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Perspective

Advances and prospects of physics-based and data-driven approaches for CO_2 geological storage safety assessments

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Abstract:
Assessing the long-term safety of geological CO_2 storage remains a critical technical challenge. CO_2 migration in porous media is governed by the coupling of multiphase flow, capillary trapping, dissolution, geochemical reactions, and geomechanical effects. In addition to geophysical monitoring methods, experimental and mathematical models can estimate CO_2 leakage volumes and associated risks by simulating fluid transportation processes. This perspective offers a comprehensive comparison of the recent experimental studies, physics-based models, and data-driven approaches for evaluating CO_2 storage safety. Laboratory investigations provide fundamental insights into plume evolution and trapping mechanisms. Analytical and semi-analytical models generate rapid storage capability screening. Numerical simulators serve as essential tools for evaluating long-term storage performance. Data-driven methods can accelerate computational-demanding numerical workflows and support uncertainty quantification. Based on the strengths and limitations of the physics-based and data-driven approaches, this paper further identifies future research directions in experimental design and mathematical modeling for CO_2 storage safety assessment.

1. Introduction

Although deep saline aquifers and depleted hydrocarbon reservoirs are widely considered promising storage sites, ensuring the long-term safety of injected CO_2 remains the primary technical challenge. Detecting potential leakage and evaluating storage integrity typically rely on geophysical surveys and pressure/temperature measurements from monitoring wells. However, these direct monitoring approaches can be expensive and operationally demanding. Experimental studies and mathematical modeling therefore play a critical role in understanding CO_2 flow behavior in porous media. They provide insights into storage mechanisms and support the optimization of injection strategies for long-term storage performance. A robust experimental and modeling framework must account for multiphase flow, capillary trapping, dissolution, geochemical reactions, and geomechanical effects in order to realistically represent the coupled multi-physics processes governing the CO_2 storage process.

Laboratory experiments quantify key hydrodynamic, geomechanical, and geochemical parameters of formation fluids in the presence of CO_2. Multiscale imaging techniques are employed to directly observe the interactions among CO_2, formation fluids, and reservoir rocks. These measurements also provide essential input parameters for mathematical modeling. Physics-based approaches, including analytical and numerical models, simulate CO_2 transport in porous media by solving governing equations for flow, geomechanics, and chemical kinetics. Analytical models generate rapid predictions from

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field pressure and production data, making them suitable for preliminary storage screening and early-stage site evaluation. Numerical simulators, by coupling multiple trapping mechanisms, offer a more comprehensive representation of CO_2 migration and retention processes and are widely applied to assess long-term storage performance, including leakage risk and mechanical integrity. Data-driven models are increasingly developed as alternatives or complements to physics-based tools. Because they do not explicitly solve the underlying physical equations, they can significantly reduce computational cost and remain applicable in situations where data availability or computational resources limit the use of high-fidelity simulation models. As shown in Fig.1, these approaches could assist each other and have their suitable application scenarios.

Research on the modeling approaches continues to advance as efforts are made to address their technical limitations. This paper presents a perspective analysis of these approaches and discusses their respective roles in CO_2 storage assessment.

2. Laboratory experimental approaches

(1) Core-scale multiphase flow

Core-flooding experiments are the primary laboratory approach for quantifying CO_2/brine and CO_2/brine/oil flow behavior under reservoir conditions, providing key parameters such as relative permeability, capillary pressure, residual gas saturation, and flow instability characteristics that govern plume migration and post-injection redistribution. Hysteresis in relative permeability and capillary pressure has been shown to significantly enhance residual trapping efficiency (Zhang et al., 2025). However, results often vary due to sample heterogeneity, wettability, and experimental protocols, and the limited core scale raises concerns about representativeness, particularly in anisotropic or fractured formations. Future research should prioritize the integration of high-resolution imaging (e.g., in situ X-ray CT or micro-CT) with core-flooding experiments to directly visualize dynamic phase distribution and quantify pore-scale displacement mechanisms under reservoir-relevant conditions. In addition, digital rock physics and physics-informed data-driven approaches offer promising pathways to upscale laboratory observations to field-scale predictions while systematically accounting for heterogeneity and uncertainty.

(2) Pore-scale visualization and microfluidic experiments

Microfluidic devices and transparent porous media models are increasingly used to directly visualize pore-scale interfacial dynamics and trapping mechanisms, including viscosity fingering, snap-off, ganglia formation, and dissolution-driven convection. Experiments indicate that pore geometry strongly controls residual trapping, while CO_2 dissolution induced density convection can enhance solubility trapping under favorable conditions (Ratanpara et al., 2025). Such mechanisms are considered important for enhancing long-term containment security. Nevertheless, converting pore-scale observations to field-scale predictions remains challenging. The scaling behavior of convective mixing and the impact of reservoir heterogeneity on dissolution rates require further systematic investigation. One of the most promising research directions is the establishment of robust and internally consistent scaling frameworks that quantitatively link pore-scale displacement and convective mixing processes to continuum-scale transport models. Moreover, key parameters inferred from microfluidic experiments may vary under different pore geometries and flow conditions, and developing a practical strategy to calibrate and update these parameters within reactive transport models would be a worthwhile topic for further study. Integrating microfluidic observations with adaptive, data-informed modeling approaches is therefore necessary to enhance reservoir-scale predictive capability under realistic geological heterogeneity.

(3) Geochemical reaction experiments

Geochemical interactions between CO_2, brine, and host rock may result in mineral dissolution and precipitation, altering porosity and permeability over time. Laboratory experiments are conducted to quantify dissolution rates of primary minerals, carbonate precipitation kinetics, reactive surface area evolution, and changes in hydraulic properties (Gaus, 2010). While these experiments provide critical parameters for mineral trapping assessment, most are conducted over accelerated timescales relative to geological storage periods. Future research should prioritize the development of physically consistent time-scale extrapolation frameworks that combine Arrhenius-based kinetic scaling, dimensionless similarity metrics such as Damköhler and Péclet numbers, and multiscale reactive transport upscaling from reliably extend accelerated laboratory kinetics to geological storage timescales.

3. Physics-based models

(1) Analytical and semi-analytical models

Analytical and semi-analytical models have provided fundamental and straight forward insights into the mechanisms driving CO_2 plume migration. Due to their computational efficiency and clear physical interpretability, these models remain valuable for rapid prediction, sensitivity analysis, and preliminary risk screening. Analytical frameworks based on two-phase flow theory and gravity segregation have been developed to characterize the CO_2 plume distribution. These formulations provide fast estimates of plume extent and fluid front propagation. The solution characterizes the relationships among injection rate, permeability, density contrast, and plume geometry (Nordbotten et al., 2005). After injection completes, buoyancy-driven redistribution and capillary hysteresis govern long-term plume stabilization. Semi-analytical models incorporating residual trapping mechanisms have been proposed to estimate migration distance and stabilization time (Hesse et al., 2008). Analytical solutions for pressure diffusion are widely used to estimate regional pressure propagation and assess the risk of fault reactivation or wellbore leakage (MacMinn, 2008). These models provide rapid feasibility screening and potential leakage pathways during early project evaluation. The primary limitation of these analytical tools lies in their oversimplified assumptions regarding formation homogeneity and multiphysics interactions, which restrict their applicability to realistic problems. Formulations that incorporate effective parameters to account for stratification, anisotropy, and stress-dependent permeability could extend their applicability be-

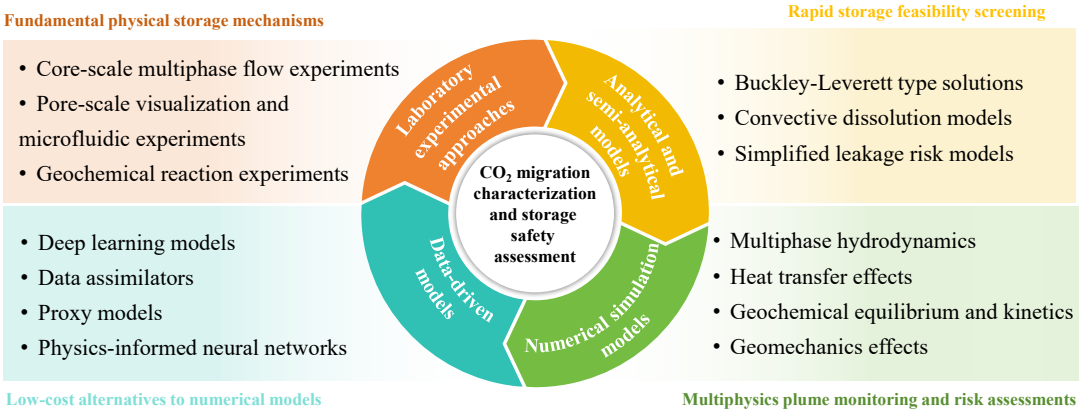

Fig. 1. Integrated methodological framework for CO_2 migration characterization and storage safety assessment

yond idealized homogeneous systems. For example, fractional diffusion formulations, which introduce a fractional exponent to modify the second-order partial differential equation, may offer a promising approach for characterizing CO2 leakage in heterogeneous formations with fractures. The development of hybrid frameworks that integrate analytical solutions with data-driven correction terms or adaptive calibration strategies may further enhance predictive performance for site-specific leakage risk assessment and injection optimization.

(2) Numerical simulators

Field scale numerical models are vital tools to model the CO_2 migrations in porous media and assess the leakage risk. Due to the physical-chemical storage mechanisms, a comprehensive modeling tool should include multi-physics solvers to characterize the hydrodynamics, thermodynamics, geochemical and geomechanical effects (Ajayi et al., 2019). Numerous commercial software packages are developed to include the aforementioned functions. Many oil and gas reservoir simulators are modified to characterize the fluid flow processes in porous media when CO_2 is injected into depleted hydrocarbon reservoirs and deep saline aquifers (for example, CMG-GEM and Eclipse). Reactive transport fluid models are also widely used to simulate CO_2 geological storage processes (for example, ToughReact and DuMux). Unlike oil and gas production, the primary challenge in CO_2 storage simulation arises during the post-injection phase. Once injection stops, simulations must extend over hundreds of years to track plume evolution and long-term CO_2 migration, during which most geochemical reactions take place. When multiple geochemical reactions are considered, the simulation becomes computationally intensive, and using large time steps may lead to convergence issues. Although incorporating geomechanical effects can further increase the computational cost, a one-way coupling strategy, in which the stress field is solved one time step behind the flow solution, can help reduce the additional computational expense. However, this approach is only valid when pressure-induced property variations are insignificant.

Therefore, one of the most promising research directions is the acceleration of large-scale multiphysics numerical simulators. Moreover, reaction parameters such as activation energy and reactive surface area may change under different reservoir conditions, even for the same geochemical reaction. Establishing a practical and consistent way to adjust these parameters within the numerical model could be a worthwhile topic for further study. Last but not the least, model tuning during the storage phase can be challenging for saline aquifer projects because of the limited availability of historical data. It involves potential leakage pathways, such as fractures, faults, or the transmissibility of abandoned wells. Developing a dynamic and adaptive model-updating approach is therefore necessary for this type of simulator.

4. Data-driven models

Deep learning models have been widely employed to characterize the CO_2 plume migrations in various formations. Advanced deep neural network architectures such as long-short-term-memory, fully-connected, transformer, encoder-decoder, etc. have been employed as regression tools to correlate unstructured sequential, feature and image data in CO_2 plume characterization problems (Nagao et al., 2024; Talabi et al., 2026). A well-trained expert system can generate predictions in a fraction of a second, making it orders of magnitude faster than a numerical model. One of the technical gaps for the aforementioned application is the lack of field data to train the deep learning models. Most of the current publications are based on the synthetic case study to demonstrate the feasibility of the workflow. The general rationale is analogous to the history matching, which tunes the hydrodynamical properties of the model and matches the observation data, then the corresponding CO_2 plume can be predicted (Ampomah et al., 2017). When most of the models are trained using the synthetic data, the data generation process could be a time-consuming process and more importantly, the application of such a methodology to a new field could be difficult. Moreover, non-unique solutions may arise in such inverse problems, thereby increasing the uncertainty of the results. To address this issue, data assimilators such as Ensembled Kalman filters are developed for CO_2 plume characterizations (Zhang and Sun, 2025). These approaches represent uncertainty through an ensemble of model states and update their prior and posterior distributions based on observational data. However, the data assimilation algorithms assess the states using either

a numerical simulator or a reduced order mode. The users must choose to pay the computational overheads on the entire data assimilation process using the high-fidelity model, or to generate data and train the proxy model. On the other hands, the physics-informed neural network (PINN) models are employed to solve the fluid dynamics of the CO_2 injection processes (Zhang et al., 2025). It has been proved that the PINNs are capable to obtain accurate pressure and saturation distributions for the CO_2-water-oil systems. A key drawback of PINN approaches is the stringent requirements imposed on boundary condition specification.

Although one approach to addressing the shortage of field data is to generate synthetic datasets using physics-constrained mathematical models, future research could also explore small-sample strategies such as few-shot learning and transfer learning to enhance the model's generalization capability. Model validation requires greater emphasis. Historical-data problems such as plume characterization can be evaluated using benchmark field cases, while forecasting tasks should be tested against blind cases generated by high-fidelity models. An open-access benchmark dataset would further enable rigorous validation and objective comparison among algorithms. Long-term predictions inevitably involve substantial uncertainty, even when based on history-matched models, as key reservoir properties may evolve over century-scale processes. Future research could explore data-driven assisted uncertainty analysis that leverages rapid prediction capabilities to efficiently quantify forecast uncertainty. Moreover, machine learning applications for predicting CO_2 leakage probability remain at an early stage, largely due to the challenges in characterizing leakage mechanisms and pathways over long time scales.

5. Conclusions

Characterizing CO_2 migration and assessing long-term storage security require collaboration between physics-based and data-driven approaches. Future experimental research should emphasize the development of robust upscaling approach and parameter calibration frameworks that translate short-term, small-scale observations into dynamically updated predictions at the reservoir scale. Analytical and semi-analytical models should focus on extending current solutions to incorporate effective representations of reservoir heterogeneity, capillary variability, and geomechanical effects, while maintaining computational efficiency. Strengthening the integration between data-driven models and high-fidelity simulators offers a practical route to accelerate multiphysics simulations and advance reservoir modeling practices. Data-driven models can be coupled into numerical simulators to replace phase behavior modules and multiphysics solvers, thereby accelerating the solution of the governing flow equations. Meanwhile, well-calibrated physics-based models can be used to generate synthetic datasets for training data-driven models.

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Conflicts of interest

The authors declare no competing interest.

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