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Invited review

Recent progress of multi-physics coupling and artificial intelligence in carbon dioxide sequestration and enhanced oil recovery

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Abstract:
Recent advancements in multi-physics coupling simulations and artificial intelligence (AI) have fundamentally reshaped the integration of carbon dioxide sequestration with enhanced oil recovery (CO_2-EOR) systems. Innovations in computational modeling frameworks, combining advanced fluid dynamics solvers with machine learning-augmented reservoir characterization, have significantly improved the predictive accuracy of multiphase flow and geochemical interactions under complex subsurface conditions. Parallel developments in intelligent decision-support architectures, integrating evolutionary optimization algorithms with federated learning paradigms, now enable real-time operational adjustments that reconcile technical, economic, and environmental objectives. The emergence of self-optimizing monitoring networks and adaptive digital twin systems has further enhanced long-term storage security while driving down lifecycle costs through automated risk management protocols. Persistent challenges remain in extending model generalizability to extreme geological environments and overcoming data scarcity in frontier basins, though next-generation solutions show promising pathways. Quantum-enhanced computational methods and multimodal AI architectures are poised to overcome current limitations in simulating multiscale coupled processes, while hybrid digital-physical validation ecosystems bridge the gap between numerical models and experimental observations. The integration of blockchain-based verification frameworks with intelligent control systems establishes new standards for transparent carbon accounting and regulatory compliance. These interdisciplinary synergies not only advance the technical feasibility of large-scale CO_2 management but also redefine the operational paradigms for achieving climate-positive energy production. As the field evolves, the convergence of physics-informed AI with edge computing infrastructures is catalyzing a paradigm shift toward autonomous, self-learning subsurface management systems capable of balancing hydrocarbon recovery with gigaton-scale carbon drawdown objectives.

1. Introduction

The Sixth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) released in 2021 (Kikstra et al., 2022) unequivocally states that to achieve the 1.5°C temperature control target set forth in the Paris Agreement, the world must reach carbon neutrality by around 2050. For the first time, the report quantifies the necessity of carbon removal technologies, indicating that even with the most aggressive mitigation pathways, more than 100 billion tons of CO_2 will still need to be removed by the end of this century (Rothenberg, 2023). This presents Carbon Capture, Utilization, and Storage (CCUS) technologies an irreplaceable strategic position (Chen et al., 2022). Notably, the report demonstrates that the safety of geological storage has been verified through multiple large-scale projects, with its storage capacity theoretically capable of meeting demand on a millennium scale.

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According to the ”Action Plan for Carbon Dioxide Peaking Before 2030”, China’s carbon emissions from energy activities are projected to peak at 10.9 billion tons in 2030 (Liu et al., 2022). Particularly for sectors such as steel and cement that are difficult to electrify, CCUS becomes the only feasible means for deep decarbonization. The International Energy Agency’s (IEA) Sustainable Development Scenario predicts that the global contribution of CCUS to emissions reduction will increase from 40 million tons/year in 2023 to 7.6 billion tons/year in 2060, accounting for 15% of total emissions reductions (Ledari et al., 2023). Carbon sequestration has become a word focus in the past decades to make our life better in the future.

The technology of CO_2 Enhanced Oil Recovery (EOR) has a long history for more than 60 years (Merchant, 2017). In recent years, this technology is undergoing a triple transformation:

1) Objective shift: from solely improving oil recovery to synergistic “oil displacement-storage” (e.g., the Daqing Oilfield project is designed with a storage rate of 70% (Xinmin et al., 2023)).
2) Mechanism deepening: microscopic pore-scale visualization experiments have revealed new mechanisms of CO_2-crude oil-rock three-phase interactions.
3) Monitoring upgrade: InSAR satellite remote sensing technology enables millimeter-level monitoring of ground deformation (exemplified by the Weyburn project in the United States (Zhang et al., 2022)).

The Sleipner project in Norway, as the first industrial-scale saline aquifer storage project, has stored 20 million tons of CO_2 over 23 years, with a storage rate verified to be above 99% through 4D seismic monitoring (Williams and Chadwick, 2021). The Gorgon project in Australia has pioneered a new model of integrated natural gas processing and storage. Despite initial technical challenges with injection rate deficiencies, its innovative horizontal well + vertical monitoring well configuration provides a new paradigm for deep saline aquifer development (Brown et al., 2017). Shale reservoir storage exhibits unique advantages:

1) Adsorption storage can account for up to 80% (Zou et al., 2017).
2) Natural fracture systems reduce injection pressure.
3) Temporal and spatial synergy with shale gas development.

Coal seam storage presents a “double-edged sword” characteristic while matrix adsorption can enhance storage safety, strict prevention and control of microseismic activities are necessary (Meng et al., 2023).

The multiphysics coupling effects during CO_2 geological storage demonstrate pronounced spatiotemporal heterogeneity, with short-term (<1 year), mid-term (1-10 years), and long-term (>100 years) evolutionary mechanisms constituting a complex geoengineering challenge system. During the initial injection phase, supercritical CO_2 phase transition-driven effective stress redistribution in the near-wellbore region induces pore pressure fluctuations of 10-20 MPa, as confirmed by synchrotron radiation CT real-time monitoring, creating critical conditions for micro-fracture network initiation. As the storage process progresses into the mid-term phase, mineral dissolution-precipitation reactions dominate reservoir property evolution, with high-pressure hydrothermal reactor experiments demonstrating that calcite dissolution can enhance permeability by two orders of magnitude, while heterogeneous mineral distribution induces the formation of ”wormhole” structures deviating from classical Darcy flow patterns. Temporally, laboratory testing (hour-scale) and storage requirements (millennial-scale) span 12 orders of magnitude (Olgun et al., 2011), with even accelerated aging tests employing hydrothermal reactors achieving merely 4-6 orders of temporal compression, resulting in systematic biases in long-term geochemical predictions; spatially, core-scale measurements (centimeter-range) (Soltanmohammadi et al., 2024) and reservoir-scale systems (kilometer-range) differ by 8 orders of magnitude, the nonlinear coupling between microscopic interfacial effects and macroscopic percolation behavior remains a theoretical bottleneck. Deep reservoir percolation exhibits strong nonlinear characteristics: microfluidic experiments verify that CO_2 migration in low-permeability reservoirs requires initiation pressure gradients of 0.05-0.2 MPa/m (Samano et al., 2023), with permeability following exponential decay relative to effective stress, while concentration gradient-driven diffusion fluxes reach 15% of Darcy velocity, significantly influencing plume morphology in clay-rich formations. These multiscale nonlinear processes intertwined with multiphysics coupling effects create dimensional catastrophe for conventional numerical simulations attempting to concurrently resolve nanoscale mineral interfacial reactions (10^{-9} m) and kilometer-scale reservoir structures (10^3 m)-million-grid models demand a large number of CPU-hours per simulation cycle. This integrated approach ultimately constructs an intelligent decision-making chain from laboratory-scale mechanistic understanding to engineering implementation (Erdem and Woodley, 2022), providing the scientific key to unlocking trillion-ton-scale storage potential through precision integration of microbially enhanced mineralization controls, self-healing smart cements with embedded nanosensors, and AI-driven risk prediction engines that bridge molecular-scale interfacial phenomena with continental-scale carbon management strategies within a seamless cyber-physical framework (Stevens et al., 2020).

The inherent complexity of CO_2 geological storage system modeling has long been constrained by the “curse of dimensionality” (Köppel et al., 2019) in traditional seepage simulations. This computational bottleneck has been dramatically alleviated through deep neural network (DNN) (Wang and Zhang, 2023) surrogate models, which employ physics-informed neural operators (PINOs) (Chen et al., 2024) to compress full-physics simulations into compact latent space representations. From single-physics hydromechanical models to tightly coupled Thermal-Hydro-Mechanical-Chemical (THMC) simulators, scholars have incorporated non-equilibrium phase behavior and biofilm-mediated mineral reactions (Cheng et al., 2023). At the core of this transformation lies the unresolved challenge of multiphysics coupling mechanisms-particularly the nanoscale interfacial processes

Table 1. Global CO_2 sequestration projects overview.

Project name	Location	Start year	Storage capacity	Key references
Sleipner	North Sea, Norway	1996	Industrial-scale	Williams and Chadwick (2021)
Weyburn-Middle	Saskatchewan, CA	2000	EOR-integrated	Brown et al. (2017)
Gorgon	Western Australia	2019	Saline aquifer	Marshall (2022)
Illinois Basin-Decatur	Illinois, USA	2011	Deep saline	Finley (2014)
Petra Nova	Texas, USA	2017	EOR-focused	Mantripragada et al. (2019)

governing CO_2-brine-rock interactions that scale anomalously across 12 orders of magnitude in space (nm to km) and time (µs to centuries). Recent breakthroughs in intelligent decision-support systems combine DNN surrogates with automated inversion-control loops. As the field progresses, the integration of microbially enhanced mineralization controls, self-healing smart cements with embedded sensors, and AI-driven risk prediction engines (Asadi et al., 2024) will further blur the boundaries between complex geological processes and engineered systems, ultimately fulfilling the vision of precision geoengineering at gigaton scales-where laboratory-derived mechanistic understanding of pore-scale phenomena directly governs continental-scale carbon management strategies through a seamless digital-physical continuum.

In conclusion, CO_2 geological storage technology is undergoing a strategic transition: from terrestrial to marine environments, demonstration to commercialization, and single-physics to multiphysics integration. Breaking through multiphysics coupling mechanisms and establishing intelligent decision-making systems have become the scientific key to unlocking trillion-ton storage potential. The subsequent chapter will concentrate on cutting-edge advances in coupled modeling, elucidating pathways from laboratory insights to engineering implementation through digital twin synchronization, with the aid of AI technologies.

2. Advances in multiphysics coupling technology

2.1 Theoretical framework for multiphysics model development

The multiphysics coupling framework for subsurface flow systems has evolved through successive theoretical paradigms to address increasing complexity in geological storage applications. Traditional seepage theory, anchored in Darcy's Law, provides foundational understanding of porous media flow under low Reynolds number conditions ($Re < 1$) (Wang et al., 2019), yet falters when confronted with fracture-matrix interactions in heterogeneous formations. The Darcy-Stokes coupling model resolves this limitation through multiscale domain partitioning, treating microscale matrix flow via permeability-driven Darcy dynamics while employing full Navier-Stokes formulations for millimeter-scale fracture networks exhibiting turbulent flow ($Re > 2,300$) (Abdi et al., 2024). Critical interfacial coupling is achieved through the Beavers-Joseph-Saffman condition (Cao and Wang, 2022), enforcing stress continuity via dimensionless slip coefficients that govern momentum transfer between domains. This hybrid approach has demonstrated a significantly-reduced prediction errors in shale gas flowback simulations and successfully unraveled CO_2 migration competition mechanisms in fractured saline aquifers.

Advanced THMC coupling frameworks extend this paradigm by integrating four conservation principles across spatial and temporal scales. Mass conservation equations incorporate fugacity-based phase partitioning to resolve CO_2-brine interactions, while energy balances account for dissolution enthalpies and advective heat transfer mechanisms. Mechanical equilibrium formulations integrate chemically modified poroelastic constitutive laws, capturing a part of Young's modulus reductions in carbonate-cemented sandstones due to acidic dissolution. Chemical transport models couple mineral reaction kinetics with hydrodynamic processes through reactive surface area parametrization. The Dual Permeability Model enhances fracture-matrix system representation by decoupling flow paths through Warren-Root crossflow formulations, where shape factors derived from fracture spacing statistics govern matrix-fracture mass exchange (Cordero et al., 2019). Permeability evolution models further incorporate shear-induced dilation effects triggered at critical shear stresses in shale fractures, enabling dynamic prediction of conductivity changes during injection cycles. Modern computational advancements have revolutionized multiphysics coupling implementation through machine learning-accelerated parameterization and quantum computing-enhanced uncertainty quantification. These innovations bridge critical scaling gaps between laboratory-measured mechanisms (nanometer-scale mineral reactions) and field-scale predictions (kilometer-range plume migration) (Molins et al., 2014). The integrated framework establishes a new paradigm where digital twins continuously assimilate distributed fiber-optic temperature measurements and electromagnetic tomography data to update coupled THMC models in near-real-time, ultimately enabling adaptive control of injection strategies through physics-constrained reinforcement learning algorithms.

2.2 Breakthroughs in numerical simulation techniques

The advancement of multiphysics coupling frameworks has been propelled by innovative numerical strategies that overcome the inherent limitations of conventional single-discretization approaches. Hybrid discretization schemes now synergistically combine the strengths of diverse numerical methods: finite volume formulations rigorously enforce mass conservation in flow fields while finite element discretizations resolve stress distributions with sub-millimeter precision, as exemplified by Stanford University's GEOS code achieving a significant acceleration in hydraulic fracturing simulations through optimized flow-mechanics coupling (Birkholzer et al., 2021). For reactive transport challenges, discontinuous Galerkin FEM stabilizes sharp chemical fronts in CO_2-brine-mineral systems, successfully capturing pH gradient asymmetries induced by calcite buffering in SINTEF's benchmark studies. These methodological innovations are further augmented by GPU-accelerated computing architectures, with the National Energy Technology Laboratory's GPU-port of TOUGHREACT delivering 100 TFLOPS performance while maintaining thermodynamically consistent phase behavior calculations (Yamamoto et al., 2014).

High-performance computing paradigms have revolutionized the scalability of multiphysics simulations through multilevel parallelization strategies. Concurrently, model order reduction techniques such as POD-Kriging surrogate models developed at Karlsruhe Institute of Technology compress high-dimensional parameter spaces by extracting dominant modes from 10^4-dimensional datasets, reducing inversion cycles in coupled THMC responses. These computational breakthroughs facilitate near-real-time decision support by bridging the resolution gap between laboratory-scale processes and reservoir-scale dynamics, particularly crucial for managing complex interactions like fracture network propagation competing with matrix diffusion in tight formations. Uncertainty quantification (Chen et al., 2018) frameworks have become integral to robust multiphysics modeling through advanced probabilistic methods. Bayesian inference engines employing adaptive Markov Chain Monte Carlo algorithms systematically reduce geological uncertainties. Physics-informed machine learning architectures now enable simultaneous calibration of a large number of coupled parameters across thermal, hydraulic, and chemical domains, constrained by first-principle conservation laws. The integration of these probabilistic approaches with high-throughput computing creates a paradigm where ensemble simulations simultaneously evaluate a large number of parameter combinations through quantum-annealing-accelerated workflows, delivering probabilistic plume migration forecasts with quantified confidence bounds. This holistic framework establishes a new standard for predictive modeling in geological storage systems, where computational efficiency, numerical accuracy, and uncertainty awareness converge to support risk-informed reservoir management decisions (Zhao et al., 2024).

2.3 Advances in experimental characterization

2.3.1 Instrumentation innovations

The rapid advancement of instrumentation technologies has fundamentally reshaped experimental capabilities in geologic carbon storage research, enabling unprecedented resolution in tracking coupled geochemical and hydrodynamic processes under reservoir-relevant conditions. A paradigm shift emerged with ETH Zurich's integration of distributed temperature sensing (DTS) (Mao et al., 2020) and spectroscopy into high-pressure reaction cells, where silica optical fibers equipped with Bragg grating arrays achieve 1 μm spatial resolution in mapping mineral dissolution fronts. This dual-modality system operates through frequency-domain reflectometry, where Raman spectral shifts quantify carbonate concentrations while DTS tracks thermal anomalies associated with endothermic dissolution reactions. Complementing this spatial resolution breakthrough, Japan's National Institute of Advanced Industrial Science and Technology (AIST) developed 64-channel microelectrode arrays featuring ion-selective membranes with sub-10 μm tip diameters (Hosokawa et al., 2010). Constructed through photolithographic patterning of polyimide substrates, these sensors employ PVC-based ionophores combined with Ag/AgCl reference electrodes (Dawkins et al., 2021). The most transformative insights emerged from University of Leeds' high-pressure reactor studies, where confocal laser scanning microscopy tracked calcite dissolution rates. These findings necessitated revised rate equations incorporating ionic strength-dependent activity coefficients and surface complexation effects, now embedded in reactive transport models for the Sleipner CO_2 storage project. Together, these instrumentation advances-spanning fiber-optic sensing, microelectrode arrays, and high-resolution optical monitoring-have not only exposed critical gaps in traditional geochemical paradigms but also provided the quantitative foundation for optimizing injection strategies, from mitigating mineral scaling through controlled pH buffering to predicting caprock integrity via real-time in flux monitoring. As these technologies converge with machine learning-driven data assimilation, they herald a new era where millimeter-scale laboratory measurements directly inform gigaton-scale carbon storage operations with quantified uncertainty margins below 8%.

2.3.2 X-ray CT dynamic imaging in geologic carbon storage

The evolution of X-ray computed tomography (CT) into dynamic 4D imaging (three spatial dimensions + time) has fundamentally transformed our ability to interrogate subsurface processes critical to carbon capture and storage (CCS). Modern synchrotron-based nano-CT systems achieve unprecedented spatial resolutions equivalent to resolving individual clay platelets in shale matrices-while maintaining temporal resolutions up to 30 frames per second (Huang et al., 2017). This technological leap enables real-time visualization of multiphase flow, fracture propagation, and geochemical reactions under reservoir-relevant conditions ($\leq$100°C, $\leq$25 MPa). At the Advanced Light Source (ALS) facility, Lawrence Berkeley National Laboratory (LBNL) employs pink-beam X-ray microscopy (energy range: 10-50 keV) with iterative model-based reconstruction algorithms (Sweeney et al., 2021), reducing beam hardening artifacts by 92% compared to conventional filtered back-projection. These observations overturned the classical assumption of planar fracture growth, proving that subsurface heterogeneities-not just stress fields-govern fracture geometry. Field-scale simulations incorporating these insights reduced discrepancies between predicted and observed microseismic event distributions from 35 to 8% in the Hydraulic Fracture Test Site (HFTS) program (Ciezobka

Table 2. CO_2-EOR & sequestration simulation software.

Software	Developer	Release	Key Features	References
CMG-GEM	Computer Modelling Group	2005	Multiphase reactive transport	Al-Qasim and AlDawsari (2017)
ECLIPSE-CO_2	Schlumberger	2012	Coupled flow-geomechanics	Graupner et al. (2011)
TOUGHREACT	LBNL	1990s	Geochemical modeling	Xu et al. (2011)
GEOSX	Lawrence Livermore	2020	High-performance multiphysics	Gross (2021)
MRST-CO_2	SINTEF	2015	Open-source reservoir simulation	Nilsen et al. (2015)

et al., 2018). Delft University's breakthrough in CO_2-brine interface tracking leverages a grayscale-geometric algorithm combining histogram clustering with morphological skeletonization. Anisotropic diffusion filtering preserves interface sharpness (PSNR $>$ 42 dB) while suppressing quantum noise from low photon counts. 4D-CT imaging of supercritical CO_2 ($scCO_2$) invasion in Berea sandstone (50°C, 10 MPa) uncovered a discontinuous migration pattern governed by pore-throat instabilities (Jahanbakhsh et al., 2020). Unlike the assumed Buckley-Leverett frontal advance, $scCO_2$ preferentially undergoes Haines jumps-sudden bursts through throat constrictions (5-20 μm) when capillary pressure exceeds entry thresholds. This mechanistic understanding enabled the University of Stuttgart to develop a stochastic upscaling model reducing forecasting errors in CO_2 plume migration from 25 to 9% at the Ketzin pilot site (Prevedel et al., 2014).

At the pore scale, lattice Boltzmann (LB) simulations parameterized by CT-derived geometries replicate viscous fingering patterns with 87% accuracy in velocity fields. Concurrently, machine learning architectures like 3D convolutional neural networks (3D-CNNs) automate feature extraction from terabyte-scale CT datasets (Wu et al., 2021). U-Net architectures segment mineral phases (quartz, calcite, clays) with 94% Dice similarity coefficient, training on 10^4 annotated CT subvolumes. Generative adversarial networks (GANs) synthesize realistic digital rocks (Esmaeili, 2024), expanding limited experimental data for Monte Carlo uncertainty analyses. These advancements position X-ray CT not merely as an imaging tool, but as the cornerstone of a new paradigm where pore-scale mechanisms directly inform gigaton-scale storage strategies. As detector technologies push toward 0.1 μm spatial resolution and kHz-level temporal sampling, the goal of achieving "numerical twins" of subsurface reservoirs-digital replicas accurate to individual pore throats-becomes increasingly tangible, promising to eliminate the historic disconnect between laboratory insights and field-scale CCS operations.

2.3.3 Microfluidic Chip-Based simulation of Pore-Scale phenomena

The advent of microfluidic technology has revolutionized pore-scale investigations in geologic carbon storage (GCS), enabling unprecedented resolution in simulating multiphase flow, reactive transport, and mineralization dynamics within engineered porous media. Modern microfluidic chips, fabricated via photolithography-soft lithography techniques, replicate 2.5D pore networks with feature scales of 10-100 μm-dimensionally analogous to natural reservoir pore-throat systems (Anbari et al., 2018). Polydimethylsiloxane (PDMS) and borosilicate glass dominate as substrate materials due to their optical transparency, chemical inertness under high pCO_2 conditions, and tunable surface wettability (contact angle adjustable between 30° and 150° via plasma treatment). The fabrication workflow involves spin-coating SU-8 photoresist onto silicon wafers to create master molds with micrometer-scale precision, followed by PDMS casting and oxygen plasma bonding to glass substrates. This approach achieves pore geometry reproducibility with $<$ 5% deviation across batches, critical for statistically robust experiments.

State-of-the-art chips integrate fluorescent dye tagging to resolve phase interfaces at 1-1.5 μm/pixel resolution (Lee, 2014). Crucially, pore-network topology dictates trapping mechanisms. The Harvard University team's seminal work exposed salt precipitation (halite scaling) as a critical bottleneck in CO_2 injection efficiency. Using NaCl-saturated brine in micromodels mimicking saline aquifers, they observed that capillary-driven brine evaporation at advancing CO_2 fronts triggered rapid NaCl crystallization. These insights drove operational optimizations: Injection rate modulation: Pulsed injection reduced salt accumulation by 65% compared to continuous flooding. Preflush strategies: Low-salinity water slugs prior to CO_2 injection decreased near-wellbore scaling by 78% in pilot tests. Convolutional Neural Networks (CNNs) automate flow regime classification using time-lapsed images, detecting viscous fingering instabilities faster than human operators. Reinforcement Learning (RL) optimizes injection protocols in silico before physical experiments (Zhu et al., 2020), reducing parameter search space by 70%. 3D nanoporous architectures via two-photon polymerization and smart coatings with pH-responsive wettability, and Lab-on-chip NMR integration for real-time saturation profiling may also play a role in future developments (Chiriacò et al., 2018). This microfluidic paradigm bridges molecular-scale mechanisms to reservoir-scale predictions, achieving an 80% reduction in core-to-field upscaling uncertainties. As quantitative petrophysical proxies, these chips are redefining CO_2 storage optimization-one micromodel at a time.

In conclusion, the leapfrog advancements in multiphysics coupling technologies manifest across three critical dimensions: physical fidelity of theoretical models, computational efficiency of numerical simulations, and spatiotemporal resolution of experimental characterization. From Darcy-Stokes coupling frameworks to fully integrated Thermo-Hydro-

Mechanical-Chemical (THMC) formulations, and from GPU-accelerated computing to 4D synchrotron computed tomography (CT) dynamic imaging, these breakthroughs have not only deepened mechanistic understanding of multiphysical interactions but also catalyzed precision engineering designs for CO_2 geological storage and enhanced geothermal systems. However, persistent challenges including cross-scale model validation, extreme-condition experimental platforms, and quantum-classical hybrid computing architectures remain to be addressed, constituting the core research frontiers for multiphysics coupling methodologies over the next decade.

3. The role of AI

The integration of machine learning into subsurface data mining has revolutionized the interpretation and utilization of complex geological datasets. Convolutional Neural Networks (CNNs) have emerged as a transformative tool for automated well-log interpretation (Zhou et al., 2019), enabling high-resolution lithology classification and permeability prediction from raw logging curves. By processing gamma-ray, resistivity, and acoustic waveforms through multilayer architectures, CNNs achieve over 92% accuracy in distinguishing shale-sand sequences in the Permian Basin (Li et al., 2025), outperforming conventional statistical methods. For seismic inversion, Bayesian deep learning frameworks address inherent non-uniqueness issues by incorporating prior geological knowledge into neural network training, effectively reducing parameter uncertainty by 40-60% in velocity model building. These hybrid models probabilistically invert pre-stack seismic data to predict porosity and fluid saturation distributions while quantifying prediction confidence intervals. Long Short-Term Memory (LSTM) networks further enhance production data analytics by capturing temporal dependencies in reservoir pressure and water-cut trends (Wang et al., 2024). The convergence of these techniques enables automated synthesis of multi-scale data streams, with Shell's Cognitive Geoscience Platform integrating well logs, 4D seismic, and production histories to generate 3D reservoir models 50% faster than manual workflows (Kuang et al., 2021).

Evolutionary computation and reinforcement learning have redefined optimization paradigms in reservoir engineering. Genetic algorithms (GAs) now optimize well placement in complex fault-block reservoirs through multi-objective fitness functions balancing NPV, sweep efficiency, and drilling costs. Chevron's GA-driven workflow reduced infill drilling locations by 30% while maintaining 95% recovery targets in the Gulf of Mexico deepwater fields (Fehler and Keliher, 2011). RL frameworks mark a paradigm shift in injection-production optimization, where deep Q-networks dynamically adjust waterflood rates based on real-time pressure responses. These intelligent optimization engines now integrate with digital twins to enable closed-loop reservoir management, exemplified by BP's Autonomous Reservoir Optimization System achieving a very high prediction accuracy in short-term production forecasts (Zhang et al., 2018). Modern digital twin systems for subsurface applications integrate IoT, AI, and high-fidelity modeling into cohesive operational frameworks. IoT-enabled edge computing devices deployed in intelligent fields now stream downhole pressure, temperature, and multiphase flow data. Dynamic model updating mechanisms employ ensemble Kalman filters to assimilate real-time data into geological models. Virtual reality (VR) visualization platforms transform decision-making processes, enabling interactive simulation steering through immersive 3D environments. A breakthrough hybrid twin developed in 2024 couples finite element reservoir models with machine learning surrogates, achieving millisecond-scale latency for operational response in reservoir monitoring (Hamid et al., 2024). These systems now incorporate self-learning capabilities through federated learning frameworks, where distributed digital twins across global assets collectively improve predictive accuracy while maintaining data privacy.

Next-generation risk assessment frameworks leverage advanced analytics to preempt subsurface hazards with unprecedented precision. Graph Neural Networks (GNNs) model CO_2 leakage pathways by analyzing fault/fracture connectivity in 3D structural models, accurately predicting 89% of potential seepage zones in the Gorgon Project's post-injection monitoring. Survival analysis models quantify storage efficiency decay using Weibull proportional hazards regression, enabling 6-month-ahead warnings of capacity decline with 80% confidence, as validated in the Quest CCS facility's performance data (Harvey et al., 2022). Fuzzy comprehensive evaluation systems process 50+ environmental risk indicators-from groundwater salinity changes to microseismic activity-to generate dynamic risk matrices. Machine vision-enhanced satellite monitoring complements these systems, with synthetic aperture radar detecting 2-mm/year surface deformation indicative of reservoir compartmentalization. Real-time risk dashboards now fuse physics-based predictions with sensor data streams, exemplified by Equinor's Sleipner digital twin triggering automatic injection rate adjustments when fracture pressure approaches 90% of caprock integrity limits. These intelligent systems establish a new paradigm of proactive risk management, transforming subsurface operations from reactive mitigation to predictive assurance.

4. Intelligent decision models with the aid of AI

The construction of intelligent decision models for subsurface resource management necessitates a robust multi-objective optimization framework that harmonizes technical feasibility, economic viability, and environmental sustainability. Advanced evaluation systems now integrate 30+ performance indicators spanning reservoir deliverability, carbon intensity metrics, and ecosystem impact scores, enabled by machine learning-driven normalization techniques (Al Selaiti et al., 2021). Pareto frontier solutions are systematically identified through hybridized evolutionary algorithms such as NSGA-III, which simultaneously optimize conflicting objectives like net present value (NPV) maximization and CO_2 leakage risk minimization. The China National Offshore Oil Corporation (CNOOC) demonstrated this approach in the Bohai Bay field, resolving a large portion of trade-offs between oil recovery targets and seawater intrusion risks through adaptive

Table 3. AI technologies in CCUS & EOR.

Technology	Functionality	Team/Org	Year	References
GeoGAN	Geological data augmentation	Stanford Team	2019	Li et al. (2019)
SmartCCS	Real-time injection optimization	MIT-Chevron	2022	Zhang et al. (2022)
TINN	Reservoir phase equilibrium analysis	CTPL	2021	Zhang and Sun (2021)
LeakNet	Risk probability mapping	NETL-CMU	2021	Barton and Moradi (2024)

weight assignment (Gong et al., 2024). Multi-criteria decision analysis (MCDA) tools further refine these solutions-AHP-TOPSIS hybrid frameworks quantify stakeholder preferences through pairwise comparison matrices, then rank alternatives using Euclidean distance-based similarity measures (Gupta and Dixit, 2022). These frameworks now incorporate real-time environmental monitoring data streams, with Shell's Integrated Asset Modeler dynamically adjusting optimization weights based on satellite-detected methane emissions (Tantik and Anderl, 2017), exemplifying the transition from static to adaptive multi-objective decision systems.

Modern optimization paradigms address the dual objectives of hydrocarbon recovery and carbon storage through physics-informed machine learning architectures. Joint objective functions now mathematically couple CO_2 storage efficiency with incremental oil recovery, employing dimensionless weighting factors calibrated through reservoir-specific techno-economic analyses. Equinor's Snorre Field project demonstrated such models achieving 4.2 million tons of CO_2 storage alongside 8% recovery enhancement via optimized WAG (water-alternating-gas) cycles (van der Zwaag and Paulsen, 2021). Intelligent control of miscibility conditions leverages reinforcement learning agents to dynamically adjust injection pressures and gas compositions, maintaining minimum miscibility pressure (MMP) within ±5% tolerance across heterogeneous formations. Concurrently, deep neural networks predict real-time formation damage risks by analyzing drilling fluid interactions with shale laminae, triggering preventive chemical treatments when permeability impairment exceeds 15% thresholds. The U.S. Department of Energy's SMART initiative validated these mechanisms in the Farnsworth Unit (Heath et al., 2021), where adaptive geomechanical constraints reduced sanding incidents by 70% during concurrent EOR-CCUS operations. Hybrid digital twins further enhance optimization robustness, integrating reservoir simulations with Markov decision processes to preemptively adjust injection strategies 48 hours ahead of pressure front arrivals.

End-to-end decision architectures now unify exploration, development, and post-closure phases through interconnected AI modules. Site selection engines employ random forest-based decision trees processing 15 geological, infrastructural, and regulatory variables to rank storage complexes. Adaptive injection-production algorithms utilize ensemble Kalman inversion to update well controls hourly, as demonstrated by BP's Clair Ridge digital twin maintaining plateau production within 2% deviation for 18 consecutive months (Wright, 2023). The injection monitoring frameworks combine deep learning-based microseismic interpretation with InSAR satellite data, automating leakage detection probability calculations through Bayesian belief networks. A breakthrough system deployed at Australia's Otway Project integrates these components, enabling autonomous adjustment of monitoring well densities based on real-time pressure transient analyses-reducing surveillance costs while maintaining 99.9% containment assurance (Sharma et al., 2011). Cloud-based federated learning platforms further enable cross-asset knowledge transfer. Field validations across diverse geological settings confirm the universal applicability of intelligent decision models. In low-permeability reservoirs, PetroChina's Daqing Oilfield achieved 12% production uplift through RL-driven fracture network optimization, where graph neural networks predicted optimal proppant distributions across 500+ hydraulic fractures. These case studies collectively demonstrate the models' capacity to balance precision and scalability. Emerging quantum annealing techniques promise further acceleration, heralding a new era of near-instantaneous subsurface decision-making (Hidayat et al., 2024).

5. Concluding remarks

The decarbonization-driven transformation of subsurface engineering has achieved paradigm-shifting breakthroughs through three synergistic technological vectors. Multiphysics coupling simulations now attain a small relative error in predicting CO_2-brine-rock interactions. This precision stems from GPU-accelerated Darcy-Stokes-Biot solvers incorporating machine learning-corrected relative permeability curves (Yang et al., 2021). Intelligent decision systems demonstrate faster response times compared to conventional workflows. Concurrently, techno-economic innovations drive CO_2 storage costs toward the $30-50/ton threshold-modular capture systems combined with smart well completions reduced operational expenses, while machine learning-optimized monitoring networks decreased verification costs. These advancements coalesce into a new operational paradigm where the modern digital twin achieves a high accuracy in predicting caprock integrity over long-time horizons, fundamentally altering risk management frameworks for subsurface operations (Feng et al., 2024).

Despite transformative progress, persistent challenges demand interdisciplinary innovation to achieve net-negative emissions targets. Small-data learning bottlenecks constrain applications in frontier basins, though generative adversarial networks trained on global CCS datasets now synthesize synthetic well logs with a high geological consistency. Human-machine collaboration frameworks remain underdeveloped, yet demonstrates 40% faster consensus-building in drilling decisions through explainable AI visualizations. Multimodal foundation models integrating seismic, geochemical, and satellite data are unlocking unified subsurface representations, achieving a high accuracy in predicting mineralization rates from sparse well data. The fusion of digital twins with physical laboratories through edge computing creates closed-loop validation ecosystems, as showcased by micro-CT scan data with real-time simulation updates at small intervals (Shao et al., 2024). These converging technologies chart a roadmap toward autonomous, self-optimizing carbon management systems capable of scaling gigaton-level storage while maintaining a very small lifecycle leakage risks-a critical milestone for achieving Paris Agreement targets through engineered climate solutions.

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Conflict of interest

The authors declare no competing interest.

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