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Current minireview

Modeling fidelity upon competitive adsorption for underground hydrogen storage in depleted shale reservoirs: A minireview

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Abstract:
Underground hydrogen storage in depleted shale gas reservoirs has emerged as a promising option for large-scale energy storage, with feasibility assessments relying on compositional simulations. The fidelity of such simulations hinges on accurate representation of key physicochemical processes, particularly gas adsorption, which governs phase partitioning in shale formations. However, adsorption is often treated deterministically in large-scale simulations, while optimization efforts emphasize operational and geological parameters. This minireview summarizes prevailing compositional simulation workflows and key performance metrics for shale and further synthesizes recent advances and gaps in H_2/CH_4 competitive adsorption, highlighting the scarcity and experimental difficulty of multicomponent adsorption data. The propagation of adsorption-related uncertainty to large-scale predictions is further discussed. An illustrative scenario demonstrates that different multicomponent adsorption models can significantly alter the predicted fraction of adsorbed H_2 and the recovery factor. The magnitude of these variations can be comparable to or even exceed improvements achieved through typical operational optimizations. Such discrepancies indicate that adsorption representation is not a non-significant modeling input but a central factor influencing evaluation outcomes. These findings underscore the need to explicitly account for competitive adsorption in assessing underground hydrogen storage in shales. Furthermore, adsorption uncertainty should be systematically quantified and integrated into modeling workflows to secure the high-fidelity of compositional modeling underground hydrogen storage in shales.

1. Introduction

Underground hydrogen storage (UHS) is widely viewed as a key enabling technology for large-scale renewable energy integration and seasonal energy storage (Malki et al., 2024; Bagchi et al., 2025). Suitable geological settings for UHS include saline aquifers, salt caverns, abandoned mines, and depleted oil & gas reservoirs. Among these, depleted reservoirs have attracted particular attention due to the availability of existing wells and surface facilities, as well as their relatively well-characterized geological conditions (Song et al., 2025; Wu et al., 2025). More recently, research interest has expanded from conventional depleted reservoirs to unconventional ones, such as shale gas reservoirs (Table 1). This shift is driven by several intrinsic characteristics of shale formations. Shale reservoirs typically exhibit strong sealing capacity owing to ultra-low matrix permeability and thick caprock systems, which are favorable for long-term containment. In addition, their widespread global distribution

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Table 1. Comparison of studies related to UHS in depleted hydrocarbon reservoirs.

Reservoir type	Storage system	Simulation	Highlights	Limitations	Reference
Subsurface geological formations	H_2 (CO_2, N_2 as cushion gas)	GCMC	Cushion gas effects; H_2 fraction dependence	Pore-scale only	Doan et al. (2024)
Unconventional reservoir	H_2 (residual CH_4)	GCMC; compositional	Hydraulic fracture contribution; nanopore purity control	Chemical reactions not considered	Wang et al. (2023)
Depleted tight sandstone reservoir	H_2	Compositional	Injection-withdrawal strategy; fractured reservoir storage	Single-component (H_2) system	Wang et al. (2024a)
	H_2 (residual CH_4, N_2)	Compositional	Capacity projection; economic comparison	Single-cycle simulation; geochemical reactions and adsorption not considered	Singh (2022)
	H_2 (CO_2 as cushion gas)	Compositional	Multi-cycle feasibility; energy efficiency	Geochemical reactions, multi-component effects, and competitive adsorption not considered	Liu et al. (2024)
Depleted shale gas reservoir	H_2 (residual CH_4)	Numerical	Multilayer storage capacity; fracture-enhanced flow	Multicomponent effects not considered	Micheal et al. (2025)
	H_2 (residual CH_4, H_2S)	Compositional	Dissolution-diffusion loss; operational sensitivity; H_2S risk	Heterogeneity not considered	Dai et al. (2025)
	H_2/CH_4 binary mixture	GCMC	Binary adsorption experiments; pressure optimization	Simplified dry kerogen model; no mineral or water; pore-scale only	Chen et al. (2026)

and large original gas-in-place volumes suggest considerable storage potential. Extensive geological characterization and existing well infrastructure from prior production further reduce implementation uncertainties. Moreover, the presence of organic-rich nanoporous structures introduces adsorption as an additional storage mechanism, distinguishing shale formations from conventional reservoirs and adding complexity to H_2 storage behavior.

The feasibility assessment, operational design and parameter optimization of converting shale gas reservoirs into UHS sites rely prevailingly on compositional reservoir simulation (Chang et al., 2025). Although these studies have deepened the understanding of UHS feasibility in depleted shale reservoirs, they typically adopt a deterministic treatment of adsorption behavior and leave the uncertainty associated with multicomponent competitive adsorption largely unexplored.

To fill this gap, the role of H_2/CH_4 competitive adsorption that governs phase partitioning and ultimately affects H_2 recovery factor and purity is reviewed herein. This study first identifies persistent data and knowledge gaps by synthesizing recent experimental and modeling advances, and then traces how adsorption model uncertainty propagates through compositional simulations to affect large-scale performance metrics. By reframing adsorption as a source of dynamic uncertainty rather than a fixed input, existing reviews are complemented to encourage a shift toward uncertainty-aware UHS assessments.

2. Current status of UHS in depleted shale gas reservoirs

Despite the increasing simulation studies of UHS in depleted shale gas reservoirs, performance assessment is largely framed by treating the underlying physicochemical interactions in a simplified or prescribed manner. Commonly used performance metrics include: (1) Working gas capacity, typically quantified as the volume of H_2 that can be cyclically injected and withdrawn under operational pressure constraints, reflecting the effective storage deliverability of the reservoir; (2) H_2 recovery factor, defined as the fraction of injected H_2 that can be recovered after one or multiple cycles, often evaluated together with energy recovery efficiency to assess economic feasibility (Ajibona and Pandey, 2025); (3) Cushion gas requirement, i.e., the type and volume of cushion gas needed to maintain reservoir pressure and sustain withdrawal efficiency (Prigmore et al., 2024). In field practice, cushion gases commonly include residual CH_4 originally present in depleted reservoirs, as well as N_2, CO_2 introduced for pressure support. In order to ensure the purity, H_2 is sometimes used directly as the cushion gas. The selected cushion gas composition directly affects mixing behavior, H_2 diffusion, H_2 purity, and ultimately recovery performance (Zhao et al., 2025); (4) H_2 purity, particularly critical in depleted hydrocarbon reservoirs where in-situ hydrocarbons may mix with injected H_2 during cycling and reduce the purity of recovered H_2 (Chen et al., 2026); (5) Pressure management, aimed at avoiding formation integrity risks associated with excessive pore pressure while preventing insufficient reservoir energy that could reduce H_2 recovery factor (Antwi et al., 2025). These metrics are intrinsically intertwined. That is, cushion gas composition influences H_2 recovery and purity; pressure management affects working gas capacity, and multiphase flow behavior governs gas-brine displacement and plume distribution. Given the limited number of practical UHS projects, these metrics are commonly obtained from numerical simulations and used for feasibility assessment and operational strategy optimization. A representative workflow includes: (1) constructing an integrated geological model of the shale gas reservoir and caprock; (2) coupling phase behavior with multiphase flow mechanisms; (3) designing injection-withdrawal cycling schemes; and (4) evaluating controlling factors through sensitivity analysis and scenario comparison.

Within this workflow, current optimization efforts mainly focus on operational parameters and geological variations, including the number and duration of injection-withdrawal cycles, well pattern configuration and well controls, injection-withdrawal rates, cushion gas fraction, and fracture-related parameters. These factors typically affect predicted recovery factor by a magnitude of several percent. For instance, sensitivity studies on injection-withdrawal rates and well control conditions suggest that moderately increasing injection rate and injection duration can improve H_2 recovery factor by 5%, whereas shut-in operations have a limited effect on recovery factor (Wang et al., 2024a). In addition, processes such as non-Darcy flow at high velocities, geomechanical responses, and geochemical reactions are commonly examined by selectively enabling or disabling model modules to quantify their impacts on UHS performance. For example, large-scale simulations indicate that H_2 losses due to mineralization reactions remain at the per-mille level over multiple injection-withdrawal cycles (Dai et al., 2025), and H_2 injection may alter the mechanical properties of shale formations (Zhang et al., 2025). Laboratory experiments demonstrate that humic acids can enhance H_2 adsorption on shale surfaces (Abid et al., 2022).

Apparently, these studies assumed that adsorption behavior is either well constrained or of secondary importance, which may not hold for shale systems. In shale systems, adsorbed gas can constitute a substantial fraction of total gas in place, and mixture behavior is sensitive to how adsorption is represented. Under such condition, a deterministic treatment risks underestimating uncertainty in predicted UHS performance and obscure the role of competitive adsorption in H_2 losses and recovery (Fig. 1).

Overall, existing UHS simulations in shales demonstrate an increasing level of methodological sophistication at the large-scale research; however, the treatment of adsorption processes is commonly simplified and embedded as a fixed input rather than interrogated as a source of modeling uncertainty. The adsorption assumptions made in current optimization workflows are rarely tested against alternative formulations or measurement constraints.

3. Research advances and gaps in competitive adsorption of H_2/CH_4

Adsorption capacity reflects the strength of interactions between gas molecules and shale pore walls. At the pore scale, adsorption governs the partitioning between free and adsorbed phases, thereby controlling the free gas inventory and, ultimately, the recoverable gas volume (Mengal et al., 2011). A substantial proportion of CH_4 may reside in the adsorbed state, commonly reported to range from 20% to 80% (Hassan et al., 2024; Cao et al., 2025), which makes storage and production behavior highly sensitive to sorption trajectory and capacity.

The injection-withdrawal cycles of UHS in depleted shale gas reservoirs involve the coexistence of H_2 and residual CH_4. Because CH_4 is generally more strongly adsorbing than H_2 (Lou et al., 2024; Chu et al., 2025), their coexistence gives rise to competitive adsorption in which the stronger adsorbate (CH_4) preferentially occupies adsorption sites. This competition alters the partitioning of H_2 between free and adsorbed phases and can affect CH_4 carryover and H_2 purity in the recovered gas (Shu et al., 2025). In general, the competitive adsorption of CH_4 suppresses H_2 adsorption, leading to a greater proportion of H_2 remaining in the free phase, which is an outcome favorable for both storage and recovery. However, neglecting this mechanism in modeling studies can substantially compromise the evaluation of H_2 storage capacity and energy recovery in storage reservoirs. Besides, multicomponent adsorption is not a simple superposition of single-component isotherms. Selectivity often varies with pressure, temperature, and gas-phase composition (Ho et al., 2024). If gas mixture behavior is represented using fixed selectivity factors or by simply extrapolating single-component isotherms, the dependence of competitive site occupancy on operating conditions may be inadequately captured. This can bias predictions of working gas capacity, recovery factor, and gas composition (Li et al., 2025).

At present, experimental datasets for H_2/CH_4 competitive adsorption on shale remain scarce owing to technical and safety challenges. H_2 adsorption capacities are typically small, leading to low signal-to-noise ratios and strong sensitivity to blank correction and instrument resolution. Under binary conditions, accurate gas blending and reliable compositional analysis are also required. In addition, equilibration in shale micro- and nanopore systems can be time-consuming, and high-temperature, high-pressure experiments impose stringent requirements on system stability and safety (Chen et al., 2024; Raza et al., 2024). Current experimental data on multicomponent adsorption are insufficient to accurately determine adsorption selectivity under realistic UHS conditions. Consequently, molecular simulations are frequently used to probe competitive adsorption mechanisms. Available studies suggest that sulfur-containing functional groups in kerogens can provide important competitive adsorption sites for H_2 and CH_4. Although CH_4 can reduce the adsorption amount of H_2 by preferentially occupying adsorption sites and modifying the adsorption layer structure (Chen et al., 2025), CH_4 and H_2 undergo mixed adsorption on the surfaces such as kerogen,

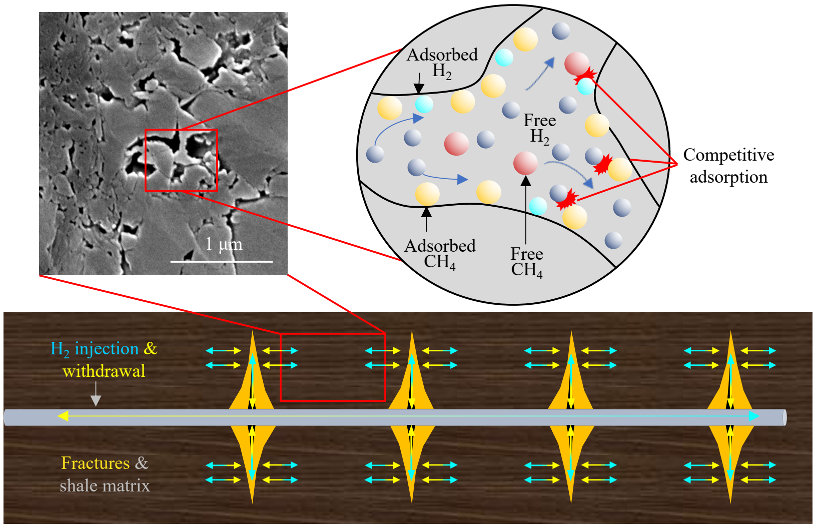

Fig. 1. Conceptual schematic of UHS in shale and H_2/CH_4 competitive adsorption.

quartz, and montmorillonite (Xie et al., 2024). In nanopores of kerogen and montmorillonite, CH_4 exhibits a stronger adsorption ability towards H_2 (Zhang et al., 2024). Among kerogens of different maturities and types, the influence of CH_4 on the thermodynamic adsorption behavior of H_2 shows inconsistent trends (Raza et al., 2023).

Currently, discrete molecular simulations often use ideal substrates of nanometers without capturing the mineral complexity, results of which may not be directly usable as inputs for realistic reservoir simulations over arbitrary temperature and pressure conditions. To incorporate competitive adsorption effects into large-scale simulations in the absence of experimental data, gas mixture adsorption is therefore commonly inferred from single-component isotherms using theoretical extensions. Two widely adopted approaches are the Extended Langmuir (E-L) model and the Ideal Adsorption Solution Theory (IAST), both of which extrapolate from single-component adsorption data. The E-L model is straightforward to implement but assumes a constant selectivity factor. In contrast, IAST also relies solely on single-component inputs but allows selectivity to vary with thermodynamic conditions. This thermodynamic flexibility makes it a more internally consistent framework for predicting multicomponent adsorption (Dutta, 2009; Asif et al., 2019). Previous studies on multicomponent adsorption systems (e.g., CO_2/CH_4) have demonstrated that, in the absence of mixture data constraints, different theoretical frameworks or different single-component isotherm formulations can lead to pronounced divergence in multicomponent adsorption predictions (Yu et al., 2008; Liao et al., 2023). Fig. 2 compares predicted H_2 adsorption in H_2/CH_4 system using the E-L model, IAST coupled with Langmuir isotherms, IAST coupled with Toth isotherms, and IAST coupled with Freundlich isotherms. Although all models fit the single-component data reasonably well with coefficients of determination above 0.96, their derived multicomponent predictions differ substantially.

Therefore, with limited experimental data, both the choice of single-component isotherm formulations and competitive adsorption extrapolation constitute major sources of uncertainty in UHS adsorption prediction. The following section examines how this uncertainty propagates through compositional reservoir simulations, affects UHS performance metrics, and discusses how it should be more appropriately quantified and upscaled into engineering assessments.

4. Uncertainty propagation from sorption model to UHS performance metrics

In compositional simulations of UHS in depleted shale, gas adsorption is generally parameterized using prescribed pure-gas isotherms or tabulated adsorption data. The simulation workflow updates the adsorbed amounts at each time step as functions of pressure, temperature, and gas composition, and couples adsorption with free-phase behavior to determine total gas storage and phase partitioning. Uncertainty in competitive adsorption prediction arises primarily from three sources. First, model uncertainty: even when single-component adsorption data are fitted well, differences in isotherm shapes among models can be amplified during multicomponent extrapolation, leading to substantial divergence in predicted selectivity and component partitioning. This effect has been widely reported in previous studies (Ward and Pini, 2022; Monsalve-Bravo et al., 2024). Second, extrapolation uncertainty: large-scale UHS simulations often cover broader pressure ranges, longer cycling periods, and more complex compositional evolution. In addition, interpolation over sparsely distributed experimental data points may introduce numerical artifacts and unreliable trends (Moubarak et al., 2023; Mayer et al., 2024). Third, data-scarcity uncertainty: H_2/CH_4 adsorption experiments on shale are time-consuming and highly sensitive to low adsorption amount, gas mixing accuracy, and compositional analysis, hence published high-quality multicomponent datasets remain very limited. Taken together, these uncertainties are not independent numerical artifacts but are physically undetermined in the to-date workflow of shale UHS modeling, which must be rigorously derived and constrained using experimental measurements. Nowadays, in the absence of sufficient experimen-

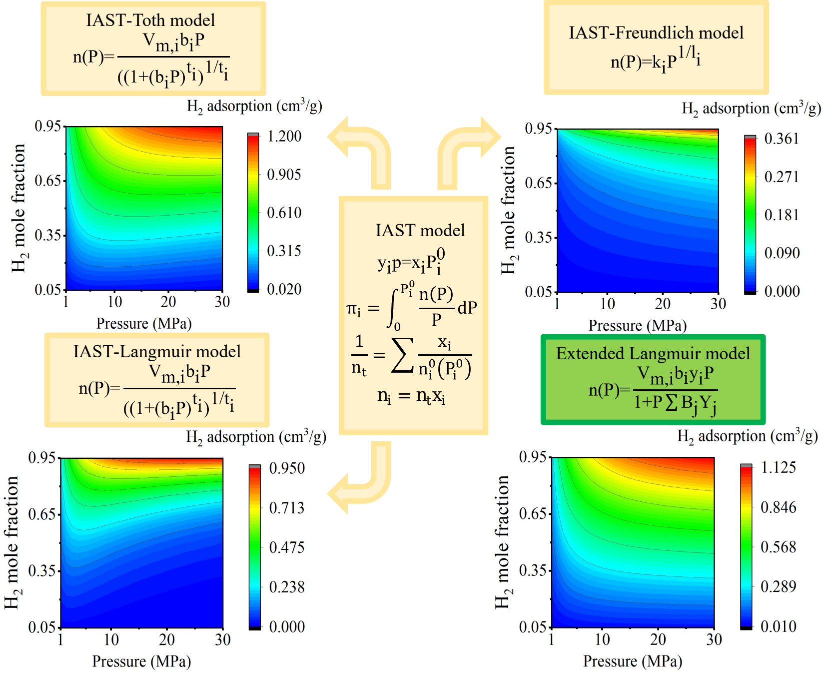

Fig. 2. H_2 adsorption capacity corresponding to different adsorption models.

tal constraints, competitive adsorption data are often estimated or predicted using molecular simulations or machine-learning models (AbdaBabaei et al., 2025; Mwakipunda et al., 2025). Without direct experimental constraints, it is difficult to justify any single isotherm formulation or extrapolation framework as the most representative of reservoir reality. A more defensible assessment paradigm is therefore to treat competitive adsorption as a non-negligible source of uncertainty and to evaluate its impact on large-scale performance metrics.

Uncertainty in competitive adsorption matters at engineering scales in compositional simulations because it fundamentally controls the partitioning between free and adsorbed phases. Injected H_2 does not reside entirely as the free-phase, the adsorbed H_2 reduces the amount available as working gas for recovery. Meanwhile, the more strongly adsorbing CH_4 can repeatedly desorb and adsorb during cycling, competitively displacing H_2 and thereby modifying phase partitioning, recovered gas composition, and purity evolution. To illustrate the magnitude of this effect, a model was constructed using the competitive adsorption predictions discussed above and examined differences in the fraction of H_2 stored in the adsorbed phase. The simulations were implemented using a compositional reservoir simulator with a large-scale depleted shale gas reservoir model at approximately 2,000 m depth. The heterogeneous reservoir consisting of embedded discrete hydraulic fractures was surrounded by low-permeability side and caprock formations. In this scenario, H_2 was selected as the cushion gas to minimize downstream separation costs and to maintain high produced-gas purity. The maximum discrepancy in adsorbed H_2 fraction reaches 29.938% (Fig. 3). This difference in adsorption partitioning directly maps onto macroscopic performance metrics, including H_2 recovery factor and purity. Statistical analysis of H_2 recovery factor for the illustrative cases confirms this relationship: the maximum difference in H_2 recovery factor among cases employing different adsorption models reaches 7.073%, approaching the magnitude of gains achieved through certain operational optimizations and far exceeding recovery factor differences attributed to mechanisms such as mineralization reactions. Because these simulations span multiple injection-withdrawal cycles, the observed divergence reflects not a transient numerical artifact but a cumulative effect of competitive adsorption uncertainty over long-term UHS operation. Therefore, it is necessary to carefully consider how the uncertainty discussed propagates into reservoir scale simulations. Presenting UHS performance metrics with uncertainty ranges provides a more convincing basis for engineering decision-making (Fig. 4).

5. Conclusions and perspectives

This minireview underscores competitive adsorption as a key factor on UHS performance in depleted shale gas reservoirs that is often simplified in large-scale modeling. Current simulation studies predominantly emphasize operational and geological parameter optimization, whereas adsorption is commonly prescribed as a fixed input. Under the data-scarcity regime, gas mixture adsorption is typically inferred from single-component data, making predicted adsorption capacity and selectivity sensitive to isotherm model forms and extrapolation. The compiled evidence indicates that this sensitivity can propagate to large-scale outcomes and lead to non-negligible differences in key performance metrics, comparable in magnitude to commonly reported gains from operational optimization. This finding suggests that adsorption representation should not be merely treated as a non-significant modeling input, but a primary factor on prediction fidelity in modeling UHS in shales.

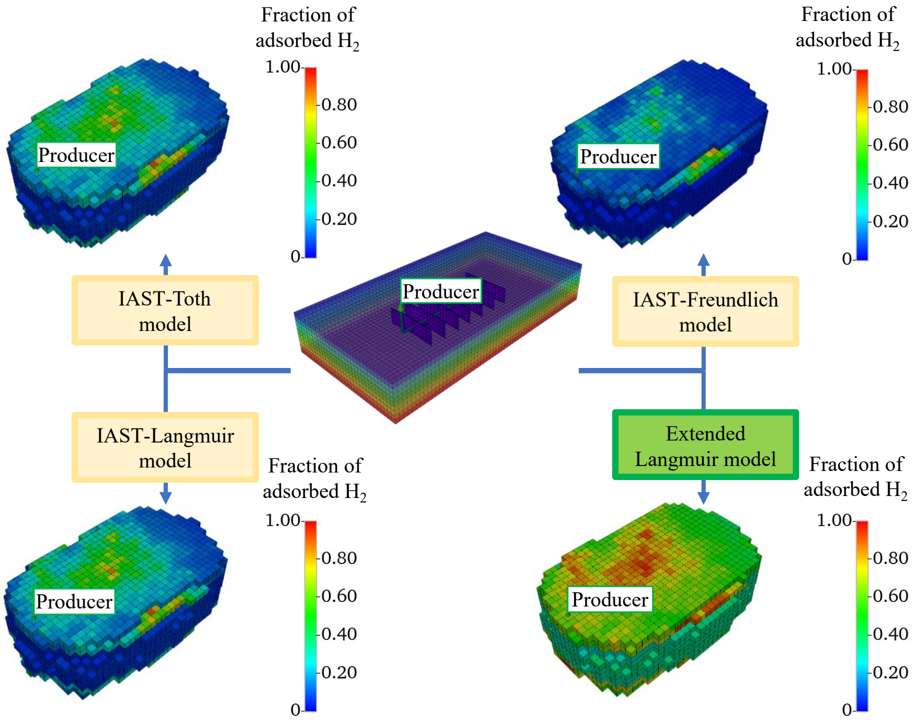

Fig. 3. The fraction of adsorbed H_2 in a shale gas reservoir predicted using different adsorption models.

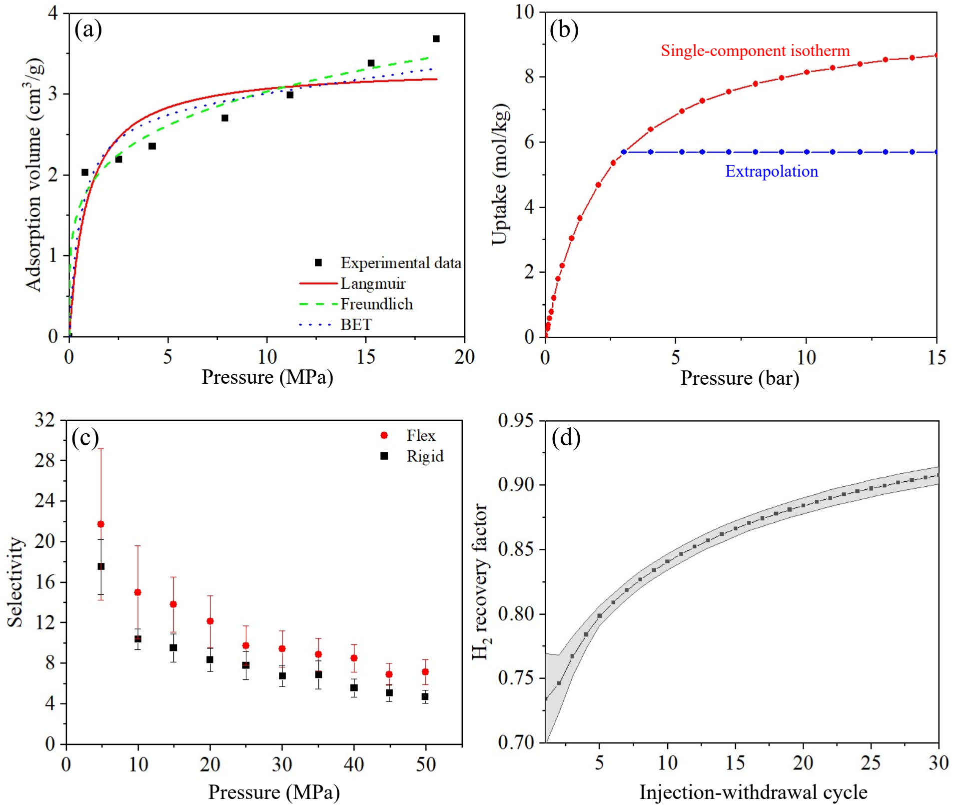

Fig. 4. (a) Model uncertainty (Wang et al., 2024b), (b) Extrapolation uncertainty (Moubarak et al., 2023), (c) Data-scarcity uncertainty (AbdaBabaei et al., 2025), and (d) Differences in H_2 recovery factor predicted using different adsorption models, presented as uncertainty bands.

To improve the modeling precision and optimization, it is recommended that UHS evaluation shifts from single deterministic predictions toward uncertainty quantification. Practically, it is suggested that adsorption should not be represented by a single best-fit isotherm. Instead, multiple plausible adsorption models could be treated as a scenario ensemble, alleviating their impacts propagated into reservoir scale predictions. In parallel, multicomponent adsorption experiments conducted at a limited set of representative pressures and gas compositions could help constrain model choices. Whereas such experiments are challenging, molecular simulations may provide complementary evidence to interpret mechanisms and cross-check experimental trends. Until more definitive mechanistic models or more practical multicomponent measurement methods become available, to conduct uncertainty evaluations by treating adsorption as an ensemble of plausible scenarios is necessary for engineering assessments.

It should also be acknowledged that other mechanisms, such as hydrogen leakage associated with caprock integrity, or multiphase migration, also influence UHS performance. These processes represent additional sources of uncertainty that could be comparable in importance to adsorption effects, yet involve distinct physical and geological conditions. A comprehensive assessment of UHS reliability will ultimately require integrating competitive adsorption dynamics with leakage and seal integrity evaluations in a unified uncertainty-aware framework.

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Conflicts of interest

The authors declare no competing interest.

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