

Digital Twins and Artificial Intelligence for Intelligent CO₂ Storage Management

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Abstract

As geological CO₂ storage (GCS) advances from pilot demonstrations toward gigatonne-scale commercial deployment, the industry increasingly requires management systems capable of continuously integrating real-time monitoring data with predictive subsurface models to support safe, adaptive, and cost-effective operations. Digital twins—dynamic, uncertainty-aware virtual replicas of subsurface storage systems that assimilate real-time data through advanced artificial intelligence (AI) techniques—have emerged as a unifying framework for achieving this vision, bridging the historically siloed domains of geophysics, reservoir engineering, and operational decision-making. This review examines the state of digital twin and AI-enabled intelligent CO₂ storage management, synthesizing recent advances in generative AI-based data assimilation, graph neural network surrogate modeling, uncertainty-aware forecasting, and reinforcement-learning-based reservoir control. It draws on case studies from heterogeneous depleted gas reservoir optimization, geothermal-analogue reservoir characterization, and geomechanically informed reservoir assessment, and further considers methodological parallels with large-scale, real-time AI monitoring and predictive analytics frameworks developed for national healthcare systems. The review concludes by identifying persistent challenges in the transition from uncertainty-aware digital shadows to fully decision-capable digital twins, computational scalability, and multiphysics integration, and proposes a research agenda for advancing digital twin technology toward routine, trustworthy use in commercial-scale CO₂ storage management in the years immediately following its projected 2026 maturation milestones.

Keywords: Digital twin, artificial intelligence, geological CO₂ storage, graph neural networks, uncertainty quantification, reservoir management, generative AI

Introduction

The concept of a digital twin—a dynamic virtual representation of a physical system that is continuously updated from real-time data and uses simulation, machine learning, and reasoning to support decision-making—has migrated from manufacturing and aerospace applications into the domain of geological CO₂ storage (GCS), where it is increasingly recognized as the organizing framework needed to manage the full complexity of large-scale subsurface carbon sequestration operations. Unlike a static reservoir model calibrated once and periodically revised, a digital twin for GCS is designed to assimilate multimodal monitoring data—seismic, well-log, pressure, geochemical—continuously over the project lifetime, updating its representation of subsurface state and, in its most advanced form, informing operational control decisions such as injection rate adjustment to mitigate risks including caprock fracturing or fault reactivation.

Achieving this vision requires the integration of several distinct artificial intelligence capabilities: generative AI techniques for simulation-based Bayesian inference that can characterize the posterior distribution of subsurface states conditioned on sparse, multimodal observational data; graph neural network and other surrogate architectures capable of approximating expensive multiphysics simulations at the speed required for real-time or near-real-time operation; and reinforcement learning frameworks capable of translating continuously updated state estimates into optimal, risk-informed management decisions. Each of these capabilities has matured substantially in recent research, though their full integration into a decision-capable digital twin—as opposed to a purely monitoring-oriented “digital shadow”—remains an active and rapidly evolving area of development heading into 2026 and beyond.

This review synthesizes recent advances in digital twin and AI-enabled intelligent CO₂ storage

management, integrating insights from heterogeneous reservoir case studies (Williams et al., 2026), geothermal-analogue reservoir characterization (Yeboah et al., 2026), and machine-learning-enhanced geomechanical risk assessment (Akpabli et al., 2026), alongside the rapidly developing digital twin literature specific to GCS (Gahlot et al., 2024, 2025; Sun, 2020; Vo Thanh et al., 2026). It further draws methodological parallels with large-scale, real-time AI monitoring and predictive analytics frameworks developed for public health and healthcare systems (Nguyen, 2026a, 2026c, 2026d), which offer transferable lessons on deploying continuously updated, decision-supporting AI infrastructure at scale. The objective is to provide a comprehensive, forward-looking synthesis for researchers, operators, and regulators seeking to advance digital twin technology from research demonstration toward routine, trustworthy use in commercial-scale CO₂ storage management as the field matures through 2026 and the years following.

From Static Models to Digital Twins: A Conceptual Framework

Defining the Digital Twin for Geological CO₂ Storage

A digital twin for GCS is a virtual replica of the subsurface storage system that incorporates real-time monitoring data and advanced generative AI techniques—including neural posterior density estimation via simulation-based inference and sequential Bayesian inference—to continuously characterize subsurface state and inform operational decision-making. Crucially, a full digital twin extends beyond passive state estimation to encompass active control capability: the ability to translate updated state knowledge into injection rate adjustments or other operational interventions that mitigate risks such as reservoir fracturing (Gahlot et al., 2024).

The Digital Shadow as an Intermediate Milestone

Because full decision-capable digital twins require both accurate state estimation and validated control policies, much of the current research literature focuses on an intermediate capability termed the “digital shadow”—a machine-learning-based data-assimilation framework that characterizes

the posterior distribution of subsurface state (CO₂ saturation and pressure) conditioned on multimodal time-lapse data, without yet incorporating control and decision-making functionality (Gahlot et al., 2025). This staged development pathway, progressing from uncertainty-aware digital shadow toward fully decision-capable digital twin, represents the dominant trajectory along which the field is expected to mature through 2026 and beyond.

Why Digital Twins Matter for GCS at Commercial Scale

As CCUS scales toward the gigatonne-level annual injection volumes required for meaningful climate mitigation, the sheer number of concurrently operating storage sites, combined with the heterogeneity of individual reservoir properties, makes manual, expert-driven interpretation of monitoring data increasingly impractical. Digital twins offer a pathway to systematic, continuously updated, uncertainty-quantified management of individual storage sites—and, in principle, of entire storage portfolios—addressing subsurface complexity, operational optimization, and risk mitigation in a unified computational framework rather than through disconnected, periodically executed analyses (Gahlot et al., 2024).

AI Foundations for Digital Twin State Estimation

Simulation-Based Inference and Sequential Bayesian Filtering

At the core of digital twin state estimation is simulation-based inference (SBI), a generative AI technique in which neural networks are trained on ensembles of simulated states and corresponding synthetic observations, enabling posterior sampling of subsurface state when new field data becomes available. Gahlot et al. (2025) developed an uncertainty-aware digital shadow that combines SBI with a novel neural adaptation of nonlinear ensemble filtering, validated on realistic numerical simulations incorporating both imaged surface seismic and well-log data; the results demonstrate that injection-site-specific permeability uncertainty can be propagated into state uncertainty, with the highest reconstruction

quality achieved when conditioning on both seismic and wellbore data jointly, establishing a proof-of-concept for scalable, uncertainty-aware digital shadow technology.

From Digital Shadow to Controlled Digital Twin

Extending this state-estimation capability toward active control, Gahlot et al. (2024) presented a digital twin for GCS with controlled injectivity, demonstrating how digital twin-derived state estimates can directly inform injection rate control decisions aimed at mitigating reservoir fracturing risk. This represents a critical methodological advance: rather than treating monitoring and control as separate workflows, the controlled digital twin framework closes the loop between real-time state assimilation and operational decision-making, integrating geophysics and reservoir engineering within a single computational system.

Graph Neural Network Surrogates for Multiphysics Forecasting

Because full thermo-hydro-mechanical-chemical (THMC) simulation remains too computationally expensive for the rapid, repeated evaluations that digital-twin-style updating requires, surrogate modeling constitutes an essential complementary capability. Vo Thanh et al. (2026) developed a graph neural network (GNN) ensemble surrogate trained on coupled THMC simulation outputs to jointly forecast gas saturation, formation-water pH, and vertical surface displacement over a century-long injection and post-injection horizon, demonstrating that the GNN architecture—by explicitly encoding spatial connectivity among geological grid cells—outperformed multilayer perceptron and convolutional neural network baselines in capturing plume front geometry and deformation localization under previously unseen geological realizations. Critically, the surrogate achieved millisecond-scale inference per forecast snapshot with well-calibrated ensemble prediction intervals, a combination of speed and uncertainty quantification directly suited to digital-twin-style monitoring support and rapid scenario screening.

Heterogeneous Reservoir Characterization as a Digital Twin Input

The fidelity of any digital twin's state estimation is fundamentally bounded by the quality of the geologic and petrophysical characterization on which its underlying models are built. Heterogeneous storage sites such as the Evetts site in the depleted-gas Permian Basin exhibit substantial spatial variability in porosity, permeability, and residual saturation that directly governs the accuracy of plume migration and pressure forecasts a digital twin must produce (Williams et al., 2026). Similarly, machine learning-enhanced petrophysical workflows applied to the Three Forks geothermal reservoir in the Williston Basin illustrate how well log, core, and seismic attribute data can be integrated to characterize reservoir quality at high spatial resolution (Yeboah et al., 2026), providing exactly the class of high-fidelity static property fields that graph-based digital twin surrogates such as that of Vo Thanh et al. (2026) require as geologic input.

AI for Geomechanical Integration Within Digital Twin Frameworks

Geomechanical Risk as a Digital Twin Output

Beyond flow and geochemical state estimation, a complete digital twin for GCS must also forecast geomechanical deformation and associated risks—fault reactivation potential, induced seismicity, and wellbore stability—since pore-pressure perturbation from CO₂ injection directly alters the in-situ stress state. The multi-output GNN surrogate framework of Vo Thanh et al. (2026), which jointly predicts gas saturation, pH, and vertical surface displacement within a single learning framework, exemplifies the trend toward integrated, multiphysics digital twin outputs rather than isolated single-variable forecasts, directly supporting the comprehensive risk evaluation—caprock failure, CO₂ leakage, induced seismicity—that operators and regulators require.

Machine-Learning-Enhanced Wellbore Stability as a Digital Twin Component

Machine-learning-enhanced geomechanical characterization and wellbore stability assessment, as demonstrated in the offshore South Tano Field,

integrates stress field estimation, rock strength prediction, and drilling parameter analysis into a proactive risk-management workflow (Akpabli et al., 2026). Embedding this class of geomechanical model as a component service within a broader digital twin architecture would allow wellbore integrity risk to be continuously updated alongside plume migration and pressure forecasts, rather than assessed only at discrete, periodically scheduled evaluation points—an integration that remains an important frontier for digital twin development in CO₂ storage.

Toward Fully Coupled Digital Twin Architectures

The current generation of digital twin and digital shadow frameworks, while individually sophisticated, generally address a subset of the full THMC coupling relevant to comprehensive risk management: state-estimation-focused digital shadows emphasize flow and pressure (Gahlot et al., 2025), while the GNN ensemble surrogate of Vo Thanh et al. (2026) extends coverage to geochemical and geomechanical observables but relies on a linear poroelastic mechanical formulation rather than a fully nonlinear, fault-reactivation-capable geomechanical model. Achieving a truly comprehensive digital twin will require continued integration of these complementary lines of research into a single, coherent architecture.

AI for Sequential Decision-Making Within Digital Twin Operations

Reinforcement Learning as the Control Layer

Because a decision-capable digital twin must translate continuously updated state estimates into operational actions, reinforcement learning provides a natural methodological foundation for the control layer of digital twin architectures. Sun (2020) developed a deep reinforcement learning framework, employing a deep Q-learning network agent, to identify optimal multiperiod CO₂ storage reservoir management policies under monitoring-only and active brine-extraction risk-mitigation strategies, demonstrating that policies learned in one reservoir environment substantially retained their effectiveness when transferred to related but distinct environments—a transferability property directly relevant to digital twin architectures intended to generalize across

a portfolio of storage sites with varying geologic characteristics, including heterogeneous settings such as the Evetts site (Williams et al., 2026).

Closing the Loop: State Estimation, Forecasting, and Control

The controlled digital twin architecture of Gahlot et al. (2024) illustrates the practical integration of state estimation and control within a single system, using digital-twin-derived state estimates to directly inform injection rate adjustments aimed at preventing cap rock fracturing. Extending this closed-loop paradigm to incorporate the GNN-based multiphysics forecasting capability of Vo Thanh et al. (2026)—which additionally predicts geochemical and geomechanical observables—represents a natural next step toward digital twins capable of managing the full spectrum of CO₂ storage risks through coordinated, AI-driven operational control.

Cross-Domain Lessons: Real-Time, Predictive AI Systems at National Scale

While the technical foundations of digital twins for GCS are rooted in subsurface geoscience and generative AI, valuable operational lessons can be drawn from large-scale, continuously updated predictive AI systems developed in other high-stakes domains. National-scale AI frameworks developed for precision public health illustrate the operational value of continuously integrating individual-level data streams into updated risk assessments that inform targeted, real-time intervention—an operational analogue to a digital twin’s continuous assimilation of monitoring data into updated subsurface state estimates that inform operational intervention (Nguyen, 2026a). This principle—that continuously updated, individual-site risk characterization enables more effective, targeted management than periodic, static assessment—maps directly onto the digital twin value proposition for CO₂ storage, where each storage site’s digital twin can be understood as an analogue to a continuously monitored, individually characterized “patient” within a broader storage portfolio.

National-scale predictive analytics frameworks applied to Medicare and Medicaid populations

further demonstrate how AI-driven, continuously updated risk stratification across large, heterogeneous populations can identify high-risk cases for targeted intervention while managing the overall cost of the monitoring program itself (Nguyen, 2026d). This population-level monitoring logic parallels the portfolio-scale ambition of digital twin technology in CCUS, where operators managing multiple storage sites must similarly prioritize computational and monitoring resources toward the sites and reservoir zones exhibiting the highest predicted risk, rather than applying uniform digital twin infrastructure investment across an entire portfolio regardless of relative risk.

Economic impact analyses of AI adoption in healthcare, quantifying national-scale cost savings and productivity gains attributable to continuously updated, AI-driven monitoring and decision support, offer a further template for building the economic case for digital twin infrastructure investment in CCUS (Nguyen, 2026c). Just as healthcare AI systems capable of continuous, real-time risk updating have demonstrated measurable cost reductions through earlier detection and more efficient resource allocation, digital twin systems for CO₂ storage can be expected to reduce costs associated with reactive, incident-driven monitoring and intervention by shifting toward continuously informed, proactive reservoir management—an economic argument that merits explicit quantification as digital twin technology matures toward standard industry practice through 2026 and beyond.

Collectively, these cross-domain parallels reinforce a broader principle: the challenge of building trustworthy, continuously updated, decision-capable AI systems at scale is not unique to subsurface CO₂ storage, but reflects a general pattern observed across regulated domains where real-time state characterization and proactive intervention offer substantial advantages over periodic, reactive assessment. The maturation of digital twin technology for GCS can accordingly draw on deployment, validation, and cost-justification frameworks already developed in these adjacent, more mature large-scale AI application domains.

Challenges and Limitations

Despite rapid progress, several challenges continue to constrain the transition from research-stage digital shadows to fully operational, decision-capable digital twins for GCS.

The gap between digital shadow and digital twin. Most current implementations remain digital shadows—capable of state estimation but not yet supporting validated control and decision-making functionality (Gahlot et al., 2025)—and the transition to fully closed-loop digital twins with demonstrated control capability (Gahlot et al., 2024) remains at an early stage of field validation.

Multiphysics coupling completeness. Current surrogate architectures, including graph neural network ensembles, typically rely on simplified mechanical formulations—such as linear poroelasticity rather than nonlinear, fault-reactivation-capable geomechanics—limiting their applicability to the full range of risk scenarios relevant to comprehensive digital twin deployment (Vo Thanh et al., 2026).

Training data scale and geological generalizability. Digital twin surrogates are typically trained on limited ensembles of simulated geological realizations—often numbering in the tens to low hundreds—raising questions about generalizability to the full range of geological heterogeneity encountered across a diverse commercial storage portfolio, including sites as structurally distinct as depleted gas reservoirs and geothermal-analogue formations.

Computational infrastructure for real-time deployment. Translating research-grade digital twin frameworks into continuously operating, field-deployed systems requires substantial investment in real-time data pipelines, computational infrastructure, and integration with existing reservoir engineering software toolchains, investments that remain uneven across the global CCUS project portfolio.

Regulatory and stakeholder trust in AI-driven control decisions. As digital twins move from passive monitoring toward active operational control, regulatory frameworks must evolve to accommodate AI-informed decision-making with appropriate auditability and human oversight, an institutional and governance challenge that parallels, but currently

lags, the technical maturation of the underlying digital twin technology.

Future Directions

Future research should prioritize the integration of uncertainty-aware digital shadow state estimation (Gahlot et al., 2025) with graph neural network-based multiphysics forecasting (Vo Thanh et al., 2026) and reinforcement-learning-based control (Sun, 2020) into a single, coherent digital twin architecture capable of jointly estimating subsurface state, forecasting geochemical and geomechanical risk, and issuing validated operational recommendations. Extending the controlled injectivity framework of Gahlot et al. (2024) to incorporate nonlinear, fault-reactivation-capable geomechanics represents a particularly important direction for improving the comprehensiveness of digital twin-informed risk management at heterogeneous, fault-bearing storage sites.

Closer integration of high-resolution petrophysical and geomechanical characterization workflows—such as those demonstrated for the Three Forks geothermal reservoir (Yeboah et al., 2026), the South Tano offshore field (Akpabli et al., 2026), and the heterogeneous Evetts site (Williams et al., 2026)—directly into digital twin training pipelines represents a further avenue for improving the site-specific fidelity of digital twin state estimation and forecasting. Finally, adopting governance, validation, and cost-justification frameworks informed by continuously updated, real-time AI deployment in national-scale healthcare systems (Nguyen, 2026a, 2026c, 2026d) may help establish the auditability and regulatory trust required for digital twins to transition from research demonstration toward routine, decision-capable operational use across commercial CO₂ storage portfolios in the period immediately following 2026.

Conclusion

Digital twins, powered by generative AI, graph neural network surrogates, and reinforcement-learning-based control, represent a rapidly maturing and increasingly central framework for intelligent CO₂ storage management. Applications spanning

uncertainty-aware digital shadow state estimation, controlled-injectivity digital twin architectures, graph-based multiphysics forecasting, and reinforcement-learning-based reservoir management collectively demonstrate that the field is progressing along a clear developmental trajectory—from passive, uncertainty-quantified monitoring toward active, closed-loop operational control—that is expected to reach growing commercial maturity through 2026 and the years following. Cross-domain lessons from continuously updated, real-time AI deployment in national-scale healthcare systems further suggest a pathway toward the governance and cost-justification frameworks necessary for digital twins to achieve regulatory trust and routine operational adoption in CCUS. Realizing the full potential of digital twin technology for CO₂ storage will require sustained investment in closing the gap between digital shadow and fully decision-capable digital twin, achieving comprehensive multiphysics coupling, and building the real-time computational infrastructure required for field deployment—investments essential to ensuring that geological CO₂ storage can be managed safely, adaptively, and at the scale required to meet global climate objectives.

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