

Research Paper

Energy capacity and injection strategy evaluation for the conversion of natural gas storage to hydrogen storage

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ABSTRACT

Hydrogen has emerged as a key energy carrier in the global transition toward low-carbon energy systems, driving increasing interest in Underground Hydrogen Storage (UHS) as a large-scale energy balancing solution. Repurposing existing Underground Gas Storage (UGS) facilities provides a practical pathway for early UHS deployment by leveraging established subsurface infrastructure. This study investigates the technical feasibility of converting a depleted gas reservoir from UGS to UHS using an energy-based framework, in which storage and withdrawal performance are evaluated in terms of energy units (TJ/day) rather than gas volume or mass.

A three-dimensional compositional reservoir model of a dome-shaped depleted gas reservoir was developed using CMG-GEM to simulate cyclic natural gas and hydrogen storage operations. The results indicate a pronounced reduction in deliverable energy following conversion, with hydrogen storage providing approximately 12 TJ/day compared to about 48 TJ/day during natural gas storage under equivalent volumetric operating conditions. Increasing the hydrogen injection rate to four times that of natural gas restores the energy injection capacity to levels comparable to UGS. Several operational strategies were evaluated to enhance UHS performance, including cushion gas reduction, extension of the hydrogen injection period, and the use of horizontal wells. Among these, reducing cushion gas volume proved most effective in improving early-cycle hydrogen injectivity. Caprock integrity was assessed under cyclic loading using geo-mechanical scenarios representing stress-independent, elastic, and elasto-plastic behavior. The results demonstrate that stress-induced deformation and hysteresis can significantly increase hydrogen leakage, highlighting the critical role of pressure management in UHS operations. In addition, a screening-level assessment of hydrogenotrophic methanogenesis was incorporated through a simplified reaction model, indicating that microbial hydrogen consumption remains limited under the temperature and salinity conditions of the studied reservoir.

1. Introduction

It is well known that, storage is an essential component in completing the distribution chain of any type of energy to enhance flexibility and ensure the security of consumer markets [1,2]. Utilizing underground structures enables large-scale energy storage, particularly for gaseous energy. Consequently, when the natural gas distribution chain is recognized as a mature chain worldwide, Underground Gas Storage (UGS) is identified as a key element [3–5]. It should be mentioned that, over 70% of underground natural gas storage facilities have been developed in depleted gas reservoirs, making this storage method the most conventional approach to securing the global gas supply [6].

With global warming and increasing environmental concerns, the energy transition from fossil fuels to clean and renewable energy sources has garnered unprecedented attention. Hydrogen, as a clean and sustainable energy carrier, is a key element in the transition toward renewable energies and reducing fossil fuel consumption [7–9]. The role of hydrogen as an energy carrier is crucial, as it can store and transport energy generated from intermittent renewable sources, making it available for use at different times and locations [10,11]. Hydrogen's ability to store and transport energy enhances the flexibility of energy networks and ensures the stability of the energy supply [12,13]. Moreover, hydrogen can replace fossil fuels in industrial processes such as steel production and chemical fertilizer manufacturing, significantly reducing greenhouse gas emissions in these sectors.

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Nomenclature

H_2	Hydrogen
MMScf (unit)	Million Standard Cubic Feet
CCS	Carbon Capture and Storage
UHS	Underground Hydrogen Storage
D	depth
nc	number of components
N_i	moles of component i per unit block volume
P	pressure
P_{cog}	oil-gas capillary pressure
Q	injection/production rate
T_j	transmissibility of phase j

V	grid-block volume
y_{ij}	mole fraction of component i in phase j
γ	specific gravity or gravity term in flow equation
Δt	timestep
ρ_m	molar density of phase m
Φ	porosity
Ψ	function
(k)	iteration level
N	old time level
$n + 1$	new time level
I	component
J	phase

Given the gaseous nature of hydrogen and the ongoing energy transition toward sustainable clean energies, a supply chain similar to that of natural gas can be envisioned for hydrogen [14–16]. Considering that the geographical distribution of renewable energy sources worldwide is broader compared to fossil fuels, it appears that the hydrogen supply chain could have an even wider geographical reach than that of natural gas. Underground hydrogen storage (UHS) technology, which can scale up the hydrogen supply chain, becomes a critical consideration in such a scenario [17,18]. Hydrogen storage requires an extensive distribution network, high pressure, and secure locations. These factors make geological structures essential for hydrogen storage.

Among fossil fuels, natural gas is expected to experience the least decline in demand during the energy transition, with predictions suggesting that its distribution network may even expand [19,20]. Consequently, UGS projects are anticipated to maintain their significance in the coming years. However, the advancement of hydrogen economy programs and hydrogen's pivotal role in the energy transition position it as a strong competitor to natural gas. As noted, gaseous energies cannot sustainably reach consumer markets without the development of underground storage. Therefore, one of the initial points of contention between the natural gas and hydrogen supply chains will likely emerge in underground storage. Given the geographic and geological limitations of suitable underground storage sites already utilized for natural gas storage, converting some natural gas storage facilities into hydrogen

storage sites appears inevitable for the sustainable development of hydrogen [21,22]. A wide range of geological options have been proposed for UHS, including unconventional gas reservoirs as potential candidates [23]. In parallel, converting existing natural gas storage hubs into hydrogen storage facilities is often considered more justifiable than developing new UHS sites from scratch, given the extensive geological knowledge, existing wells and surface infrastructure, and, in some cases, their proximity to consumer markets.

Underground storage of natural gas in depleted gas reservoirs has significantly enhanced the attractiveness of the natural gas supply chain over the past decades. As can be seen from Fig. 1-a notable difference exists between depleted gas reservoirs and other storage methods in terms of both the number of actively developed projects and the volume of natural gas storage [24]. Factors contributing to the appeal of depleted gas reservoirs include the availability of suitable storage facilities, a comprehensive understanding of reservoir structures, a lower cushion gas requirement compared to oil reservoirs and aquifers, a larger storage volume compared to salt caverns (Fig. 1-b), and fewer non-gaseous phases than other methods. Chen et al. (2023) [25] conducted a comprehensive techno-economic assessment of UHS across depleted gas reservoirs, salt caverns, and saline aquifers in the Intermountain-West region of the United States. By integrating regional energy demand analysis with geological capacity estimation, the study showed that geologic hydrogen storage could supply up to 72% of the

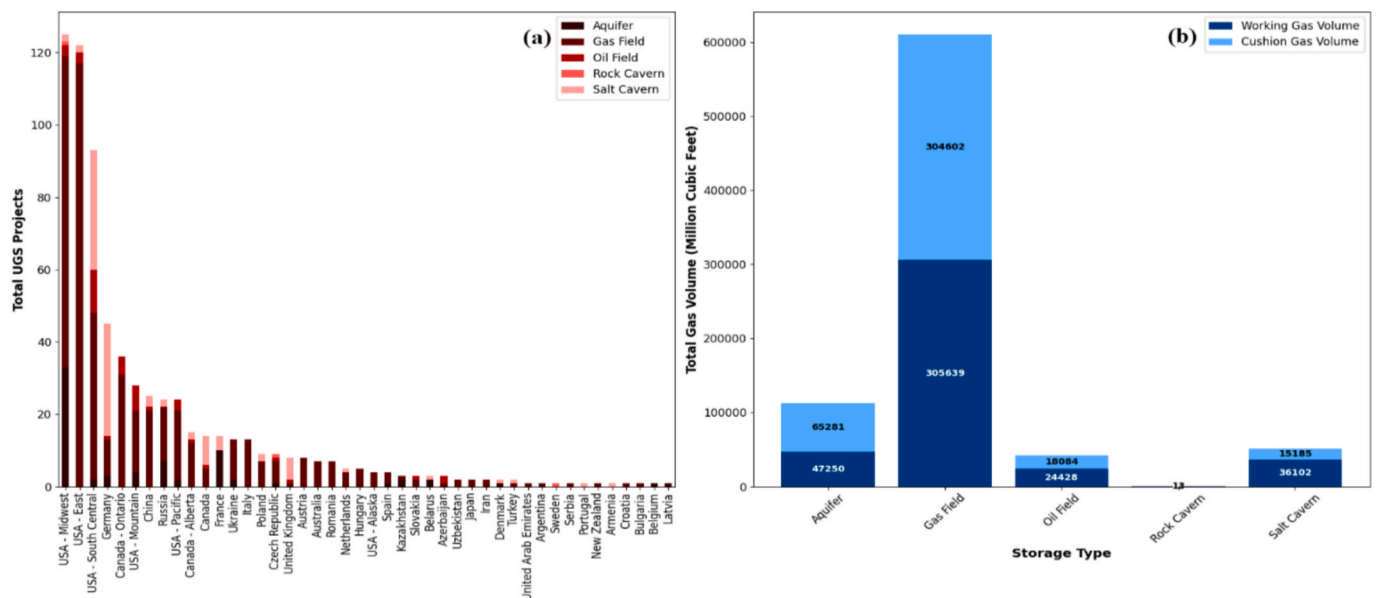


Fig. 1. (a): Quantitative distribution of UGS projects across countries worldwide. (b): Cushion gas and working gas volumes are stored using various natural gas storage methods [24].

region's 2020 energy consumption. Their results indicate that depleted gas reservoirs offer the most cost-effective storage option, with leveled storage costs significantly lower than those of salt caverns and saline aquifers, largely due to existing infrastructure and reduced site preparation requirements. These advantages can also be extended to hydrogen storage. Thus, depleted gas reservoirs emerge as the most suitable option for developing large UHS hubs. However, given the limited availability of such sites, converting existing UGS hubs into UHS hubs will become a significant focus.

The idea of converting UGS facilities into UHS is a viable option, but it comes with several challenges that need to be addressed. These challenges can be categorized into key areas, including designing suitable parameters for hydrogen storage operations, assessing gas leakage from the reservoir caprock, improving the purity of the produced hydrogen, and minimizing hydrogen loss within the reservoir. These issues are among the most critical factors that must be evaluated when transitioning a UGS hub into a UHS hub.

1.1. Proper design of operational parameters for underground hydrogen storage

One of the most important criteria for evaluating a gas storage project is the maximum volume of working gas stored in a given cycle [23,24]. This criterion depends on the reservoir's pore space, the fracture pressure of the reservoir rock, and the storage objectives. Similarly, the working gas volume achievable in a reservoir converted from UGS to UHS must be determined for UHS. A major cost in underground gas energy storage is the injection of cushion gas, which is essential for maintaining the pressure stability required for storage operations [28]. The volume and composition of the cushion gas play a critical role in enhancing storage efficiency. Following the conversion of a UGS project into a UHS facility, one of the key operational design questions is determining the appropriate volume and composition of the cushion gas [29–31]. Working gas injection and production rates during underground energy storage cycles are crucial and depend on the operational strategy. Usually, some structures are used to mitigate pressure fluctuations in the energy distribution chain, commonly referred to as peak shaving. These facilities must inject their energy content into the distribution network in the shortest possible time and quickly receive energy injections to prepare for future peak demand periods. Therefore, the deliverability and injectivity of hydrogen in the converted reservoir must be appropriately designed for such scenarios. Another critical parameter in designing UHS operations is the number of wells used in the process. The need for drilling additional wells compared to UGS operations, as well as the potential for reducing the number of operational wells, must be evaluated before the commencement of operations.

1.2. Evaluation of gas leakage from the reservoir caprock

The caprock of depleted gas reservoirs has demonstrated the ability to retain gas without leakage over millions of years. This stability has been further confirmed during several years of UGS operations. Safety and stability must also be verified when converting a gas storage facility into hydrogen storage. Concerns about hydrogen leakage from the caprock of underground reservoirs remain one of the most challenging and longstanding issues in UHS operations [32–34] [NO_PRINTED_FORM] The petrophysical properties and the balance of reservoir forces in the caprock must be carefully evaluated to ensure its safety in retaining hydrogen within the depleted reservoir structure. Recent studies have shown that hydrogen interactions with caprock can alter its sealing capacity through both geochemical and physical mechanisms. Hashemi and Sedaei (2025) demonstrated that changes in pH, temperature, pressure, and salinity affect mineral stability and porosity [35]. Ajibona and Pandey (2024) found that prolonged hydrogen exposure increases porosity and permeability in shale due to micro-fracturing [33]. Hashemi et al. (2025) highlighted the importance of vertical

permeability and injection parameters in hydrogen leakage risk [36]. However, these studies did not consider reservoirs previously used for UGS, where caprocks are cyclically stressed. This mechanical fatigue can further compromise sealing integrity, making hydrogen leakage more likely in such settings. Careful evaluation of caprock condition in repurposed UGS sites is therefore essential for safe UHS deployment.

1.3. Hydrogen reactivity: Microbial consumption and geochemical controls

UGS has traditionally relied on natural gas, a fluid that is not foreign to the subsurface environment and has existed within geological formations over millions of years. Through long-term geochemical equilibration with reservoir minerals, connate water, and native microbial communities, natural gas typically exhibits a stable and predictable behavior, with minimal risk of triggering significant biochemical or geochemical alterations during storage operations. As a result, UGS systems have historically required limited consideration of microbially mediated reactions or mineral–fluid interactions beyond standard integrity assessments. In contrast, hydrogen represents a chemically and biologically reactive molecule that is not naturally abundant in most subsurface reservoirs and can behave fundamentally differently from natural gas when injected into geological formations. Its small molecular size, high diffusivity, reducing potential, and role as an energy source for various anaerobic microorganisms introduce new uncertainties that were not relevant in conventional UGS systems. Previous studies on UHS have predominantly focused on hydrodynamic and operational aspects, such as flow behavior, mixing, and cyclic performance, while geochemical and microbial processes have received comparatively less attention [37]. Experimental studies indicate that hydrogen exhibits wettability and adsorption behavior markedly different from natural gas in reservoir rocks, underscoring the need to explicitly account for hydrogen–rock interactions in UHS assessments [38]. Hydrogen can participate in several microbial metabolic pathways or engage in abiotic redox reactions with iron-bearing or carbonate minerals, depending on the prevailing geochemical conditions [39,40]. These potential reaction pathways raise important questions about hydrogen stability, storage integrity, gas purity, and long-term reservoir performance in UHS projects. As a result, understanding the spectrum of microbial and geochemical processes that can influence hydrogen behavior in the subsurface has become a central theme in current UHS research. Table 1 provides an overview of these processes, their mechanistic pathways, and the environmental constraints that govern their activity.

Before converting a UGS site to UHS, a site-specific assessment of the processes listed in Table 1 is required to clearly distinguish the behavior of hydrogen from that of natural gas in the same reservoir. This evaluation should consider reservoir history, fluid composition, rock mineralogy, formation temperature, and brine salinity, as these factors control whether microbial or geochemical reactions may occur. Such an assessment is necessary to determine how hydrogen storage may differ from conventional gas storage and to identify which processes, if any, are relevant for a given reservoir.

1.4. Enhancing the purity of produced hydrogen gas and reducing hydrogen loss in the reservoir

The ideal scenario for a UHS project is achieving 100% purity in the produced gas stream and a 100% recovery factor. However, reservoir heterogeneities, mixing of hydrogen with natural gas or cushion gases, and interactions with other phases make this ideal challenging to achieve [32,33]. In converting a UGS project into a UHS, continuous monitoring of these two parameters, aimed at improving the quality of the produced gas stream and ensuring the economic efficiency of the project, can guarantee the operation's success. These two parameters can also serve as the basis for project optimization.

Previous studies have covered multiple aspects of the conversion of

Table 1

Overview of microbial and abiotic (geochemical) reactions involving hydrogen in subsurface environments and key environmental constraints controlling their activity.

Reaction Category	Representative Reaction Pathway	Products / Consequences	Conditions Required for Activity	Environmental Limitations / Inhibitors	Key References
Sulfate Reduction (Microbial SRB)	$\text{SO}_4^{2-} + 4\text{H}_2 + 2\text{H}^+ \rightarrow \text{H}_2\text{S} + 4\text{H}_2\text{O}$	H_2S , acidification, mineral scaling	Presence of sulfate; anaerobic conditions; moderate-to-high temperature (25–100°C); salinity up to ~120 g/L	Absence of sulfate; extreme salinity (>150 g/L); temperatures > 100°C; nutrient limitation	Dopffel et al., 2021 [41]; Viveros et al., 2025 [40]
Hydrogenotrophic Methanogenesis	$\text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{H}_2\text{O}$	Methane generation; carbon isotope shifts	Strict anaerobiosis; CO_2 availability; wide temperature range (30–110°C species-dependent); salinity 45–200 g/L; neutral pH	Outcompeted by SRB when sulfate exists; very high salinity (>200 g/L); low nutrient availability	Dopffel et al., 2021 [41]; Vasile et al., 2023[42]
Acetogenesis (Microbial)	$2\text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_3\text{COO}^- + \text{H}^+ + 2\text{H}_2\text{O}$	Acetate formation	Low-moderate salinity (<40 g/L); temperatures < 50–60°C; neutral pH	Strongly inhibited by high salinity (>40 g/L) and high temperature (>60°C)	Viveros et al., 2025 [40]
Iron Reduction (Microbial IRB)	$\text{Fe (III)} + \text{H}_2 \rightarrow \text{Fe}^{2+} + \text{H}_2\text{O}$	Dissolution of iron minerals; Fe^{2+} release	Bioavailable Fe(III) minerals; moderate temperature; availability of organic carbon	Limited in high salinity; limited in hydrocarbon-rich reservoirs; absent when Fe (III) scarcity exists	Viveros et al., 2025 [40]
Nitrate Reduction / Denitrification	$\text{NO}_3^- + \text{H}_2 \rightarrow \text{N}_2 + \text{H}_2\text{O}$	Nitrogen gas production	Presence of nitrate; anaerobic or suboxic conditions	No activity when nitrate is absent; inhibited under extreme salinity or high temperatures	Dopffel et al., 2021 [41]
Abiotic Hydrogen–Iron Mineral Reactions	H_2 reducing Fe(III) oxides to Fe(II)	Fe^{2+} formation; minor mineral alteration	Reactive Fe-oxide surfaces; acidic-neutral pH; elevated temperature (>120°C)	Reaction rates extremely slow below ~120°C; strongly inhibited in saline brines	Viveros et al., 2025 [40]
Carbonate Precipitation (Indirect, pH-driven)	H_2 -driven pH shifts $\rightarrow \text{CaCO}_3/\text{MgCO}_3$ precipitation	Carbonate scaling; porosity alteration	Presence of $\text{Ca}^{2+}/\text{Mg}^{2+}$; high alkalinity; microbial alkalinity generation	Requires microbial activity; inhibited in hypersaline or water-limited systems	Viveros et al., 2025 [40]
Sulfide Mineral Precipitation	$\text{H}_2\text{S} + \text{Fe}^{2+} \rightarrow \text{FeS} / \text{pyrite}$	Pyrite/FeS formation; permeability alteration	Requires microbial H_2S generation (SRB) + dissolved Fe^{2+}	Absent if SRB inactive or sulfate unavailable	Viveros et al., 2025 [40]

UGS to UHS. Reitenbach et al., in 2015, examined the capacity of porous underground storage facilities for hydrogen storage alongside natural gas and assessed the effects of hydrogen on the integrity of the underground structure and the technical equipment of these facilities. The study concluded that, due to the microbial activity of hydrogen, there is a significant risk of losing the sealing capacity of the caprock and chemical reactions when converting a UGS hub to a UHS or when storing hydrogen simultaneously with natural gas, unless significant changes are made to the design of operations and equipment [22]. Lackey et al. in 2022 investigated the feasibility of repurposing natural gas underground storage facilities for hydrogen storage, yielding important results. They estimated that switching from natural gas storage to pure hydrogen storage would significantly reduce the energy yield of these facilities, from 1,282 TWh to 327 TWh, a decrease of about 75%. This reduction is due to hydrogen's lower energy density than natural gas; each unit volume of hydrogen provides less energy than natural gas. Additionally, the lower molecular weight of hydrogen means that, for the same volume, less hydrogen can be stored. Furthermore, the differing thermodynamic properties of hydrogen may affect the optimal performance of systems designed for natural gas storage, reducing their efficiency. However, the study suggests that using a blend of 20–60% hydrogen with natural gas in these facilities could effectively meet energy needs and also reduce the demand for new hydrogen storage facilities [21]. Camargo et al., in 2023, further explored the conversion of natural gas underground storage systems into hydrogen storage systems. They developed a new viscosity model for gas mixtures containing hydrogen and evaluated cost-effective injection and withdrawal strategies for this process through reservoir simulations. The newly developed model introduced modifications to the viscosity model of mixtures, improving the accuracy of predictions. The results showed that creating and maintaining a stable hydrogen layer above the injection point of the well helps prevent large fluctuations in the composition of the produced gas. Additionally, managing buoyancy forces and overcoming gravity is crucial for optimizing the efficiency of these systems [45]. Hibbard and Gilfillan, in a study published in 2024, investigated the feasibility of hydrogen storage at both active and inactive natural gas storage sites in

the USA. They estimated that active sites could store 312 TWh of hydrogen, which exceeds the energy required to supply a 100% renewable grid in the country. Furthermore, for the first time, the storage capacity of inactive sites was assessed, revealing that these sites could store 3.9 TWh of hydrogen. Their conclusions indicate that inactive sites are suitable for initiating seasonal hydrogen storage, but active sites with larger capacities will be necessary to meet future demands [46].

So far, only a few studies have focused on reservoir simulation for converting UGS to UHS, and these studies have primarily referred to the mass and injected/produced hydrogen. However, in addition to the challenges of converting UGS to UHS, it is also essential to assess the stored and produced energy alongside these challenges. Although the energy density of hydrogen by weight (120 MJ/KG) is higher than that of natural gas (55 MJ/KG), the lower density of hydrogen gas compared to natural gas means that, for the same volume in an underground storage reservoir, the stored energy in a UHS facility is lower than in a UGS facility. As a result, converting a natural gas storage reservoir to hydrogen significantly reduces the energy capacity of the reservoir, and to store the same amount of energy, a much larger volume of hydrogen must be stored. Secondly, this reduction in capacity means that more storage space or higher pressures will be required to compensate for the lower stored energy. One of the main goals of this study is to evaluate various technical factors for increasing the energy output of a UHS project. This study goes beyond the existing literature by integrating dynamic reservoir simulation with a comprehensive energy-based analysis, providing a holistic evaluation of the technical factors influencing the energy output of UHS projects. Unlike previous research, which has predominantly focused on mass flow and hydrogen purity, this work emphasizes the energy storage and delivery efficiency of converted reservoirs, addressing a critical gap in the understanding of UHS performance. Further novelty of this study lies in the explicit evaluation of hydrogen leakage under different geo-mechanical caprock response scenarios, recognizing that seal integrity proven in UGS operations does not necessarily guarantee comparable performance in UHS systems. By modeling elastic, elastic-plastic, and base-case conditions,

the study quantifies the impact of stress-induced deformation and hysteresis on long-term sealing capacity, highlighting the necessity of operational pressure control to mitigate leakage risks and ensure both storage integrity and energy retention.

2. Methodology

To assess the feasibility of converting natural gas storage operations into UHS, a robust and numerically stable reservoir dynamic model was developed. In this study, a three-dimensional reservoir model with a dome-shaped structure and heterogeneous properties was constructed using the CMG GEM compositional simulator. The numerical model consists of a corner-point grid with a total of 9,000 grid blocks, of which 2,890 cells are active. The grid is discretized into 17×17 cells in the lateral directions (X and Y) and 10 layers in the vertical direction (Z). The inactive cells correspond to non-reservoir regions outside the structural closure and do not affect flow or storage behavior within the active domain. The grid resolution was selected based on a grid sensitivity analysis to ensure an adequate balance between numerical accuracy and computational efficiency, and the resulting grid configuration was applied consistently across all simulation scenarios. All simulations were performed using the fully implicit compositional formulation implemented in CMG GEM, which solves the coupled mass conservation equations for multicomponent, multiphase flow in porous media. The resulting nonlinear system of equations was solved using a Newton–Raphson iterative scheme, ensuring numerical stability under cyclic injection and production conditions. Automatic timestep control was enabled to adaptively adjust timestep size based on convergence behavior and system nonlinearity. The reservoir model was initialized under hydrostatic equilibrium using the final state of the natural gas storage operation as the initial condition for hydrogen storage simulations. Initial pressure, phase saturations, and gas composition were assigned consistently throughout the model to represent the depleted reservoir state prior to hydrogen injection. Time discretization was handled using adaptive time stepping with an upper bound imposed on the maximum timestep to ensure stable resolution of transient pressure and compositional changes. The selected timestep range was verified to adequately capture the dynamic response of the system without affecting the reservoir-scale trends reported in this work. The geophysical properties of the created reservoir are briefly presented in Table 2.

Fig. 2 shows a cross-sectional view of the reservoir model. As can be seen the porosity and permeability are highest at the crest of the dome-shaped reservoir. As depth increases, both porosity and permeability decrease. The reservoir is considered depleted at a pressure of approximately 1000 psi based on field production indicators. At this stage, the recovery factor is high and the water–gas ratio shows a consistent increase, indicating the late-life production phase of the reservoir. These conditions are representative of typical depleted gas reservoirs considered for conversion to underground energy storage.

Fluid movement in a porous medium in a multiphase system follows the saturation of each phase and the relative permeability of the phase. The created gas reservoir has two phases: gas and water. The relative

permeability of each phase as a function of the gas phase saturation is presented in Fig. 3. The values provided in Fig. 3 were applied in the dynamic model.

Three-time periods must be simulated in a depleted gas reservoir to create a natural gas storage hub. The first period involves the depletion of the reservoir and the preparation of conditions for natural gas storage. The second period simulates the operation of natural gas storage in the reservoir, and the final period assesses the feasibility of establishing a UHS hub in the reservoir.

2.1. Modeling caprock mechanical response under cyclic stress for hydrogen leakage assessment

In addition to simulating fluid dynamics and energy performance during the transition from UGS to UHS, this study incorporates a novel geo-mechanical modeling approach to assess caprock integrity under cyclic stress conditions. The caprock is modeled as a low-permeability sealing layer using effective porosity and permeability values within the continuum-flow framework of the CMG reservoir simulator. The objective of this approach is to provide a reservoir-scale assessment of hydrogen containment rather than a pore-scale leakage analysis. While the base case scenario assumes a mechanically stable caprock with constant porosity and permeability, it fails to capture the potential effects of repeated injection and production cycles on the sealing capacity of the overburden. To address this limitation, three caprock stress-response scenarios were developed and integrated into the simulation workflow. Unlike previous studies that rely on generalized assumptions or idealized rock behavior, this work utilizes rock mechanical data obtained from the actual caprock formation of the studied reservoir. These data include stress–strain relationships, compressibility, and failure thresholds derived from laboratory measurements and field-based characterization. The three scenarios are:

Base Case – Stress-Independent Caprock: Assumes constant porosity and permeability regardless of cyclic loading.

Elastic Deformation Scenario: Captures reversible changes in porosity and permeability based on elastic stress–strain behavior. The caprock deforms under pressure but returns to its original state after unloading.

Elasto-Plastic Scenario with Hysteresis: Introduces irreversible deformation, where cyclic loading causes gradual damage accumulation. A stress-dependent porosity–permeability relationship was constructed using laboratory-measured hysteresis loops and plastic thresholds specific to the studied shale caprock. After each cycle, caprock permeability incrementally increases due to micro-fracturing and matrix dilation.

The base scenario, while practically unrealistic, is considered as a reference case for comparison purposes. The second scenario may occur in certain reservoirs where the caprock has a large elastic domain, or where the operational pressure range does not activate plastic deformation.

The third scenario represents the most complete and realistic caprock response under high-pressure storage operations and may develop in limited but critical storage conditions (Table 3).

Fig. 4 illustrates the qualitative representation of the three caprock mechanical response scenarios considered in this study. In the Base Case, the petrophysical properties of the caprock remain constant regardless of pressure variations, representing a stress-independent behavior. In the Elastic Case, the properties vary linearly with pressure changes, but the deformation is fully reversible, as indicated by the opposing arrows. In contrast, the Elasto-Plastic Case incorporates irreversible plastic deformation, producing a hysteresis loop in the pressure–property relationship. During each loading cycle, an initial elastic deformation is followed by plastic deformation, leading to a permanent shift in the caprock properties. This progressive alteration in porosity and

Table 2
Geophysical properties of the created reservoir model.

Reservoir Model Input Parameters	Value	Unit
Total grids	9000	–
Initial Reservoir Pressure	2700	psi
Temperature	160	F
Top depth	2800	ft
Thickness	200	ft
Average porosity	0.13	fraction
Average horizontal permeability	100	md
Average vertical permeability	12	md
Reservoir Water Salinity	130,000	ppm

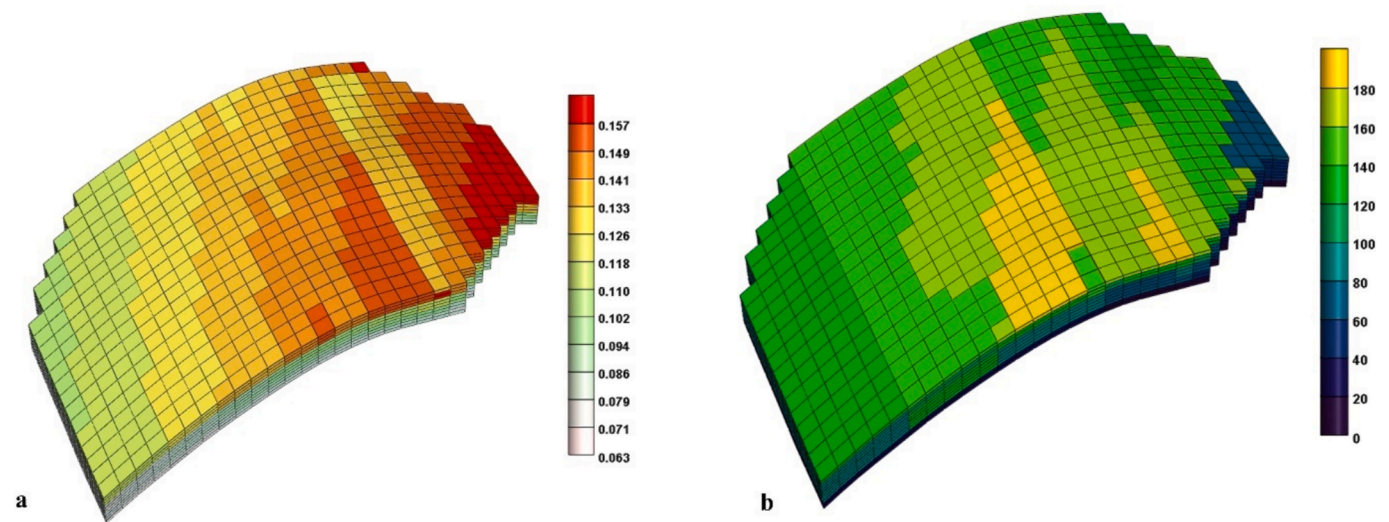


Fig. 2. Reservoir dynamic model view. (a) Porosity distribution of the reservoir, (b) Horizontal permeability (md) distribution the reservoir.

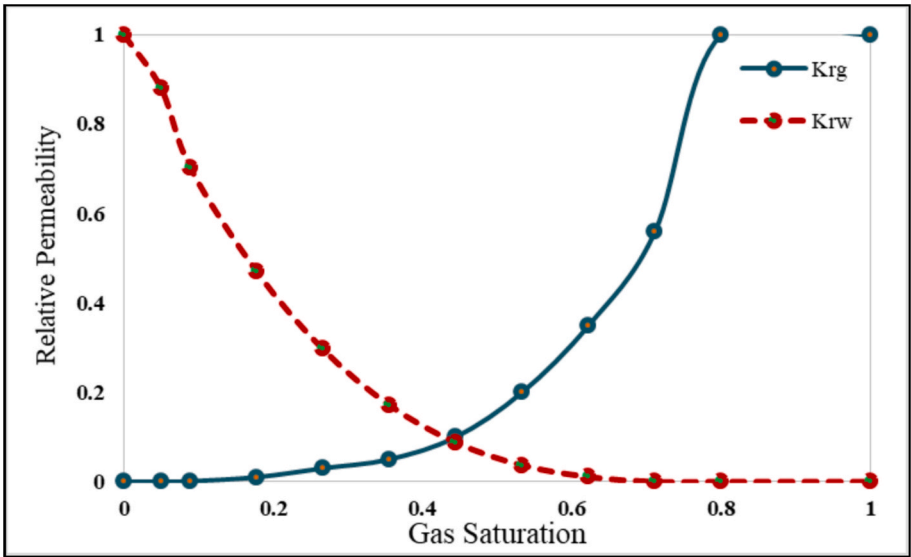


Fig. 3. Relative permeability of gas–water as a function of gas saturation in the reservoir dynamic model.

Table 3
Classification of caprock stress-dependent behavior scenarios developed in this study, highlighting the transition from idealized fixed-property assumptions to realistic hysteresis-informed elasto-plastic modeling based on actual rock mechanical data.

Scenario	Caprock Behavior	Stress Dependence	Porosity/Permeability Update	Hysteresis	Leakage Risk
Base	Fixed	No	No	No	Minimal
Elastic	Reversible	Yes	Dynamic (reversible)	No	Low
Elasto-Plastic	Irreversible	Yes	Dynamic (accumulative)	Yes	Medium–High

permeability can accumulate over multiple storage cycles, increasing the risk of hydrogen leakage.

This caprock behavior modeling was coupled with reservoir pressure data over multiple injection and production cycles. The simulations were conducted using a user-defined routine within CMG-GEM that dynamically updated caprock properties based on stress conditions. This approach enables a realistic assessment of hydrogen leakage risk due to mechanical fatigue, a key concern for long-term UHS operations in repurposed UGS sites.

2.2. Screening-level assessment of microbial hydrogen consumption

To address potential microbial hydrogen consumption during UHS, a screening-level evaluation was incorporated into the simulation framework. Microbial hydrogen consumption is represented using an equivalent reaction-based formulation within the CMG simulator. The objective is to evaluate the reservoir-scale impact of hydrogen consumption rather than to model detailed microbial kinetics or population dynamics. This approach provides an effective, upscaled representation of microbial effects within the conventional reservoir simulation framework. Based on a review of reported microbial pathways (Table 1)

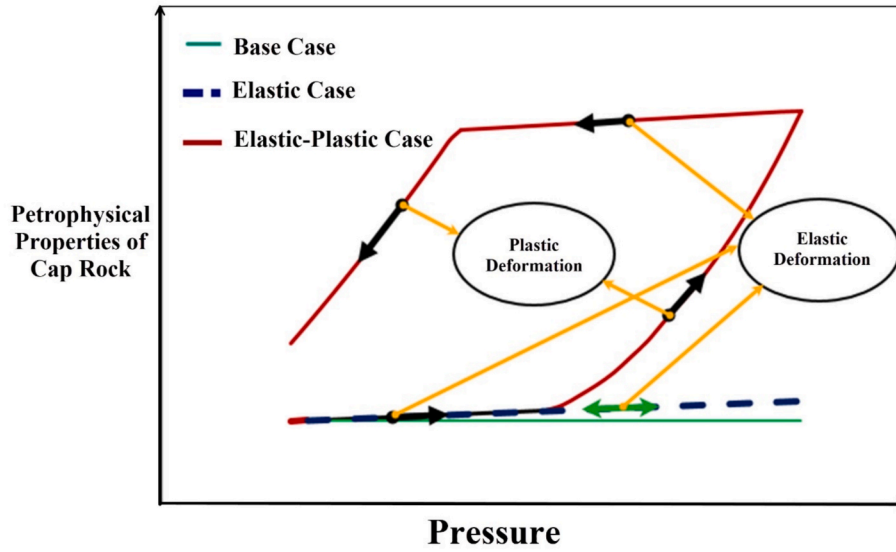


Fig. 4. Schematic comparison of base, elastic, and elasto-plastic caprock behaviors.

and their environmental constraints, a preliminary screening was performed considering key reservoir conditions, including formation temperature and formation-water salinity. This screening indicated that hydrogenotrophic methanogenesis represents the most plausible microbial pathway to be considered under the prevailing reservoir conditions, compared to other reported microbial processes. Therefore, a simplified representation of hydrogenotrophic methanogenesis was implemented using a pseudo-kinetic reaction within the compositional reservoir simulator. The reaction was defined according to the stoichiometric relationship:

and was enabled by the presence of CO_2 in the initial reservoir gas composition. A constant, low reaction rate was adopted to reflect unfavorable conditions for microbial growth associated with elevated temperature, high formation-water salinity, and limited gas–water contact. Microbial biomass growth, nutrient availability, and competitive microbial interactions were not explicitly represented; instead, the reaction was implemented as a weak, time-dependent hydrogen sink to obtain a screening-level estimate of the potential energy loss associated with microbial activity under reservoir conditions.

2.3. Governing equations

Here, four main categories of equations are used to simulate natural gas and hydrogen storage in a depleted gas reservoir, each addressing different aspects of the storage process.

1. Phase equilibrium equations

These equations define the equilibrium conditions between different phases for the components present in the system. Equations (1) represent the phase-equilibrium conditions that govern the distribution of each chemical component among the coexisting fluid phases. These relations ensure equality of fugacity for each component in all phases and form the thermodynamic foundation of the compositional simulation used in the present study:

$$g_i \equiv \ln f_{ig} - \ln f_{io} = 0 \quad i = 1, \dots, n_c \quad (1)$$

where f_{ig} and f_{io} denote the fugacities of component i in phases gas and oil, respectively.

2. Saturation equations

The saturation of each phase (water, natural gas, or hydrogen) is calculated using relations (2) and Equations (2)–(3) describe the phase-saturation relationships, linking component moles to the volumetric distribution of water, gas, and oil phases within the porous medium. These expressions provide the essential closure relations needed for tracking phase volumes during multiphase, multicomponent flow.

$$S_w = N_{nc+1} / (\Phi \rho_w) \quad (2)$$

$$S_g = 1 - S_w - S_o \quad (3)$$

where S_w is the water saturation, N_{nc+1} is the total number of moles of water in the system.

3. Flow equations in porous medium

The following equations are used to describe fluid flow in a porous medium. Equations (4–6) represents the generalized multicomponent flow equation used to compute the molar flux of each component between adjacent grid blocks. This formulation is based on Darcy-type flow and incorporates pressure gradients, gravity effects, phase-dependent transmissibilities, and component molar fractions. It corresponds to the standard nonlinear mass-balance residual solved internally by CMG-GEM in compositional multiphase simulations. Flow equations are calculated for all phases of reservoir fluids, and based on the type of reservoir and the fluids present, the terms of these equations will be utilized in the simulation.

$$\begin{aligned} \Psi_i = & \Delta T_o^m y_{io}^m (\Delta p^{n+1} - \gamma_o^m \Delta D) + \Delta T_g^m y_{ig}^m (\Delta p^{n+1} + \Delta p_{cog}^m - \gamma_g^m \Delta D) \\ & + q_i^m - \frac{V}{\Delta t} [N_i^{n+1} - N_i^n] = 0 \end{aligned} \quad (4)$$

$$N_i = \Phi (\rho_o S_o y_{io} + \rho_g S_g y_{ig}) \quad i = 1, \dots, n_c \quad (5)$$

$$N_{nc+1} = \Phi \rho_w S_w \quad (6)$$

where Ψ_i represents the flow equation for component i , ΔT_o^m and ΔT_g^m denote the transmissibilities of oil and gas phases, and Δp and ΔD denote the pressure and depth differences between adjacent grid blocks.

4. Mass conservation equations

The mass conservation of the system is ensured through equation (7). Equation (7) expresses the overall mass-balance residual for each grid

block, coupling the accumulation of component moles with the net inflow/outflow over the time step. This equation ensures mass conservation in the nonlinear solution process and is the core governing relation used by CMG-GEM to advance the compositional state of the reservoir.

$$\Psi_p \equiv \sum_{i=1}^{n_c+1} N_i^{n+1} - \Phi^{n+1} (\rho_o S_o + \rho_g S_g + \rho_w S_w)^{n+1} = 0 \quad (7)$$

where Ψ_p denotes the overall mass-balance residual for the control volume, ensuring conservation of all components across the time step. All of these equations have been fully implemented in the GEM module of the CMG software. The descriptions of each parameter used in these equations are provided in the Nomenclature section. Based on the results reported by Camargo et al. (2023) [43], the SRK equation of state was adopted in this study to model the phase behavior of hydrogen-containing gas mixtures. Previous studies have demonstrated that SRK provides reliable predictions of density, compressibility, and phase behavior for hydrogen–natural gas systems under reservoir pressure and temperature conditions. Given the scenario-comparison nature of this work, the consistent use of SRK ensures robust relative trends in fluid behavior.

2.4. Calculation of stored and produced energy

Due to the inherent differences between hydrogen and natural gas, a volumetric comparison of the gas delivered by a UGS facility with a UHS facility cannot serve as a suitable comparison criterion. The primary goal of underground energy storage is to enhance the flexibility of the energy supply network for downstream sectors. Regardless of the energy carrier fluid stored in underground reservoirs, the stored and delivered energy of an underground energy storage facility must be evaluated. To calculate the stored and produced energy for each cycle of underground natural gas and hydrogen storage, the values from Table 4 will be used.

3. Results

This study designed a comprehensive simulation scenario to assess the feasibility of converting a depleted natural gas reservoir, which was used as an UGS facility, into a UHS. The base model includes an operational period of 22 years, consisting of a 1-year cushion gas injection period, 11 years of natural gas storage operation, and 10 years of hydrogen storage operation. This two-phase simulation was designed to examine the dynamic behavior of gas injection, production, and storage over time, addressing the technical challenges related to the transition to hydrogen storage. The results of this scenario will be presented and analyzed in the following sections.

3.1. Base scenario

The base scenario serves as the benchmark for comparison in this study. After reservoir depletion, when the gas recovery factor reached approximately 80%, the reservoir pressure dropped from 2700 psi to 1000 psi. Cushion gas injection was conducted for one year using four vertical wells into the top six layers of the reservoir, with each well injecting at a rate of 40 (million standard cubic feet per day) (MMSCF/D).

Table 4

Comparison of density energy density (by weight and volume) of natural gas and hydrogen gas.

	Mass density (kg/Sm ³)	Lower heating value (LHV, MJ/kg)	Volumetric Lower Heating Value (LHV @ Standard Condition, MJ/L)
Natural Gas	0.68	55	0.0367
Hydrogen Gas	0.083	120	0.010

The injected cushion gas occupied 50% of the reservoir pore volume. The composition of the injected cushion gas was equivalent to the composition of the working gas during UGS operations. Following the injection of the cushion gas, the reservoir pressure increased to 1600 psi. This achieved pressure and injected volume are responsible for maintaining the stability of UGS operations and supporting the subsequent UHS operations.

It should be mentioned that, the UGS operations consisted of 11 cycles of natural gas injection and production, with each year including a six-month injection period and a six-month production period. During each UGS cycle, four wells injected gas at a rate of 10 MMSCF/D, with a maximum bottom hole pressure of 2100 psi. Based on geo-mechanical analysis of the reservoir rock, the fracture pressure of the caprock was estimated to be approximately 3000 psi. To ensure operational safety and account for the cyclic nature of underground energy storage, which increases the likelihood of rock fatigue, 70% of the fracture pressure was set as the maximum allowable injection pressure. The present study, the safety criterion was also applied to the UHS operations. During the six-month gas production phase, natural gas was produced at a rate equivalent to the injection rate. UHS operations were initiated at the end of the 11th year of UGS operations, following the same injection and production schedule as in UGS. Fig. 5 presents the results of UGS and UHS operations regarding reservoir pressure and injection rates. Both natural gas and hydrogen were injected into the reservoir at the maximum designed rate, indicating that the maximum injection pressure did not impose a limitation on the design rate. During UHS operations, the average reservoir pressure was higher than that observed during UGS. This pressure difference is attributed to variations in compressibility factors and the number of injected moles between hydrogen and natural gas. These differences persist despite equal injection volumes under standard conditions. Over time, the reservoir pressure during UHS increased further as the operational life extended. This trend requires further analysis to evaluate its implications on other operational parameters.

A volumetric comparison of the injection and production rates of natural gas in UGS operations with the volumetric rates of UHS operations cannot serve as a suitable criterion for managing the energy supply chain of an energy storage hub. During the injection of natural gas or hydrogen, energy is cumulatively stored in the reservoir, and during withdrawal, this energy is delivered to consumption destinations. As shown in Fig. 6, the energy injection and production rates in the UGS and UHS processes are presented. In the designed UGS operations, the injected volume of natural gas stores energy at a rate of 48 terajoules per day during each cycle. Similarly, the same amount of energy is withdrawn daily during production. However, upon converting the reservoir into a hydrogen storage hub, the daily stored energy significantly decreases to 12 terajoules per day. This reduction is primarily due to the considerably lower mass of hydrogen injected into the reservoir compared to natural gas, thereby reducing the stored energy in UHS operations compared to UGS. Consequently, the energy supply chain for a complete replacement of a UGS project with a UHS project, under similar operational conditions, cannot meet the required storage capacity.

From the production perspective, UHS operations exhibit greater complexity than UGS. During each production cycle, the produced gas stream consists of a mixture of cushion gas and hydrogen, and the composition of this mixture evolves over time. In the early UHS cycles, strong mixing between hydrogen and the remaining cushion gas leads to a lower hydrogen fraction in the produced gas, resulting in a relatively small hydrogen energy contribution despite the higher total energy production rate in these cycles. At the beginning of each production period, a higher proportion of hydrogen is produced due to its lower density and faster migration toward the wells. This results in an initially higher hydrogen energy production rate. However, as pressure depletion progresses and cushion gas moves toward the wellbore, mixing intensifies and the hydrogen fraction in the produced stream decreases.

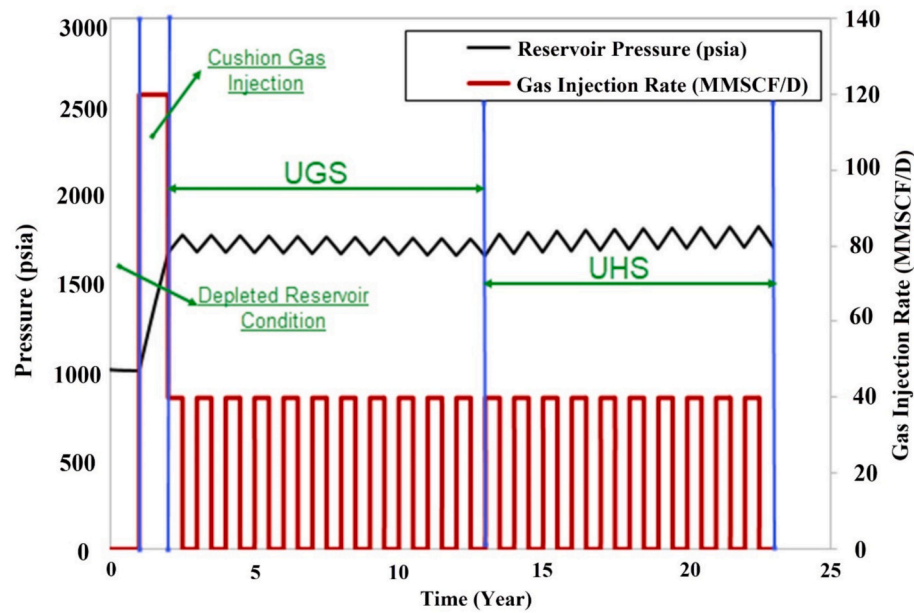


Fig. 5. Simulation Plan for UGS and UHS Processes in a Depleted Gas Reservoir.

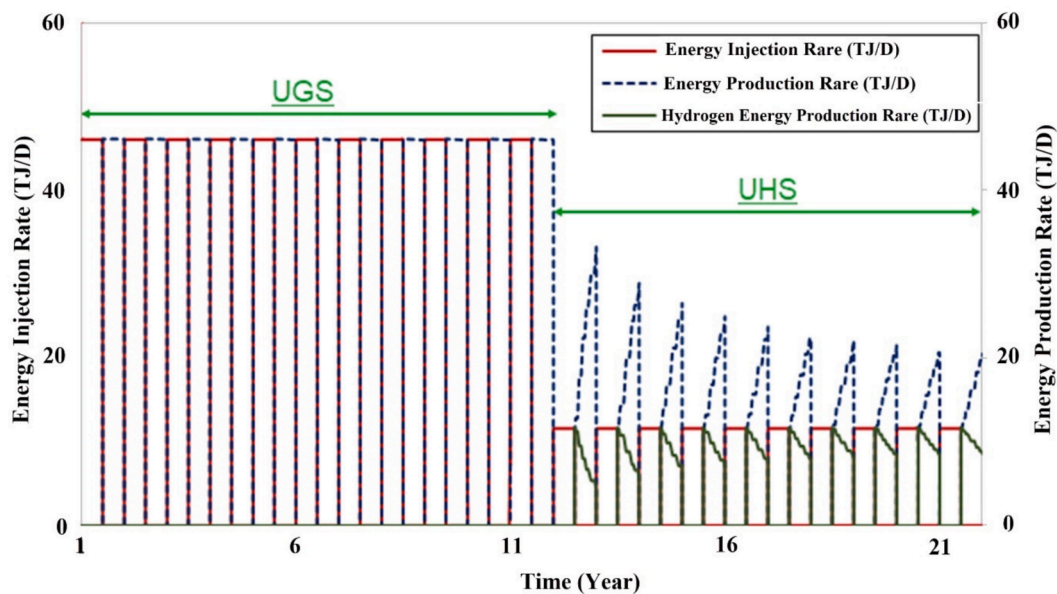


Fig. 6. Energy Injection and Production Rates.

This behavior is most prominent in the early cycles and gradually diminishes as the amount of cushion gas in the reservoir decreases over time. As UHS operations progress over multiple cycles, two trends emerge simultaneously:

- the total energy production rate decreases due to reservoir pressure decline and reduced overall deliverability
- the hydrogen energy production rate increases because the reservoir composition becomes more hydrogen-rich as cushion gas is progressively produced and some hydrogen remains trapped between cycles.

For example, the maximum total energy production rate decreases from 38 terajoules per day in the first cycle to 20 terajoules per day in the final cycle, while the hydrogen-derived share of the produced energy increases. This simultaneous decrease in total energy and increase in

hydrogen-derived energy is therefore consistent with the evolving reservoir composition and pressure behavior during UHS operations, and does not indicate a contradiction. Although mixing between hydrogen and natural gas remains a challenge—reducing hydrogen recovery efficiency and necessitating surface separation facilities—the co-production of natural gas and hydrogen during the early UHS cycles can still be beneficial within the broader energy transition context. In the early years of a UHS project, the natural gas produced alongside hydrogen can be effectively utilized in existing markets. As the operational life progresses and the hydrogen fraction in the produced gas naturally increases, UHS operations become increasingly aligned with the evolving needs of a hydrogen-oriented energy system. From the production perspective, UHS operations exhibit greater complexity than UGS. The energy production rate in UHS operations during each cycle has been higher than the injection rate. Consequently, the produced gas flow includes a mix of cushion gas and hydrogen. This mixing, caused by

interaction within the reservoir's porous medium, negatively impacts hydrogen recovery efficiency. In none of the 10 evaluated cycles was the hydrogen energy production rate fully aligned with the planned rate. At the beginning of each production cycle, the produced gas flow contains a higher proportion of hydrogen, initially leading to a higher hydrogen energy production rate. However, as pressure depletion spreads within the reservoir and the cushion gas moves toward the wells, mixing intensifies, reducing the hydrogen mass fraction in the produced gas flow. This effect is more pronounced in the early cycles of UHS operations and diminishes in later cycles. As the operational life of UHS increases, the overall energy production rate decreases while the hydrogen energy production rate increases. In the first storage cycle, the maximum energy production rate was 38 terajoules per day, which declined to 20 terajoules per day in the final cycle. The main reason for this behavior is the reduction of cushion gas in the reservoir during production and the increased hydrogen saturation due to incomplete production.

Mixing hydrogen with the reservoir's natural gas while increasing the energy extracted during UHS production cycles poses significant challenges. This includes reduced hydrogen recovery efficiency, a decreased proportion of hydrogen energy in the total energy produced, and the need for surface separation equipment, all of which can threaten the economic viability of a UHS project. On the other hand, as the hydrogen energy supply chain matures, the demand for natural gas will decrease, and the additional energy produced may not effectively contribute to hydrogen production and consumption control. Despite these weaknesses, it is important to note that converting UGS to UHS occurs within an energy transition context. During the early years of this transition, the additional energy resulting from the co-production of natural gas and hydrogen can be utilized effectively. Therefore, in the early stages of a UHS project, the mixing of hydrogen and natural gas can benefit from diverse energy markets characteristic of the transition period, helping to make the energy supply chain more flexible. As the project matures and the hydrogen energy share in the produced gas flow increases, it becomes better aligned with the evolving needs of energy markets, supporting sustainable hydrogen consumption.

The main drawback observed from converting UGS to UHS is the significant reduction in both stored and produced energy, which must be compensated by increasing the volume of stored hydrogen. Hydrogen gas, like natural gas in UGS operations, was injected into the six upper layers of the reservoir. Fig. 7 illustrates the distribution of hydrogen in the reservoir. Due to the low molecular weight of hydrogen and the effect of gravitational force on this gas in the porous medium, after injection, it tends to migrate towards the reservoir's cap rock. As a result, a large portion of the injected gas has migrated to the top three layers of the reservoir. After the production cycle, most of the remaining hydrogen in the reservoir is trapped in the upper layers. This remaining hydrogen, along with the reduction of cushion gas due to production alongside hydrogen, has led to the hydrogen share of the reservoir gases being at its highest level at the end of the production phase of the 10th storage cycle. This factor has resulted in the highest pressure in the reservoir at the end of the UHS process.

3.2. Increase in injected hydrogen volume

The hydrogen injection rate was increased compared to the base scenario to increase the energy stored in each cycle of the UHS operation. In the three cases examined, the hydrogen injection rate was doubled, tripled, and quadrupled relative to the base scenario. Fig. 8 illustrates the energy injection rate into the reservoir for both the UGS process and various UHS cases. By quadrupling the hydrogen injection volume rate into the reservoir, the daily energy injection rate into the reservoir reaches 48 terajoules, which is equivalent to the energy injection rate of the UGS operation. With doubling and tripling the hydrogen injection volume rate, the daily energy injection rate reaches 24 and 36 terajoules, respectively.

It is well known that, increasing the hydrogen injection volume rate can balance the energy generated by the UGS project. However, in the initial cycles, the injection was not fully continuous at the maximum hydrogen injection rate. This factor can be attributed to activating the maximum injection pressure constraint.

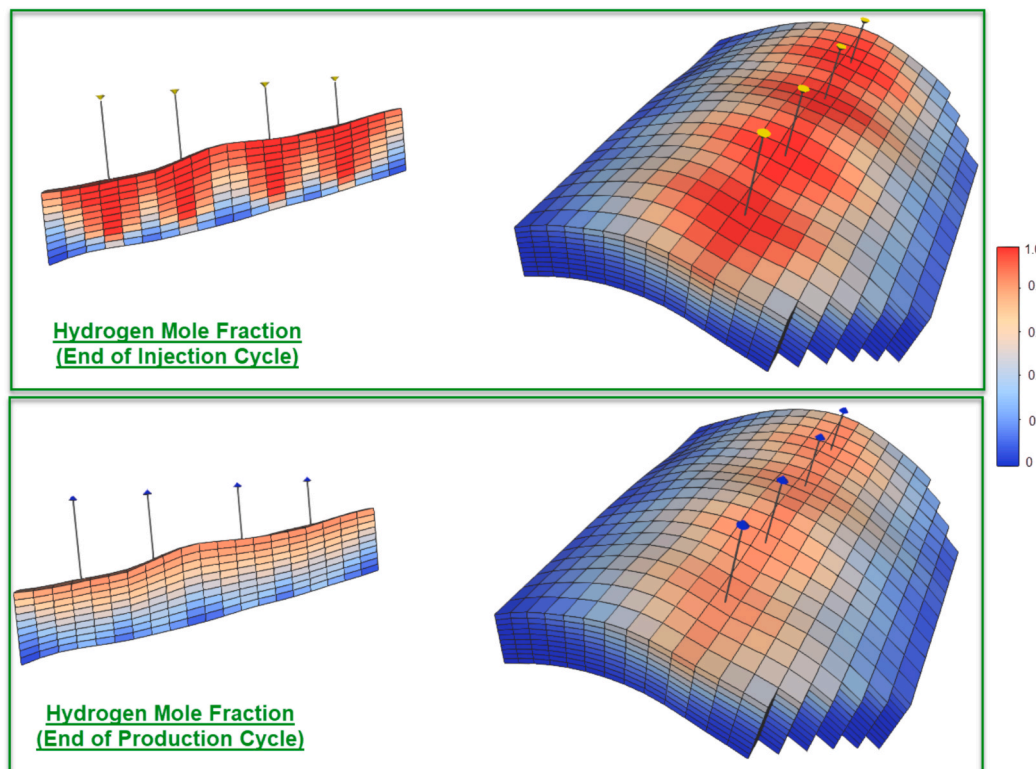


Fig. 7. Hydrogen gas distribution in the reservoir at the beginning and end of the 10th cycle of the UHS operation.

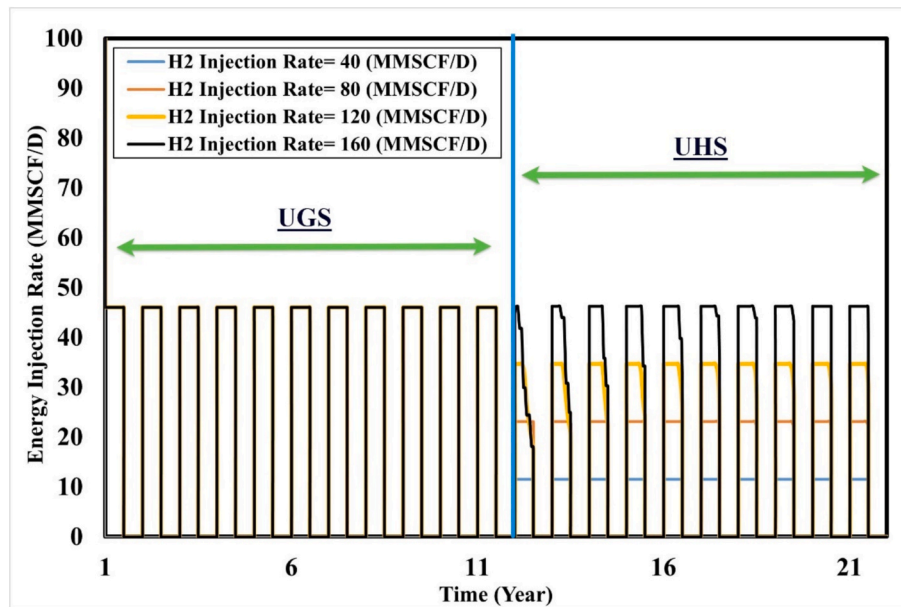


Fig. 8. Energy injection rate into the reservoir in the UGS process and different UHS scenarios.

Fig. 9 presents the status of the 160 MMSCF/D hydrogen injection case. During the first six cycles of hydrogen gas injection, the pressure limitation consistently prevented hydrogen injection into the reservoir at the maximum designed rate throughout the entire 6-month injection period. Production cycles were carried out at the maximum scheduled rate. This behavior indicates the presence of natural gas in the production flow from the wells. The reservoir pressure during the UHS operation with a hydrogen injection rate of 160 MMSCF/D showed a decrease until cycle 6, after which it stabilized (Fig. 9-A).

The energy produced in each production cycle exhibited behavior similar to the base scenario. In the early cycles, hydrogen contributed a small share of the produced energy (Fig. 9-B). Still, as the UHS operation progressed, hydrogen's share in the produced gas flow improved, and the dominant portion of the produced energy came from the hydrogen-derived gas flow. However, the UHS process must be able to both inject and produce energy in line with the planned volumes. Therefore, the 160 MMSCF/D hydrogen injection case was identified as the ideal case for replacing the UGS process with the UHS process in terms of injected and produced energy. In the following, strategies for improving hydrogen injection and production in this case will be evaluated.

3.3. Reduction of cushion gas volume

The increase in pressure due to hydrogen gas injection in the 160 MMSCF/D injection case, reaching the maximum injection pressure, prevented the hydrogen gas from being injected at the maximum planned rate. One of the initial proposed solutions to increase the injectivity of the reservoir wells was to reduce the cushion gas volume, thus lowering the reservoir pressure before the UHS operation. Therefore, the 11th cycle of the UGS operation was converted into a cushion gas depletion period lasting one year. Two scenarios were considered to examine the effect of cushion gas volume. In the first scenario, cushion gas was depleted from the reservoir at a rate of 6 MMSCF/D for one year, so that cushion gas filled 40% of the reservoir's pore space. In the second scenario, cushion gas was extracted at a rate of 12 MMSCF/D to reduce the cushion gas volume to 30% of the reservoir's pore space. The UHS operation was carried out as planned, with a hydrogen injection rate of 160 MMSCF/D.

It should be noted that the reservoir model used in this study does not include an active aquifer, and no external water-drive mechanism was defined in the boundary conditions. Therefore, the observed differences

between the 30–50% cushion gas scenarios are not associated with aquifer influx or external water invasion. Instead, the system behaves as a volumetric reservoir with only connate water present within the pore space. The differences in injectivity and pressure behavior are primarily governed by pressure redistribution and the effective pore volume available for hydrogen storage. Higher cushion gas volumes maintain a higher average reservoir pressure at the beginning of UHS operations, which reduces the available pore space for hydrogen injection and leads to earlier activation of the injection-pressure constraint at the wells. In contrast, lower cushion gas volumes reduce the initial pressure level, increase the effective pore volume available for hydrogen, and widen the operational pressure window during cyclic storage.

Reducing the cushion gas volume reduces the reservoir pressure at the beginning of the UHS operation. This factor creates more pore space for hydrogen gas, resulting in a significant improvement in hydrogen injection in the early cycles for the 30% cushion gas volume case compared to the 40% cushion gas volume case and the initial case (Fig. 10-A). Therefore, considering the high-pressure nature of the UHS operation compared to the UGS operation, reducing the cushion gas volume from the reservoir can enhance the injectivity of the wells. Reducing cushion gas in the reservoir and decreasing the pressure during operations reduces the mixing of hydrogen and natural gas within the reservoir. This factor facilitates the movement pathways of hydrogen in the reservoir. This hypothesis was evaluated based on the energy rate produced and the recovered hydrogen energy. As shown in Fig. 10-B, in the early cycles, the case with 30% cushion gas volume provided the highest rate of hydrogen energy production. The reduction in the mixing of hydrogen and natural gas results in decreased energy produced in the early cycles for the cushion gas volume reduction cases compared to the initial scenario. As the project progresses and a significant amount of cushion gas is produced, the initial scenario behaves similarly to the cushion gas volume reduction cases.

In the 30% cushion gas case, the minimum pressures during production reach lower values, while the peak injection pressures remain farther from the operational limits. This creates a wider operational pressure window and improves injectivity in the early cycles. In contrast, larger cushion gas volumes (40%–50%) maintain higher average reservoir pressures and narrower pressure oscillations, resulting in more stable but less flexible injection conditions. Overall, the pressure response demonstrates that cushion gas reduction enhances injectivity and pore-space availability, particularly during the initial UHS cycles

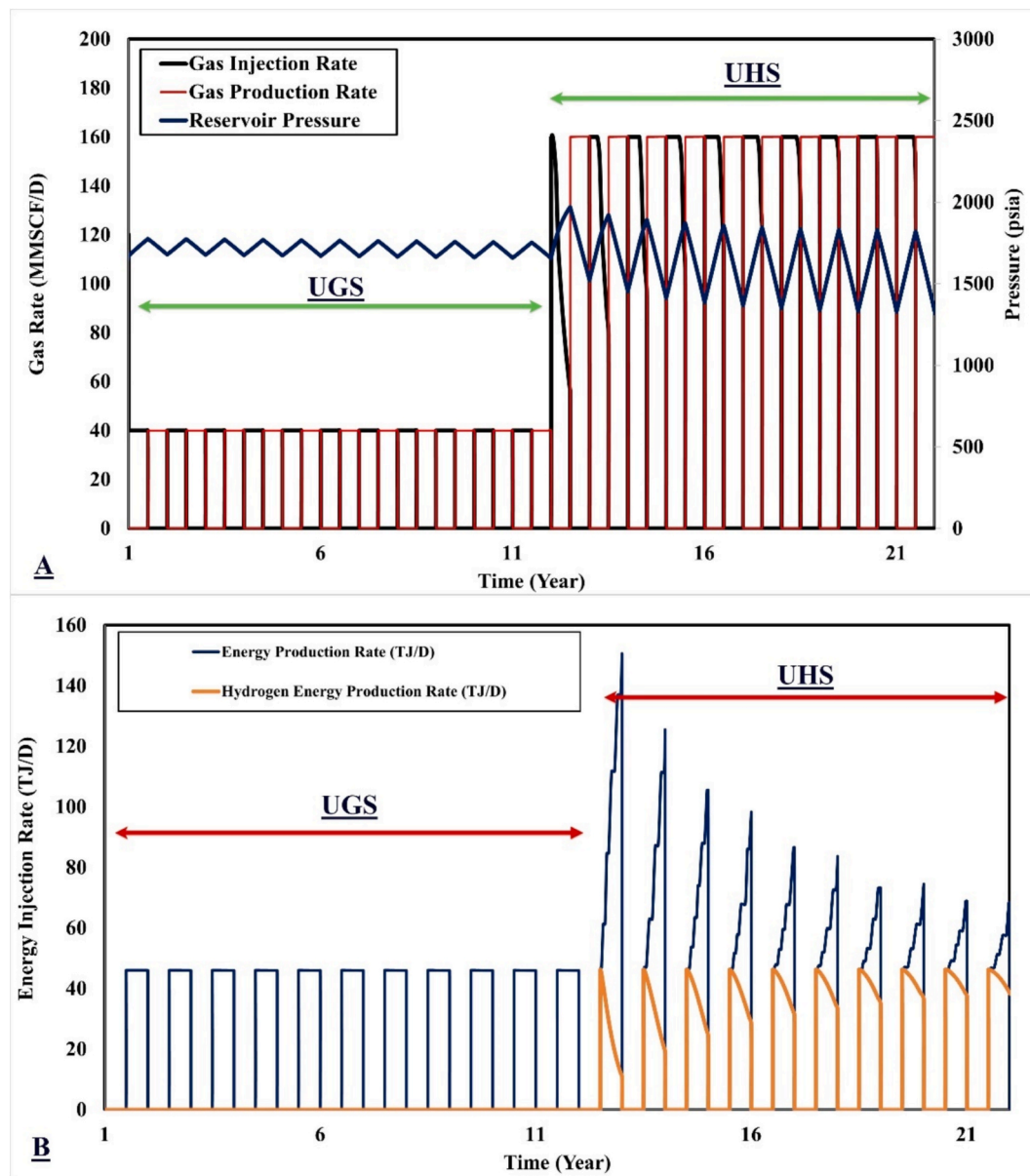


Fig. 9. Natural Gas and Hydrogen Injection and Production Rates in the UGS and UHS Processes for the 160 MMSCF/D Hydrogen Injection Case (A). Energy Production Rate and Hydrogen Energy in the 160 MMSCF/D Hydrogen Injection Case (B).

(Fig. 11). Importantly, this analysis confirms that using one of the final UGS injection–production cycles as a dedicated cushion-gas depletion period is an effective and practical strategy. This approach reduces the initial reservoir pressure before UHS startup, increases the available pore volume for hydrogen, and enhances injectivity without requiring any additional field operations beyond the existing UGS framework.

Reducing cushion gas during a depletion period before conducting the UHS operation is identified as a practical measure to improve hydrogen injection and production in the conversion of a UGS hub to a UHS. Given the nature of the energy transition, if there is a market for natural gas, cushion gas can be considered as part of the energy supplied in the early years of the UHS operation. Such an operational assumption can be implemented by considering the injectivity limitations of the wells for hydrogen and thoroughly evaluating the continuity of the cap rock.

3.4. Increasing the injection period duration

The volume of hydrogen injected into the reservoir during each storage cycle depends on the hydrogen gas injection rate and the duration of the injection period. Extending the injection period for injecting a specified volume of hydrogen reduces the injection rate. Consequently, one month was added to the hydrogen gas injection period, reducing the production period to 5 months. With the injection period extended to 7 months, the injection rate decreased to 137.15 MMSCF/D across four wells. Fig. 12 illustrates the total stored and produced energy during the UHS process for 7-month and 6-month injection periods. In the initial hydrogen injection and production cycles, approximately 2% more energy was stored in the reservoir due to the extended injection period. This difference remained constant as the injectivity of the initial scenario improved in the later cycles. From a production perspective, the two scenarios were compared based on the produced hydrogen energy. The total hydrogen produced in the two scenarios showed no significant difference. However, reducing the

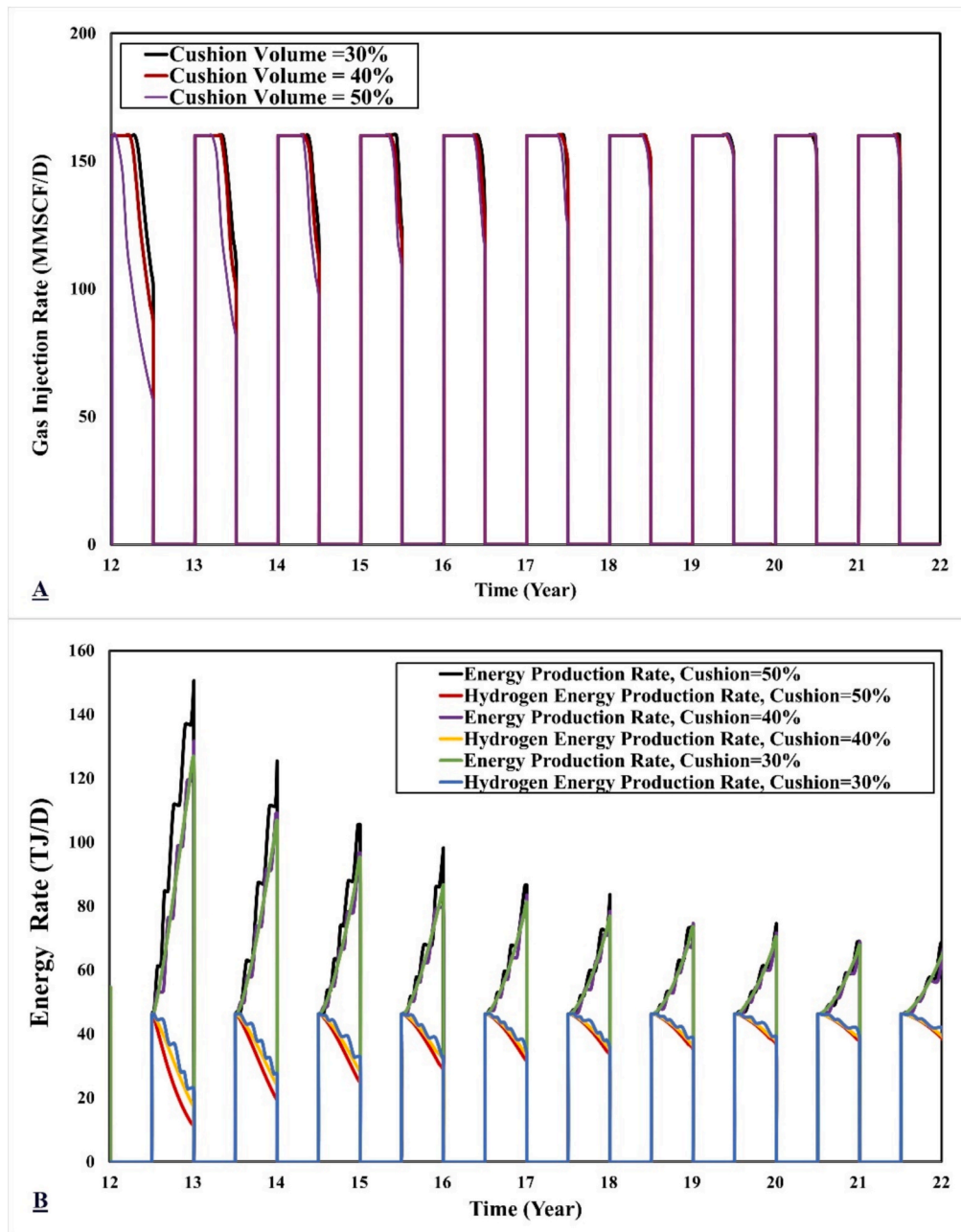


Fig. 10. Hydrogen Gas Injection Volume Rate into the Reservoir in Scenarios with Different Cushion Gas Volumes (A). Energy Production Rate and Hydrogen Energy from the Reservoir in Scenarios with Different Cushion Gas Volumes.

production period to 5 months led to a decrease in hydrogen recovery. Extending the injection period has a lesser impact on improving the quality of UHS operations than reducing cushion gas volume and even lowering the production recovery factor. Therefore, a strategy could be adopted where the injection period is extended in the initial cycles, and as the UHS operation stabilizes in the final cycles, equal durations for hydrogen injection and production periods are implemented.

Although the total planned hydrogen injection volume is identical in the 6-month and 7-month scenarios, the actual injected volume can differ in practice due to the maximum injection-pressure constraint at the wells. Extending the injection period reduces the instantaneous injection rate and modifies the near-well pressure behavior. Fig. 13 compares the injection-rate and bottom-hole pressure (BHP) responses for a representative injection well in the two scenarios. In the 7-month case, the lower instantaneous injection rate leads to a slower pressure buildup during the injection phase. As a result, the injection-pressure

constraint is reached more gradually, and the well operates within the allowable pressure limits for a longer portion of each cycle. In contrast, in the 6-month scenario, the higher instantaneous injection rate causes a faster pressure increase near the wellbore, which leads to earlier activation of the injection-pressure constraint. Under these conditions, the injection rate is effectively limited by the pressure constraint for a longer duration, and the planned injection volume cannot be fully delivered. Consequently, the effective injected hydrogen volume becomes slightly lower than the target value.

Therefore, the observed difference in retained hydrogen energy between the two scenarios is primarily a constraint-driven, near-well pressure effect rather than a consequence of intrinsic reservoir properties. Under the studied reservoir and operational conditions, this mechanism results in a modest improvement of approximately 2% in stored energy for the 7-month injection scenario. This effect is case-specific and secondary compared to the influence of cushion-gas

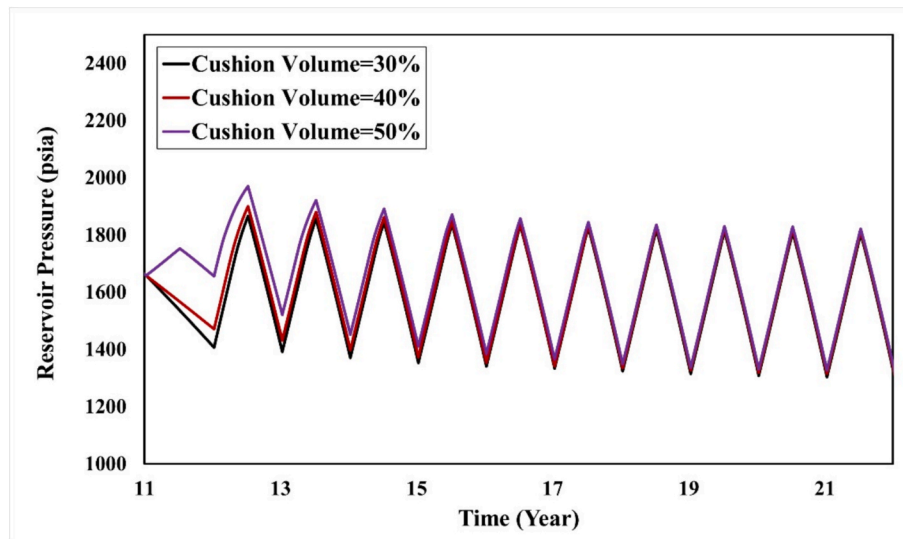


Fig. 11. Reservoir pressure profiles for different cushion gas volumes (30%, 40%, and 50%) during cyclic UHS operation.

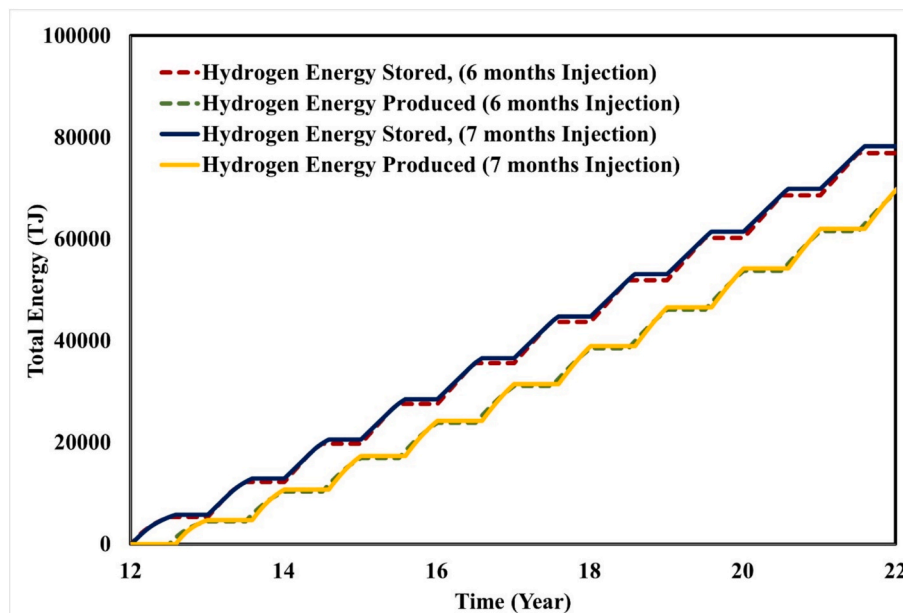


Fig. 12. Total Stored and Produced Hydrogen Energy in the UHS Process for Scenarios with Different Injection and Production Periods.

reduction.

3.5. Using horizontal wells

Among the methods for UHS, depleted reservoirs offer an advantage due to the presence of existing surface and subsurface infrastructure and a comprehensive understanding of reservoir structures. However, one of the significant costs associated with such projects is drilling new wells for hydrogen injection and production. If proven safe, existing wells in depleted reservoirs or UGS hubs can significantly reduce the initial capital investment required for UHS projects. Nevertheless, the reuse of existing wells is conditional upon a thorough evaluation of material compatibility and well integrity under hydrogen service conditions, as hydrogen embrittlement and sealing performance may represent critical safety and economic constraints. That said, the flexibility of hydrogen supply chains and the high value of hydrogen production raise the notion that improving UHS equipment quality and implementing well-planned operational strategies can enhance hydrogen injectivity and

production. Horizontal wells can play an effective role in improving the injection and production processes of hydrogen from underground reservoirs. One of the main advantages of horizontal wells is the increased contact area with the reservoir. Due to its low density, hydrogen tends to migrate upward, potentially accumulating in the upper sections of the reservoir in vertical wells. Horizontal wells, however, mitigate this localized accumulation and create a more balanced injection and production process. From an economic perspective, horizontal wells offer cost advantages by covering a larger reservoir area and reducing the need for multiple wells, thus lowering operational expenses and improving economic returns. This broader coverage facilitates more uniform hydrogen injection and distribution, preventing localized gas accumulation. Similarly, hydrogen production from horizontal wells tends to be more uniform due to extraction from various reservoir parts, reducing pressure drop along the flow path and enhancing production efficiency. The use of horizontal wells in UGS operations is not standard practice. Therefore, the likelihood of existing horizontal wells is minimal in converting a UGS project into a UHS hub. Drilling horizontal

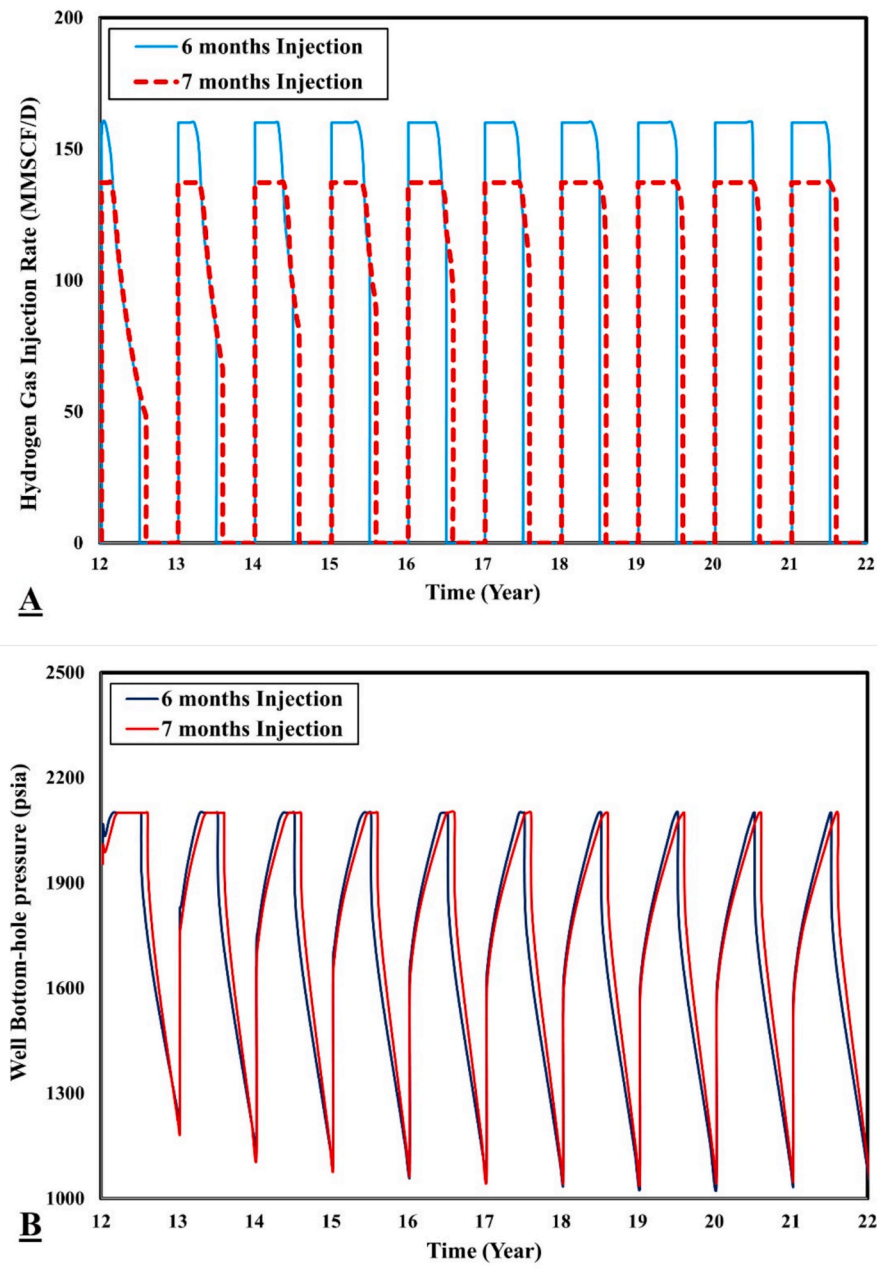


Fig. 13. Comparison of (A) hydrogen injection rate and (B) bottom-hole pressure (BHP) for the 6-month and 7-month injection scenarios (representative injection well).

wells is more costly and requires complex designs compared to vertical wells. Thus, implementing horizontal wells in UHS processes must create significant added value to justify their drilling and use.

The scenario involving the use of horizontal wells was carried out following the injection and production plan of the 160 MMSCF/D scenario, utilizing four dual-lateral horizontal wells. The horizontal legs designated for injection were perforated across six grids in the sixth layer of the reservoir. The perforated leg in the third layer of the reservoir was utilized for hydrogen production. Fig. 14 illustrates the perforation layout of the horizontal wells in the reservoir.

Utilizing horizontal wells reduces hydrogen accumulation around injection and production wells. Consequently, injected hydrogen gas is transported to more distant areas of the reservoir immediately after injection. This reduces pressure in the injection wells, preventing pressure limitations from hindering additional hydrogen injection.

According to the results shown in Fig. 15-A, horizontal wells enable gas injection at the maximum planned rate. Therefore, the injected hydrogen energy in this scenario reaches its maximum level. From a production perspective, hydrogen energy production using horizontal wells demonstrates significant improvement in the initial cycles of injection and production compared to vertical wells. The overall produced energy also decreases compared to vertical wells (Fig. 15-B). The increased hydrogen volume injected into the reservoir reduces the mixing between working gas and cushion gas. However, hydrogen recovery has not yet reached its maximum potential. One critical factor in the remaining hydrogen in the reservoir with the horizontal well scenario is the dominance of viscous forces over gravity forces, hindering movement from the upper layers of the reservoir to the third layer where the horizontal well is located. This is evident in the remaining hydrogen shown in Fig. 14, where a substantial portion occupies the top two layers

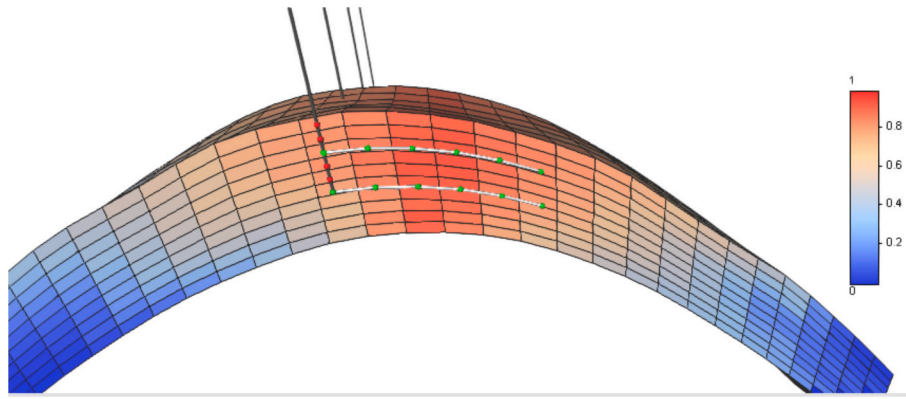


Fig. 14. Perforation Layout of Horizontal Wells for Hydrogen Injection and Production and Distribution of Hydrogen Gas in the Reservoir Using Horizontal Wells at the End of the UHS Process.

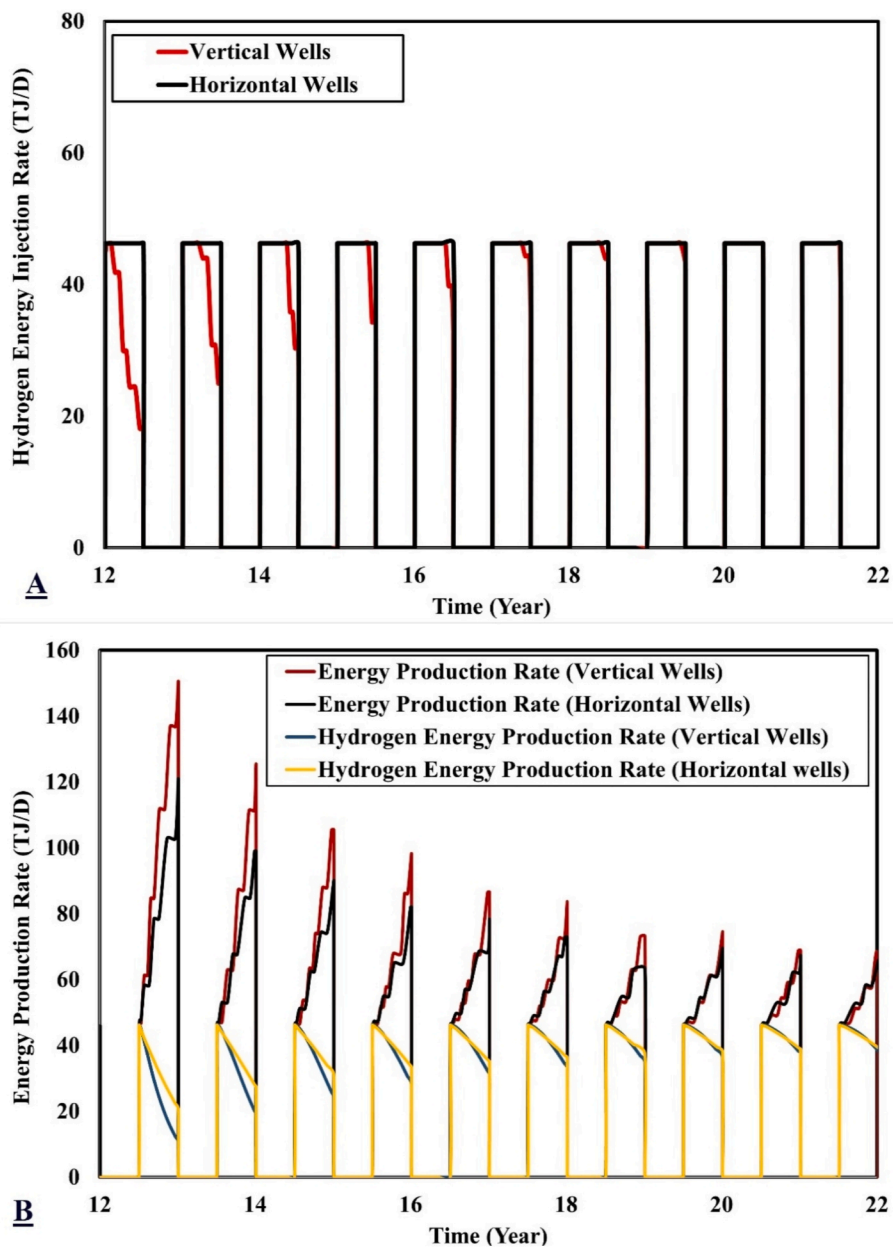


Fig. 15. Energy Injection and Production in the Reservoir. Rate of hydrogen energy injection in horizontal and vertical well scenarios (A). Rate of energy production and hydrogen energy recovery from the reservoir (B).

of the reservoir.

In the vertical well configuration (Fig. 7), the remaining hydrogen after the tenth cycle is concentrated in a more localized region, reflecting the point-source nature of injection and production. This leads to a less uniform lateral sweep and a more confined hydrogen plume within the reservoir. In contrast, the horizontal well configuration (Fig. 14) shows a more laterally distributed pattern of remaining hydrogen, due to the larger reservoir contact area and distributed flow along the horizontal section, which promotes a more uniform displacement and improved sweep efficiency over the storage cycles.

While using horizontal wells might lack economic and operational feasibility during the energy transition period when natural gas consumption is necessary, it could become a viable option during the hydrogen economy era. At that time, the need for a complete hydrogen energy supply chain will justify the adoption of horizontal wells.

3.6. Hydrogen leakage assessment from the caprock

To evaluate the potential for hydrogen leakage from the storage reservoir, the second layer above the reservoir was designated as the caprock, while the overlying formation was modeled as the overburden layer. The average petrophysical and mechanical properties of the caprock, derived from laboratory measurements on core samples from the study site, are summarized in Table 5. These parameters were applied consistently across all leakage simulations.

Following the operational schedule of the base-case injection and production scenario, three mechanical response cases for the caprock — as described in the methodology section — were simulated over a five-year operational period. This approach enabled a direct comparison between: (i) a stress-independent caprock, (ii) a stress-dependent elastic caprock, and (iii) an elasto-plastic caprock with hysteresis effects. The objective was to quantify the influence of cyclic stress behavior on hydrogen migration through the sealing formation and to identify conditions under which the sealing capacity may be compromised.

In this study, the mass of hydrogen molecules migrating from the caprock into the overburden layer was used as the primary metric for quantifying hydrogen leakage in the three investigated mechanical response cases. This metric provides a direct measure of the sealing efficiency of the caprock under cyclic storage operations. As expected, an increase in hydrogen migration into the overburden corresponds to a greater loss of stored hydrogen from the reservoir, which in turn reduces the effective energy capacity and overall economic value of the underground storage process. Therefore, minimizing leakage is essential not only for ensuring the long-term integrity of the storage site but also for maximizing the energy return on storage operations.

Fig. 16 Temporal evolution of hydrogen leakage fraction over a five-year operational period for three caprock mechanical response cases: stress-independent base case, stress-dependent elastic deformation, and elasto-plastic deformation with hysteresis effects. The results indicate that the mechanical behavior of the caprock has a pronounced influence on hydrogen leakage rates. The elasto-plastic deformation case exhibits the highest leakage fraction, increasing steadily throughout the operational period and reaching approximately 3.8% after five years. This behavior highlights the detrimental effect of irreversible deformations and hysteresis on the sealing efficiency of the caprock, as these processes can significantly enhance hydrogen migration into the overburden. The elastic deformation scenario results in lower leakage than the elasto-

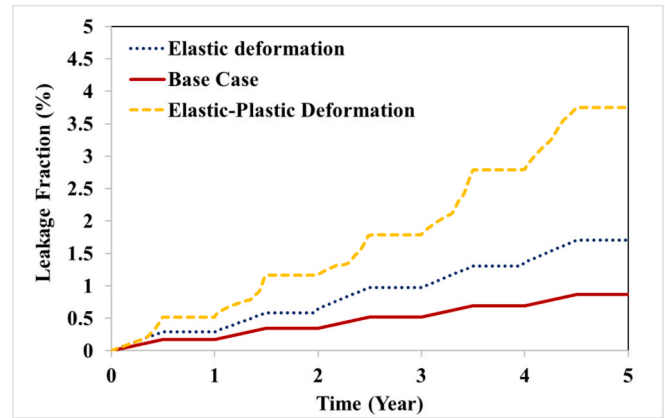


Fig. 16. Evolution of hydrogen leakage fraction over a five-year operational period for three caprock mechanical response cases.

plastic case but remains higher than the base case, suggesting that even stress-dependent elastic strain can alter the effective permeability and compromise containment performance over time. The base case, which neglects stress-dependent mechanical effects, exhibits the lowest leakage fraction, with losses primarily governed by the intrinsic properties of the shale caprock. These findings underscore the necessity of incorporating realistic mechanical responses, particularly plasticity and hysteresis, into the geo-mechanical modeling of hydrogen storage systems to ensure the long-term integrity and energy efficiency of subsurface storage sites. These findings highlight that caprock stability demonstrated during UGS operations cannot be assumed to guarantee stability under UHS conditions. Due to hydrogen's smaller molecular size and higher diffusivity, sealing performance can be more susceptible to stress-induced mechanical alterations. The elastic and elasto-plastic scenarios underline the necessity of controlling operational pressures in UHS projects to mitigate leakage risks. Maintaining pressure within safe limits is therefore essential for preserving the long-term integrity of the storage site and maximizing the energy retention efficiency of hydrogen storage operations.

3.7. Screening analysis of potential methanogenesis effects

To simulate the potential impact of hydrogenotrophic methanogenesis, the corresponding reaction was incorporated into the base reservoir model operating at a hydrogen injection rate of 40 MMSCF/D. This reaction was added as an additional process to the base UHS scenario in order to evaluate its influence on hydrogen availability under cyclic storage conditions. To quantify the progression and impact of methanogenesis at the reservoir scale, the molar balance of carbon dioxide was selected as the primary diagnostic indicator. This choice is based on the fact that the amount of CO₂ remaining in the reservoir is governed by only two mechanisms: removal through production and consumption through the methanogenesis reaction. As no other geochemical reactions affecting CO₂ were considered in the model, changes in the in-place CO₂ inventory beyond production-related losses can be directly attributed to microbial consumption.

Accordingly, the cumulative CO₂ consumption associated with methanogenesis was estimated from the difference between the initial CO₂ in-place and the sum of produced and remaining CO₂ over time. Once the amount of CO₂ consumed by the reaction was determined, the corresponding hydrogen consumption was inferred indirectly using the stoichiometric relationship of hydrogenotrophic methanogenesis (CO₂ + 4H₂ → CH₄ + 2H₂O). This approach provides a consistent and conservative estimate of hydrogen loss attributable to microbial activity, while remaining fully compatible with the compositional simulator framework. Fig. 17 presents the screening-level evaluation of hydrogenotrophic methanogenesis implemented in the base UHS scenario.

Table 5

Petrophysical properties of shale caprock formation.

Cap Rock Property	Value (Unit)
Porosity	0.00003 (Fraction)
Horizontal permeability	0.0001 (md)
Vertical permeability	0.00001 (md)
Gas capillary entry pressure	8 (Mpa)

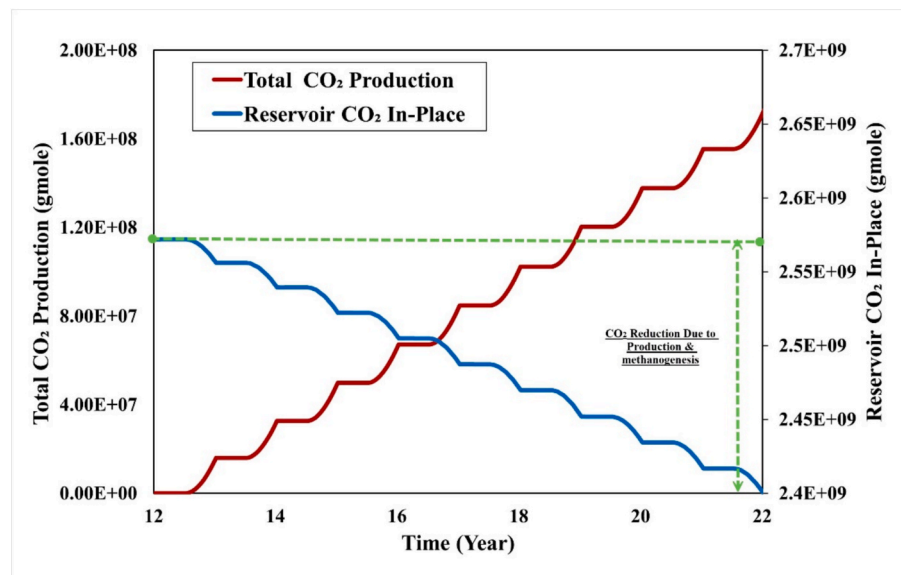


Fig. 17. Screening-level assessment of hydrogenotrophic methanogenesis in the base UHS scenario. Cumulative CO₂ production and remaining CO₂ in-place in the reservoir over time.

Fig. 17 shows the cumulative CO₂ production alongside the remaining CO₂ in place within the reservoir over the course of cyclic UHS operation. The steady increase in cumulative CO₂ production reflects continuous co-production of CO₂ with the produced gas during successive cycles. Simultaneously, the gradual and monotonic decline in the in-place CO₂ inventory indicates the combined effect of production-related removal and consumption through methanogenesis. The absence of abrupt changes or sharp inflection points suggests that methanogenesis does not exhibit early-time dominance and instead progresses gradually over multiple storage cycles.

Based on the analysis presented in Fig. 16, the total amount of CO₂ consumed due to methanogenesis over the simulated period is approximately 1.6×10^8 gmol. According to the stoichiometry of hydrogenotrophic methanogenesis, this corresponds to a cumulative hydrogen consumption of approximately 6.4×10^8 gmol attributable to microbial reactions. Over the same operational period, the total amount of injected hydrogen in the base scenario was approximately 8.66×10^{10} gmol. Consequently, the inferred hydrogen consumption associated with methanogenesis represents only about 0.83% of the total injected hydrogen. Accordingly, the estimated hydrogen loss provides a screening-level indication of the magnitude of energy that may be associated with microbial processes in similar UHS settings.

Overall, this study systematically evaluates the key technical parameters governing the feasibility of converting UGS facilities into UHS systems, including energy injection and delivery limits, hydrogen injectivity, cushion gas management, gas mixing behavior, caprock leakage risk under cyclic stress, and screening-level hydrogen loss due to microbial activity. These parameters constitute essential design and decision variables that must be considered in any UGS-to-UHS conversion project. While this study does not present a standalone economic analysis, the investigated parameters directly define the inputs to any techno-economic evaluation by controlling deliverable energy, operational constraints, storage efficiency, and risk-related losses. In addition, strategies such as increased hydrogen injection rates or transitional cushion gas production inevitably introduce surface-facility, compression, regulatory, and market considerations that are site- and context-dependent. Consequently, the results of this work provide a technical and energy-based foundation upon which reliable and project-specific economic assessments of UHS conversion can be constructed.

4. Conclusion

In this study, reservoir simulations were performed to evaluate energy balance during the conversion of a UGS project into a UHS system. Reservoir simulation studies on UGS-to-UHS conversion have been limited, focusing mainly on the mass of injected and produced hydrogen. However, the stored and delivered energy must also be considered beyond conversion challenges. Despite hydrogen's higher gravimetric energy density than natural gas, its lower volumetric density results in less energy stored in the same volume in a UHS reservoir than in a UGS system. This leads to reduced reservoir energy capacity, necessitating the storage of larger volumes of hydrogen or applying higher pressures to compensate for this shortfall. This study examined the technical factors influencing the enhancement of stored and deliverable energy in UHS conversion projects. The following findings were obtained:

1. The results of this investigation indicate that increasing the volume of hydrogen injected into the reservoir is essential compared to UGS projects to maintain energy flexibility and balance between energy production and consumption. To store the same amount of energy as in UGS projects, the volumetric injection rate of hydrogen must be at least four times that of natural gas.
2. Due to the mixing of hydrogen gas with natural gas, which acts as cushion gas in the reservoir, a portion of the hydrogen remains in the reservoir. However, the natural gas produced alongside hydrogen can meet part of the energy demand during the energy transition period, where there is still a market for natural gas consumption. This feature can enhance the reservoir's efficiency during this transitional phase.
3. Specific strategies are required to increase the volume of hydrogen injected into the reservoir safely. In this study, three main approaches were evaluated: reducing the volume of cushion gas to increase the reservoir's effective capacity, extending the hydrogen injection period to improve gradual and uniform storage, and utilizing horizontal wells to enhance reservoir contact, ensuring better distribution and higher efficiency. These strategies can contribute to safer and more effective hydrogen storage in the reservoir.
4. Reducing the volume of cushion gas in the reservoir by 20% improved the injectivity of reservoir wells by up to 10% in the early cycles. In contrast, extending the injection period by one month resulted in a 2% improvement in well injectivity. These findings

suggest that reducing cushion gas has a more significant impact on enhancing injectivity, particularly during the initial stages of operation.

5. Utilizing horizontal wells is the only strategy capable of fully executing gas injection as planned and significantly reducing the mixing of gases in the production stream. Although the use of horizontal wells may not be economically viable during the energy transition period, they can be considered an effective and efficient solution within the framework of a complete hydrogen-based energy supply chain.
6. The caprock integrity assessment revealed that mechanical behavior plays a critical role in controlling hydrogen leakage during UHS operations. While caprock stability under UGS conditions does not guarantee the same performance in UHS projects, the elastic and elasto-plastic scenarios demonstrated that stress-induced deformation, particularly irreversible plastic strains and hysteresis effects, can significantly increase leakage rates. Therefore, operational pressures in UHS must be carefully managed to limit stress-driven permeability changes and maintain long-term sealing efficiency, ensuring both energy retention and storage site stability.
7. A screening-level assessment of hydrogenotrophic methanogenesis indicates a gradual consumption of CO₂ over multiple storage cycles, from which hydrogen loss was inferred using reaction stoichiometry. Under the temperature and salinity conditions of the studied reservoir, the estimated hydrogen consumption represents a limited fraction of the total injected hydrogen and provides an order-of-magnitude indication of potential energy loss associated with microbial activity in UHS operations.

CRediT authorship contribution statement

Arash Daneshfar: Writing – original draft, Visualization, Validation, Software, Resources, Methodology, Investigation, Formal analysis, Data curation. **Zahra Khazaei:** Writing – original draft, Software, Investigation, Formal analysis. **Armin Homaei:** Visualization, Validation, Methodology, Investigation, Formal analysis. **Ali Vatani:** Writing – review & editing, Supervision, Project administration, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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