 (Supplementary file) summarizes major regulatory approaches across selected jurisdictions. In Europe, Directive 2009/31/EC mandates a structured assessment for geological CO<sub>2</sub> storage that includes comprehensive data collection, dynamic simulation, sensitivity analysis, and hazard evaluation, with explicit requirements for demonstrating site capacity and safety throughout the project lifecycle (Shogenova et al., 2014). In North America, the CSA Z741-12 (R2018) standard guides the entire storage lifecycle. In the United States, CO<sub>2</sub> storage is regulated under the EPA Underground Injection Control Class VI program, which provides detailed requirements for site characterization, injection operation, monitoring, and post-closure stewardship (Orujov et al., 2023).

Other jurisdictions, including Australia, China, and parts of the Middle East, have developed region-specific approaches that often build on petroleum, groundwater or environmental legislation, adapting these frameworks to accommodate CO<sub>2</sub> and NG storage (Zhang, 2021). Complementary guidance from organizations such as DNV and the IEA GHG reinforces the basin-to-regional-to-site progression and risk-based gating.

Despite these developments, regulatory maturity remains uneven, particularly for emerging applications and transboundary storage systems. Differences in permitting processes, pore-space ownership, monitoring requirements, and liability struc-

tures, and international regulatory coordination can significantly affect project timelines, investment risk, and cross-border deployment strategies (Dixon et al., 2015).

Across jurisdictions, regulatory clarity is closely linked to commercialization because long project timelines, high capital costs, and long-term liability exposure require predictable permitting, monitoring, and financial responsibility frameworks (Liu et al., 2025). Existing carbon capture, storage (CCS) regulations increasingly address site characterization, operational monitoring, closure, and post-closure stewardship, but uncertainty surrounding liability transfer, remediation obligations, and long-term monitoring responsibilities continues to influence investment confidence and project economics, even in relatively mature regulatory systems (Zhang, 2021). Clear rules for pore-space access, monitoring obligations, environmental risk management, and post-closure responsibility are therefore essential to reduce uncertainty and support large-scale deployment.

Regulatory frameworks for H<sub>2</sub> storage are still evolving and remain less well defined in most jurisdictions (Mioic et al., 2023). Existing regulations are often adapted from NG storage standards and may not fully account for hydrogen-specific risks such as higher diffusivity, potential material compatibility issues, and gas quality management. Clear guidelines for monitoring, leakage thresholds, microbial impacts, and long-term liability are not yet established. These uncertainties can delay project development, increase perceived risk for investors, and complicate permitting and commercialization pathways for large-scale deployment. Advancing hydrogen storage at scale will require dedicated regulatory frameworks that explicitly address these technical and operational challenges while integrating lessons learned from CCS and underground NG storage regulation.

Policy instruments strongly influence project economics and risk distribution. Jurisdictions with targeted support, such as tax credits (e.g., 45Q), low-carbon fuel standards, public demonstration programs, carbon pricing systems, and hub/cluster development strategies, tend to see more projects reaching final investment decision because these mechanisms can stabilize revenues, share infrastructure and reduce financing uncertainty associated with subsurface and regulatory risks (Fan et al., 2018; Colombe et al., 2024). Geopolitical and institutional readiness are also important. Some high-potential basins are in jurisdictions with limited regulatory capacity, unclear pore-space ownership, fragmented institutional oversight, or competing development needs, which can delay CCS and underground gas storage deployment (Abdulla et al., 2021). Effective regulatory systems therefore require coordination between geological assessment, environmental oversight, infrastructure planning, and long-term stewardship responsibilities.

Community acceptance is equally important. Public attitudes reflect local experiences with industry, land-use conflicts, perceived benefits, and trust in institutions. Evidence from CCS pilots and regional partnerships shows that early, transparent engagement, credible monitoring, and visible local benefits reduce opposition, delays, and cost overruns (Breukers and Upham, 2015). Conversely, insufficient outreach has

repeatedly derailed technically suitable projects (Huijts et al., 2007; Wallquist et al., 2012). Meaningful participation processes and credible commitments on monitoring, grievance mechanisms, and benefit sharing affect project timelines and outcomes.

Practical screening, therefore integrates socio-regulatory readiness with the geological, technical, and economic filters described earlier, removing high-conflict locations at an early stage and concentrating detailed evaluation on areas where subsurface suitability and community support are both strong and likely to remain durable over the project lifecycle.

Overall, the site-selection criteria applied across gases are broadly similar, although their relative importance and interpretation vary with gas behavior and storage objectives. CO<sub>2</sub> storage places greater emphasis on long-term containment and monitoring, whereas H<sub>2</sub> and NG storage prioritize cyclic performance and deliverability, with H<sub>2</sub> additionally affected by mobility, mixing, and reactivity. The framework is therefore unified across scales but gas-aware in its application.

## 5. Decision-making methods

The increasing complexity of subsurface storage site selection has shifted practice from qualitative judgment toward quantitative, transparent, and scalable decision support. Early source-sink allocation methods for CO<sub>2</sub> and NG matched large sources to candidate reservoirs using capacity, distance, and simple cost proxies (Bachu, 2002). These approaches highlighted the importance of logistics and showed that regional portfolio planning is often more relevant than single-site selection, but their coarse assumptions limited differentiation among sites with similar capacity but different containment, injectivity, or monitoring risks.

As datasets and standards improved, practice moved toward parametric screening, which applies geological, engineering, and regulatory criteria in a structured way (Bachu, 2003). This is often complemented by risk-informed screening of leakage, well-integrity, and HSE hazards, so that failure modes and mitigation measures are considered alongside capacity and cost (Oldenburg, 2008). Parametric screening is fast, auditable, and conservative, but it is less effective when criteria conflict or when uncertainty and expert judgment must be combined. This has led to increasing use of MCDM methods.

MCDM methods combine different indicators into transparent rankings and are especially useful at the regional scale, where many candidate structures must be prioritized, and gas-specific objectives may differ. Because expert judgments are often imprecise, many studies also use fuzzy MCDM to represent linguistic assessments and incomplete data (Mardani et al., 2015). GIS add spatial intelligence by combining constraint layers, weighted raster criteria, and network analysis to generate suitability maps and identify storage clusters (Greene et al., 2011). Reservoir simulation adds physics-based evaluation of injectivity, plume migration, pressure evolution, and cycling performance, and its outputs can be reduced into proxy models for faster screening (Askari et al., 2020). More recently, ML has been introduced to support non-linear prediction, surrogate modeling, and probabilistic screening, although its application

requires careful attention to extrapolation, explainability, and data quality (Nassabeh et al., 2024).

Decision-support methods should be selected according to decision scale, data availability, uncertainty, and gas-specific risk. GIS is most appropriate for basin-scale screening, MCDM for regional ranking, reservoir simulation for site-specific dynamic validation, and ML for surrogate modeling, uncertainty analysis, and monitoring interpretation. For CO<sub>2</sub> storage, simulation and monitoring are central because long-term containment and plume evolution dominate project risk. For H<sub>2</sub> storage, uncertainty, reactivity, mixing, and limited field data require stronger integration of simulation, sensitivity analysis with cautious ML use. For NG storage, established operational datasets make optimization and ML more mature, but deliverability and cycling performance remain the dominant evaluation targets. Table 4 summarizes the strengths, limitations, and recommended use of commonly applied methods. Rather than independent approaches, these methods are better viewed as complementary components of a unified, multi-scale decision-support workflow.

### 5.1 MCDM

MCDM provides a structured framework for evaluating subsurface storage options when multiple competing factors must be considered together. The general workflow is summarized in Fig. 3. Methods differ mainly in how they represent trade-offs and whether they allow poor performance in one criterion to be compensated for by strong performance in another.

MCDM methods can be broadly classified into compensatory and non-compensatory approaches. Compensatory, value-based methods such as Analytic Hierarchy Process (AHP) and Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS) allow trade-offs among criteria, meaning strong performance in one criterion may offset weaker performance in another. These approaches are often suitable for early-stage screening where flexibility in trade-offs is acceptable. In contrast, non-compensatory or outranking methods such as Preference Ranking Organization Method for Enrichment of Evaluations (PROMETHEE) and ELECTRE restrict full compensation and are better suited to safety-critical decisions where poor performance in key criteria, such as seal integrity or leakage risk, should not be offset by economic or logistical advantages. VIKOR occupies a compromise position by identifying solutions that balance overall utility and individual regret (Opricovic and Tzeng, 2004). In the context of subsurface storage site selection, the choice of MCDM method therefore has important implications beyond ranking performance. Table S4 (Supplementary file Appendix B) summarizes the strengths, limitations, and representative applications of these methods.

Uncertainty and correlation among criteria further influence method behavior. Many geological and operational parameters, such as depth, pressure, temperature, and geomechanical stability, are interdependent, which can violate independence assumptions in methods like AHP and TOPSIS (Huang and Chen, 2024). Under such conditions, methods that

**Table 4.** Recommended use of decision-support methods across decision scale and storage context.

Method	Decision scale	Key strengths	Key limitations	Best use cases (CO <sub>2</sub> /H <sub>2</sub> /NG)
GIS	Basin/Regional	Efficient spatial screening; integrates environmental, regulatory, and infrastructure constraints	Static; dependent on data resolution and layer quality	Early-stage screening for all gases; identifying feasible basins and exclusion zones
MCDM	Regional	Transparent ranking of alternatives; integrates multiple criteria and expert judgment	Sensitive to weights and normalization; typically static	Comparing candidate reservoirs or caverns; balancing geological, technical, and economic factors
Reservoir Simulation	Site-specific	Captures dynamic processes (pressure, plume migration, cycling, well interaction); physics-based	Data- and computationally intensive; requires detailed models	CO <sub>2</sub> storage (pressure and plume control); H <sub>2</sub> /NG storage (cycling, recovery, deliverability)
ML	Site/Operational	Fast prediction; handles nonlinear relationships; enables surrogate modeling	Requires large, representative datasets; limited interpretability; poor extrapolation	Surrogate modeling, screening large datasets, monitoring interpretation; more mature for CO <sub>2</sub> /NG than H <sub>2</sub>
Hybrid Workflows	Multi-scale	Combines strengths of GIS, MCDM, simulation, and ML; supports staged decision-making	Increased complexity; requires consistent data integration	Integrated workflows linking screening, ranking, and dynamic validation

incorporate thresholds or pairwise dominance relationships may provide more robust rankings. In addition, uncertainty in input data and expert judgment can propagate differently across methods, with fuzzy and outranking approaches often offering greater flexibility in representing imprecision (Pelissari et al., 2021). These considerations highlight that method selection should be aligned with decision context, data quality, and the relative importance of safety versus economic optimization. Among these methods, AHP, TOPSIS, and PROMETHEE remain the most widely applied in subsurface storage studies and are therefore discussed in Supplementary file (Appendix C).

## 5.2 GIS

Subsurface storage is inherently spatial. Reservoir quality, seal integrity, faults, legacy wells, protected areas, infrastructure, and communities all vary geographically. GIS provides the framework for integrating these raster and vector datasets into a common spatial system for screening, mapping, and visualization (Sabzevari and Delavar, 2017).

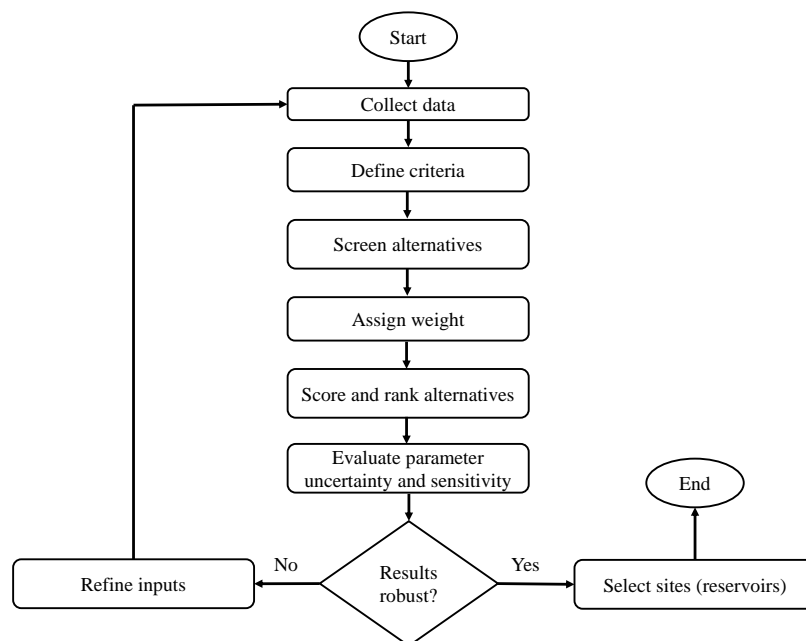
At basin and regional scales, GIS is used to build composite suitability maps by combining normalized criteria layers with weights and exclusion masks (Lankof and Tarkowski, 2023). This is common in CCS atlas development and salt-cavern siting, where depth, thickness, halite quality, population constraints, and infrastructure access are evaluated together (Irfan et al., 2014; Overy and Martins, 2024). At the site scale, GIS supports data management and visualization of wells, seismic footprints, faults, and monitoring information, enabling transparency and stakeholder communication.

GIS itself is not a decision engine. Its results depend on data quality, resolution, interpolation, weighting, and exclusion rules. Best practice therefore couples GIS with explicit

decision framework, sensitivity analysis, and documentation of layer sources, processing steps, and uncertainty. Where data are sparse or linguistic, fuzzy GIS-MCDA can provide a defensible extension (Malczewski, 1999; Morris and Jankowski, 2001).

Recent developments have expanded the role of GIS in subsurface storage screening beyond static overlay analysis. Advanced workflows increasingly integrate multi-resolution datasets, including 3D geological models, well databases, and time-dependent monitoring data, enabling more realistic spatial representation of subsurface systems (Wu et al., 2025). Coupling GIS with ML and spatial statistics has also improved the ability to identify patterns and prioritize candidate regions under uncertainty (Roy et al., 2024). In addition, network-based GIS approaches are being used to evaluate infrastructure connectivity, source-sink matching, and transport optimization, linking subsurface suitability with surface logistics and economic considerations (Budiarto et al., 2025).

Despite these advantages, GIS-based approaches have important limitations in the context of subsurface storage. Most GIS workflows rely on surface or simplified subsurface representations and therefore cannot directly capture dynamic processes such as pressure propagation, multiphase flow, or geochemical interactions (Pratama and Refani, 2023). Results are also highly sensitive to data quality, spatial resolution, interpolation methods, and weighting schemes, which can introduce bias or mask critical uncertainties (de Brito et al., 2019). In addition, the integration of heterogeneous datasets, often collected at different scales and levels of reliability, remains a major challenge. As a result, GIS is most effective as an early-stage screening and visualization tool and should be complemented by physics-based modeling and uncertainty analysis at later decision stages. For this reason, GIS outputs



**Fig. 3.** General workflow for MCDM-based subsurface storage site selection and evaluation.

are typically interpreted as indicative rather than definitive, and are most valuable when integrated within a broader, multi-stage decision-support framework.

### 5.3 Reservoir simulation

Reservoir simulation is the main physics-based tool for screening, ranking, and de-risking storage candidates at regional and site scales. It captures processes such as pressure diffusion, plume migration, capillary trapping, and fluid-rock interactions that cannot be resolved with static GIS or simple scoring approaches (Omobude et al., 2025). When coupled with geomechanics or geochemistry, it also supports evaluation of caprock integrity, fault stability, wellbore conditions, and long-term trapping (Rutqvist, 2012).

Simulation workflows typically begin with a static geological model derived from well logs, seismic interpretation, and mapping, followed by selection of appropriate physics and operating scenarios. Key uncertainties in petrophysical and structural parameters are then explored through multiple runs, and results are summarized into metrics such as storage capacity, recovery efficiency, pressure buildup, plume footprint, integrity margins, and deliverability (Feldmann et al., 2016).

Because ensemble simulation is computationally expensive, modern workflows often use surrogate models, multi-fidelity strategies, and sensitivity analysis to accelerate screening while reserving detailed models for shortlisted sites (Razavi et al., 2012). Simulation therefore provides the physics-based foundation linking subsurface behavior to operational feasibility, but its cost and complexity mean that it is best used after earlier-stage screening rather than as a first-pass tool.

Credible storage evaluation requires coupling multiple physical processes rather than relying on single-physics

flow models. For CO<sub>2</sub> storage, key couplings include flow-geomechanics (for pressure-induced deformation and fault stability) and flow-geochemistry (for mineral trapping and fluid-rock reactions) (Shi et al., 2024). H<sub>2</sub> storage introduces additional requirements, including coupling between flow, geochemistry, and microbiology to capture potential gas loss and compositional changes (Ahmed et al., 2025). For NG storage, coupled flow-geomechanical modeling is important for evaluating cycling-induced stress and long-term reservoir integrity (Nasrollahzadeh et al., 2021). Cyclic H<sub>2</sub> and NG storage increasingly require coupled thermo-hydro-mechanical or thermo-hydro-mechanical-chemical simulations because repeated injection and withdrawal can change stress, permeability, cavern shape, caprock integrity, and well performance over time (Coarita-Tintaya et al., 2025). These models help assess fault stability, salt creep, thermal stresses, and long-term cycling effects, providing realistic estimates of safe operating limits and containment than single-physics models.

Modern simulation workflows therefore increasingly rely on multi-physics modeling frameworks, although these approaches remain computationally demanding and are often applied selectively at later project stages. The choice of simulation tools and coupling strategy should be aligned with the dominant risks and decision objectives for each gas type. Table S5 (Supplementary file Appendix B) summarizes the relative importance and maturity of selected simulation capabilities across CO<sub>2</sub>, H<sub>2</sub>, and NG storage systems, together with representative modeling tools commonly used in practice.

### 5.4 ML

ML is increasingly used in subsurface storage for screening, surrogate modeling, uncertainty analysis, and monitoring (Maldonado-Cruz and Pycrz, 2022; Alqahtani et

al., 2023). However, most applications remain research-focused, simulation-based, or adapted from related fields rather than used routinely for operational site selection. Appendix B Table S6 (Supplementary file) summarizes representative applications and current limitations.

In early-stage screening, ML can help interpret geological, petrophysical, spatial, and infrastructure data to predict suitability, injectivity, capacity, or leakage risk, classify candidate storage sites, and used with GIS to transform spatial layers into feature matrices for regional ranking (Derakhshani et al., 2024).

ML has also been used as a surrogate for physics-based simulations, where simulation outputs train fast models to predict pressure, plume migration, injectivity, saturation, or trapping behavior (Alqahtani et al., 2023; Wen et al., 2023). These models can speed up uncertainty analysis and scenario testing. ML is also being explored for monitoring, forecasting, and anomaly detection during storage operations, including leakage signals, pressure changes, fracture risk, plume behavior, and geochemical anomalies in time-series monitoring data (Marvin et al., 2025). These applications could support adaptive monitoring and operations, but they still depend on reliable data, noise handling, and interpretable results before wider use in practice.

However, ML performance depends heavily on the availability and quality of data, including geological, petrophysical, operational, monitoring, laboratory, and simulation datasets. In practice, these data are often sparse, incomplete, or region-specific, making preprocessing steps such as normalization, missing-data handling, feature engineering, and uncertainty treatment important for model reliability. These limitations are especially relevant for H<sub>2</sub> storage, where operational datasets remain limited.

Subsurface storage systems are also heterogeneous and change over time, with pressure, saturation, plume movement, gas composition, and recovery influenced by geology and operational history. This makes conventional ML less suitable, leading to interest in physics-informed models that include physical constraints and connectivity-aware methods that capture flow paths, well-to-well communication, faults, and reservoir connectivity (Wang et al., 2021; Donnelly et al., 2024). However, most of these approaches are still at the demonstration stage rather than established storage workflows.

Overall, ML should be considered an enabling tool within integrated storage assessment rather than a replacement for established methods. Its strongest near-term role is to accelerate repetitive tasks, identify patterns in large datasets, support uncertainty analysis, and guide where more detailed characterization or simulation should be focused. For CO<sub>2</sub> storage, ML applications are more developed because larger simulation and field datasets exist. For H<sub>2</sub> storage, applications remain more limited and exploratory due to sparse operational data, greater uncertainty in microbial/geochemical behavior, and complex cycling-related processes. Used together with GIS, MCDM, laboratory data, monitoring, and physics-based simulation, ML can improve screening efficiency and decision support, but its outputs must remain constrained by physical understanding, validation, and expert interpretation.

## 6. Challenges, research gaps, and future directions

Despite progress in subsurface storage modeling, decision-support methods, and geoscientific knowledge, major challenges remain in selecting and deploying underground gas storage systems. These include data limitations, weak integration across scales, gas-specific knowledge gaps, methodological constraints, lack of standardization, and uncertainty in monitoring and post-closure stewardship. Addressing these issues is essential for scaling storage systems in support of climate mitigation and energy-transition goals.

### 6.1 Data availability and quality constraints

A key limitation is uneven availability and quality of subsurface data across regions and gases. Even in mature basins, uncertainty persists due to incomplete core recovery, irregular formation testing, and poorly documented legacy wells. Key parameters such as stress state, relative permeability, capillary entry pressure, and wettability remain poorly constrained. For CO<sub>2</sub> storage, multiphase flow properties, microbial and geochemical processes are not yet well quantified under reservoir conditions.

### 6.2 Integration across scales and disciplines

Key processes such as capillary trapping, mineral reactions, and microbial kinetics occur at pore or core scale, while decisions are made at reservoir and basin scales. Robust upscaling remains limited and wellbore integrity and materials compatibility are rarely integrated into site-scale evaluation. As a result, many workflows still rely on proxy indicators rather than calibrated mechanistic predictions. Integration across disciplines is also limited. GIS-based studies often provide spatial context but limited physics, while reservoir-focused studies may underrepresent permitting, land-use, and infrastructure constraints.

### 6.3 Gas-specific knowledge and criteria gaps

Important differences exist in the subsurface behavior of CO<sub>2</sub>, H<sub>2</sub>, and NG, leading to gas-specific uncertainties in storage assessment. Quantitative understanding of hydrogen transport, mixing, recovery efficiency, and long-term containment under cyclic operation remains limited, particularly in heterogeneous porous-media systems. Coupled geochemical, microbial, and geomechanical effects, including impacts on caprock integrity, wettability, and well materials, remain insufficiently constrained by laboratory experiments and field-scale observations.

### 6.4 Methodological and interpretability limitations

MCDM methods are transparent but sensitive to weighting choices, rank reversal, and static assumptions. Fuzzy approaches address vagueness but depend on membership functions, while ML methods capture complex patterns but require validation and interpretability tools to remain credible. Models may also degrade when applied across basins or

updated with new data. In all cases, results should be presented as conditional on assumptions and data quality.

### 6.5 Monitoring and post-closure uncertainty

Most frameworks focus on pre-injection feasibility, but long-term performance determines success. Monitoring should not be a one-way reporting channel but a feedback input to decision tools, so risks can be updated, and management can adapt as new data becomes available. Closure and post-closure plans must be explicit in selection studies: who owns liability, what triggers hand-off to the state (if applicable), what residual-risk metrics must be met, and how monitoring will be reduced over time under clearly defined performance criteria.

### 6.6 Future directions for subsurface storage decision support

Hybrid concepts offer additional value by expanding subsurface storage systems beyond single-purpose applications. For example, CO<sub>2</sub> plume geothermal systems may combine CO<sub>2</sub> storage with heat extraction (Uliasz-Misiak et al., 2021), while CO<sub>2</sub>-H<sub>2</sub> coupling may enable methanation (Wu et al., 2024) or alternative cushion gas strategies (Mu et al., 2019). Although these approaches remain uncertain and are not yet widely demonstrated, they highlight the potential for integrating storage with broader energy system functions and improving overall project value. Future progress will depend on the development of adaptive, gas-specific decision platforms that combine MCDM, GIS, reservoir simulation, and ML within a unified workflow.

Future research priorities are summarized in Fig. 4. In the near term, the most immediate priority is to strengthen the robustness of existing decision-support frameworks through uncertainty quantification, monitoring integration and improved data integration and standardization. This includes better propagation of uncertainty in geological properties, model assumptions, and expert-derived weights, as well as stronger coupling between screening, multi-criteria evaluation, and physics-based simulation. Key near-term research questions include: How should uncertainty in geological and operational parameters be propagated through site-selection workflows? Which monitoring variables provide the greatest reduction in decision uncertainty? How transferable are current ML and MCDM workflows across basins with different data availability and geological characteristics?

Over the medium term, research should focus on the development of integrated, multi-scale modeling frameworks including coupled multi-physics modelling, hybrid physics-ML approaches, field-scale validation, upscaling of gas-specific processes. Dynamic processes such as pressure evolution, plume migration, cyclic operations, and gas-specific reactive behavior should directly be added to decision-support workflows. Important medium-term research questions include: How can coupled flow-geomechanics-geochemistry models be efficiently integrated into decision-support workflows? What level of model complexity is required to represent H<sub>2</sub>-specific losses and reactive processes at field scale? How can hybrid physics-ML approaches maintain physical consistency while

reducing computational cost?

In the longer term, subsurface storage systems are expected to evolve toward adaptive, intelligent platforms such as digital twins, real-time optimization, AI-assisted decision support, interoperable data systems, and governance frameworks that support these tools. Achieving this vision will require advances in data sharing, model interoperability, regulatory harmonization, and physics-informed and spatio-temporal ML methods capable of representing heterogeneous and evolving subsurface systems. Long-term research questions include: How can digital twins continuously assimilate monitoring data while preserving computational efficiency and interpretability? What governance structures are required for AI-assisted operational decision-making in subsurface storage systems? How can interoperable data and model standards be developed across jurisdictions and storage types?

## 7. Conclusion

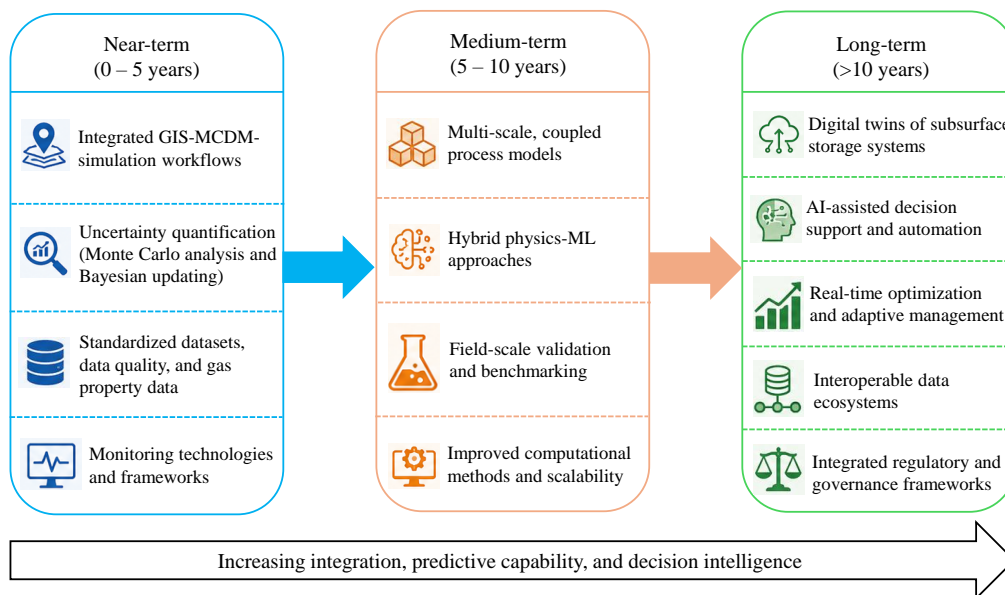
This work presents a unified, gas-aware framework for comparing site-selection criteria and decision-support methods across CO<sub>2</sub>, H<sub>2</sub>, and NG storage and across major geological options. Subsurface storage is becoming a central component of future energy systems, supporting decarbonization, energy-system flexibility, and hydrogen deployment. As a result, site selection is no longer purely a geological task but a multi-dimensional decision process that integrates reservoir physics, engineering, economics, regulation, and social considerations.

The analysis highlights how storage suitability depends on the interaction between geological properties, operational requirements, economic conditions, and regulatory context, and how these factors vary across gases and storage configurations. It also shows that while decision-support methods such as MCDM, GIS, simulation, and ML are increasingly mature, their effectiveness depends on data quality, transparent assumptions, and appropriate integration across scales.

A key finding is that no single method is sufficient on its own. Robust site selection requires hybrid workflows that combine structured ranking, spatial screening, and physics-based evaluation, while explicitly accounting for gas-specific behavior. CO<sub>2</sub> storage emphasizes containment, pressure management, and long-term trapping; hydrogen storage requires careful handling of mobility, losses, and purity; and NG storage prioritizes deliverability and cycling performance.

Looking forward, progress will depend on the development of integrated and adaptive decision platforms. These should combine transparent multi-criteria methods, spatial analysis, simulation, and data-driven tools within a staged workflow that evolves with data availability. Gas-specific criteria, clear uncertainty treatment, and continuous integration of monitoring data are essential to improve reliability and decision confidence. Standardized datasets, consistent economic metrics, and explainable decision outputs will further support regulatory acceptance and investment.

With coordinated advances in data, methods, and governance, subsurface storage can move from a technically feasible option to a reliable and scalable component of energy infrastructure. This will enable durable CO<sub>2</sub> containment, flexible



**Fig. 4.** Research priorities for advancing subsurface storage decision-support frameworks.

NG balancing, and technically credible hydrogen storage, supporting a more resilient and low-carbon energy system.

### Acknowledgements

The corresponding author gratefully acknowledges support from the Hydrogen Energy Research Center and the Mowry Shale initiative at the School of Energy Resources, University of Wyoming.

### Supplementary file

<https://doi.org/10.46690/ager.2026.06.08>

### Conflicts of interest

The authors declare no competing interest.

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