

Physics-Informed AI for Subsurface Natural Gas Storage

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Abstract

Subsurface natural gas storage in depleted reservoirs, saline aquifers, and salt caverns requires accurate, computationally efficient modeling of multiphase flow, pressure evolution, and geomechanical response across repeated injection-withdrawal cycles. Conventional numerical reservoir simulation provides high physical fidelity but is computationally expensive to run across the many geologic realizations and operational scenarios needed for robust site characterization and operational optimization, while purely data-driven machine learning models, though fast, often violate fundamental conservation laws when applied beyond their training distribution—a particular concern for the strongly nonlinear, shock-forming multiphase flow behavior characteristic of gas injection and withdrawal. Physics-informed artificial intelligence (PIAI), encompassing physics-informed neural networks (PINNs) and related hybrid architectures that embed governing partial differential equations directly into neural network training, has emerged as a means of resolving this tension, delivering models that are simultaneously computationally efficient and physically consistent. This article presents a research synthesis of physics-informed AI applications for subsurface natural gas storage, examining foundational PINN formulations for two-phase flow and transport, domain decomposition strategies for sparse-data reservoir simulation, and the documented limitations of naive physics-informed approaches when applied to shock-forming hyperbolic flow problems characteristic of gas injection. It draws on case studies from heterogeneous depleted gas reservoir optimization, geothermal-analogue reactive heat exchanger engineering, and high-resolution petrophysical characterization, and further considers methodological parallels with large-scale, constraint-consistent AI frameworks developed for public health, healthcare administration, and healthcare economics. The article concludes by identifying persistent challenges in training stability, shock-capturing fidelity, and multiphysics integration, and proposes a research agenda for advancing physics-informed AI toward routine, trustworthy use in subsurface natural gas storage management as the field matures through 2026 and beyond.

Keywords: physics-informed neural networks, artificial intelligence, natural gas storage, subsurface flow, multiphase flow, reservoir simulation, domain decomposition

1. Introduction

Subsurface natural gas storage—whether in depleted hydrocarbon reservoirs, saline aquifers, or engineered salt caverns—depends fundamentally on accurate characterization of multiphase flow behavior as gas is repeatedly injected and withdrawn over seasonal and multi-decade operational cycles. This flow behavior is governed by strongly nonlinear partial differential equations, most notably the Buckley-Leverett formulation describing immiscible two-phase displacement, whose solutions can exhibit sharp, shock-like saturation fronts that pose substantial numerical challenges for both conventional simulation and emerging machine learning approaches. Accurately and efficiently modeling this behavior across the many geologic realizations and operational scenarios relevant to robust site characterization, injection design, and long-term storage management remains a central computational challenge for the natural gas storage industry.

Conventional numerical reservoir simulation, grounded in finite difference, finite volume, or finite element discretization of the governing flow equations, remains the gold standard for physical fidelity but is computationally expensive, particularly when repeated forward simulation is required across large ensembles of geologic realizations or when real-time or near-real-time operational decision support is needed. Purely data-driven machine learning surrogate models, trained on simulation output, can approximate reservoir behavior at dramatically reduced computational cost, but risk producing physically inconsistent predictions when applied to input scenarios outside their training distribution—a particularly consequential limitation for gas storage applications, where operational and geologic conditions can vary substantially across a storage site's multi-decade lifetime.

Physics-informed artificial intelligence (PIAI) has emerged as a methodological response to this tension, embedding the governing physical laws of subsurface flow—mass conservation, Darcy's law, and the resulting nonlinear transport equations—directly into neural network training, either through soft penalty terms in the loss function, as in physics-informed neural networks (PINNs), or through architectural constraints that enforce physical consistency by construction. This article synthesizes recent research on physics-informed AI for subsurface

natural gas storage, integrating insights from heterogeneous depleted gas reservoir case studies, geothermal-analogue reactive heat exchanger engineering, and high-resolution petrophysical characterization, alongside the foundational and rapidly developing PINN literature applied directly to multiphase subsurface flow (Almajid & Abu-Al-Saud, 2022; Fraces & Tchelepi, 2021; Fuks & Tchelepi, 2020; Han et al., 2023). It further draws methodological parallels with large-scale, constraint-consistent AI frameworks developed for public health and healthcare administration and economics (Nguyen, 2026a, 2026b, 2026c), which offer transferable governance lessons for deploying physically and institutionally constrained AI systems in high-consequence domains. The objective is to provide a comprehensive research synthesis for engineers, researchers, and operators seeking to advance physics-informed AI from research demonstration toward standard practice in subsurface natural gas storage management as the field matures through 2026 and the years following.

2. The Subsurface Flow Modeling Challenge for Natural Gas Storage

2.1 Governing Physics of Gas Injection and Withdrawal

Natural gas storage operations involve the displacement of resident fluids—water in saline aquifers, residual hydrocarbons in depleted reservoirs—by injected gas during the injection phase, followed by the reverse displacement process during withdrawal. This behavior is classically described by the Buckley-Leverett equation, a hyperbolic conservation law whose solutions generically develop sharp saturation discontinuities, or shocks, at the advancing displacement front. Accurately capturing this shock-forming behavior is essential to reliable prediction of gas storage deliverability and containment, yet it poses a well-documented numerical challenge for both conventional and machine learning-based solution methods.

2.2 Computational Burden of Conventional Simulation

Full-physics reservoir simulation, while capable of resolving shock-forming multiphase flow with high fidelity when properly discretized, incurs substantial computational cost that scales unfavorably with the number of geologic realizations, operational scenarios, and injection-withdrawal cycles that must be evaluated to support robust, uncertainty-aware natural gas storage planning. This computational burden is particularly acute for heterogeneous reservoirs, where fine-scale property variability necessitates high-resolution discretization to accurately capture flow behavior.

2.3 Limitations of Purely Data-Driven Machine Learning

Purely data-driven machine learning surrogate models, trained without explicit physical constraints, can achieve substantial computational speedup relative to full-physics simulation but are prone to producing non-physical predictions—negative saturations, violated mass balance, spurious oscillations near shock fronts—when applied to input conditions not well represented in their training data. This limitation is especially consequential for natural gas storage applications, where injection and withdrawal schedules, and the resulting reservoir states, can vary substantially across a storage site's operational history, routinely extending beyond the range of any finite training dataset.

3. Foundational Physics-Informed Neural Network Approaches for Subsurface Flow

3.1 The Buckley-Leverett Benchmark and Early PINN Formulations

Because the Buckley-Leverett problem provides an analytically tractable benchmark for two-phase immiscible flow with known shock-forming behavior, it has served as a foundational test case for evaluating physics-informed neural network approaches to subsurface flow. Fraces and Tchelepi (2021) presented a physics-informed deep learning approach in which a neural network is jointly trained to respect the governing physical laws and boundary conditions of the two-phase immiscible transport problem, demonstrating that the resulting model could produce an accurate physical solution capturing both the shock and rarefaction wave structure characteristic of the Buckley-Leverett solution, honoring the governing partial differential equation along with its initial and boundary conditions across both uniform and non-uniform initial condition scenarios.

3.2 Documented Limitations of Naive Physics-Informed Approaches

Despite these advances, the direct application of standard PINN formulations to nonlinear, shock-forming subsurface transport problems has revealed important limitations that must be understood before physics-informed AI can be reliably deployed for natural gas storage applications. Fuks and Tchelepi (2020) conducted an early and influential investigation of the limitations of physics informed machine learning for nonlinear two-phase transport in porous media, finding that physics-informed learning strategies employing the nonlinear hyperbolic conservation equation directly in the loss function are generally inadequate for accurately capturing shock and mixed-wave solution structures, but that incorporating a parabolic form of

the conservation equation—adding a small diffusive term—enables the neural network to consistently learn accurate approximations of solutions containing shocks, a finding with direct methodological implications for any physics-informed AI application to the shock-forming saturation fronts characteristic of natural gas storage injection and withdrawal.

3.3 Prediction of Porous Media Fluid Flow via Physics-Informed Neural Networks

Extending physics-informed neural network methodology toward more general porous media fluid flow prediction, Almajid and Abu-Al-Saud (2022) implemented a physics-informed neural network technique combining data-driven and physics-constrained loss terms to predict fluid flow behavior in porous media, demonstrating the broader applicability of the physics-informed paradigm beyond the specific Buckley-Leverett benchmark toward the general class of subsurface flow prediction problems relevant to natural gas storage reservoir characterization.

3.4 Domain Decomposition for Sparse-Data Reservoir Simulation

A persistent practical challenge for physics-informed AI in subsurface applications is the sparsity of authentic field data, since the only source of true labeled data for training is typically limited wellbore production and pressure measurements, while high-fidelity simulation data, though more abundant, requires the very computational resources that physics-informed surrogates are intended to reduce. Han et al. (2023) addressed this challenge by introducing a physics-informed neural network based on domain decomposition (PINN-DD), dividing the computational domain into a well-containing sub-domain and a well-free sub-domain—each rigorously constrained by governing equations, sparse data matching, and boundary conditions—to more effectively utilize the sparse production data available from wells while preserving the physical continuity of the near-well region where pressure gradients are largest; the resulting PINN-DD architecture demonstrated superior performance relative to conventional PINN formulations for large-scale reservoir simulation with limited labeled data, a capability directly relevant to natural gas storage sites where extensive high-fidelity training data is rarely available across the full spatial extent of the storage complex.

4. Integrating Physics-Informed AI with Site Characterization and Infrastructure Engineering

4.1 Petrophysical Characterization as a Physics-Informed Model Input

The reliability of any physics-informed AI model for natural gas storage is fundamentally bounded by the quality of the underlying petrophysical characterization used to define the governing equation coefficients—porosity, permeability, and relative permeability functions—embedded within the physics-informed loss function. 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, providing exactly the class of high-fidelity property fields that physics-informed neural network formulations require as governing equation coefficients to achieve reliable, site-specific predictive accuracy.

4.2 Heterogeneous Reservoir Characterization and Physics-Informed Modeling Needs

Heterogeneous depleted gas reservoir management, as exemplified by the Evetts site case study in the Permian Basin, illustrates the substantial spatial variability in porosity, permeability, and residual saturation that directly motivates the domain decomposition and sparse-data handling strategies developed for physics-informed neural networks (Han et al., 2023); such heterogeneity necessitates spatially adaptive physics-informed modeling approaches capable of resolving fine-scale property variation without requiring prohibitively dense training data across the full storage complex.

4.3 Thermal-Geochemical Process Coupling from Geothermal Infrastructure

Insights from the development of reactive heat exchangers for enhanced geothermal energy recovery illustrate how coupled thermal and geochemical process models can be engineered and monitored at the wellbore scale. These coupled-process modeling principles offer valuable methodological parallels for extending physics-informed neural network formulations for natural gas storage beyond isothermal, single-component flow toward more comprehensive representations that account for thermal effects during rapid injection and withdrawal cycling, particularly relevant to salt cavern storage where thermodynamic cycling effects can be pronounced.

5. Applications Across the Natural Gas Storage Lifecycle

5.1 Site Characterization and Injection Design

Physics-informed neural network surrogates, once trained, can support rapid evaluation of injection and withdrawal scenarios across heterogeneous geologic realizations at a fraction of the computational cost of full-physics simulation, while retaining the physical consistency—shock-capturing fidelity, mass conservation—that purely data-driven surrogates cannot guarantee. This capability is directly applicable to site characterization and injection design workflows for heterogeneous depleted gas reservoirs such as the Evetts site, where evaluating storage and deliverability performance across numerous geologic realizations is essential to robust site selection and injection strategy design.

5.2 Real-Time and Near-Real-Time Operational Support

The domain decomposition approach of Han et al. (2023), by enabling effective physics-informed modeling under sparse field data conditions, offers a pathway toward real-time or near-real-time operational support for natural gas storage management, in which continuously updated wellbore pressure and production data can be assimilated into a physically consistent, computationally efficient surrogate model without requiring the extensive labeled training datasets that conventional data-driven surrogates demand.

5.3 Extending Physics-Informed Approaches to Shock-Sensitive Storage Cycling

Because natural gas storage inherently involves repeated injection and withdrawal cycles that reverse the direction of the shock-forming saturation front, physics-informed AI approaches for this application must be robust to the full range of forward and reverse displacement scenarios encountered over a storage site's operational lifetime—a more demanding requirement than the single-direction displacement scenarios addressed in much of the foundational Buckley-Leverett PINN literature (Fraces & Tchelepi, 2021; Fuks & Tchelepi, 2020), and an important direction for extending current physics-informed methodologies toward the cyclic operational reality of natural gas storage.

6. Cross-Domain Lessons: Constraint-Consistent AI Deployment at National Scale

While the technical foundations of physics-informed AI for natural gas storage are rooted in subsurface flow physics, valuable governance and deployment lessons can be drawn from large-scale, constraint-consistent AI frameworks developed in other high-stakes, regulated domains. National-scale AI frameworks developed for chronic disease prevention and early

intervention illustrate how predictive models can be constrained by clinical guidelines and established protocols, ensuring that AI-driven recommendations remain consistent with domain-established rules even when applied to novel patient populations outside the original training distribution (Nguyen, 2026a). This principle of constraint-consistent generalization is directly analogous to the physics-informed AI value proposition for natural gas storage, where embedding governing flow equations directly into model training similarly ensures that predictions remain physically valid even for injection and withdrawal scenarios not directly represented in the training data.

Frameworks for transforming prior authorization through artificial intelligence further illustrate how AI systems can be designed to operate within a fixed set of institutional and regulatory constraints, reducing administrative burden while ensuring automated decisions remain auditable and compliant with policy rules (Nguyen, 2026b). This parallels the regulatory environment surrounding natural gas storage operations, where physics-informed model outputs that are explicitly grounded in governing conservation laws offer a more defensible, auditable basis for regulatory review of storage capacity and deliverability estimates than outputs from unconstrained, purely data-driven alternatives.

Economic impact analyses of AI adoption in healthcare, quantifying national-scale cost savings and productivity gains attributable to constrained, guideline-consistent AI deployment, offer a further template for justifying investment in physics-informed AI infrastructure for natural gas storage (Nguyen, 2026c). Just as healthcare AI systems that respect clinical constraints have demonstrated measurable cost savings through more reliable, guideline-consistent decision support, physics-informed AI systems for natural gas storage can be expected to reduce costs associated with either overly conservative operational planning stemming from mistrust of unconstrained data-driven predictions, or, conversely, operational errors arising from unconstrained model extrapolation into physically inconsistent regimes—an economic case that merits explicit quantification as physics-informed AI systems mature toward standard practice in the natural gas storage industry.

Collectively, these cross-domain parallels reinforce a broader principle: the value of physics- or rule-informed constraints in machine learning is not unique to subsurface engineering, but reflects a general requirement for trustworthy AI deployment in domains where erroneous extrapolation carries substantial financial, safety, or operational consequences. The maturation of physics-informed AI for natural gas storage can accordingly benefit from governance and

validation frameworks developed in these adjacent, already-scaled AI application domains.

7. Challenges and Limitations

Despite substantial progress, several challenges continue to constrain the operational deployment of physics-informed AI for subsurface natural gas storage.

Shock-capturing fidelity. As documented by Fuks and Tchelepi (2020), naive physics-informed formulations that directly embed the nonlinear hyperbolic conservation equation in the loss function struggle to accurately capture shock and mixed-wave solution structures, necessitating careful formulation choices—such as parabolic regularization—that add complexity to physics-informed model development for natural gas storage's inherently shock-forming displacement fronts.

Training instability and loss function balancing. Physics-informed neural network training generally requires careful balancing of data-fitting and physics-residual loss terms, and can suffer from optimization pathologies that impede convergence, particularly for the highly nonlinear, multiphase flow equations relevant to gas injection and withdrawal.

Sparse field data availability. While domain decomposition approaches such as PINN-DD (Han et al., 2023) represent meaningful progress, the fundamental scarcity of authentic field data relative to the spatial extent of most natural gas storage complexes remains a persistent constraint on physics-informed model training and validation.

Cyclic, bidirectional flow modeling. Much of the foundational physics-informed literature addresses single-direction displacement problems, whereas natural gas storage inherently involves repeated, bidirectional injection-withdrawal cycling, a more demanding modeling requirement that remains only partially addressed in the current physics-informed AI literature.

Multiphysics and thermal coupling. Comprehensive physics-informed modeling of natural gas storage, particularly for salt cavern applications subject to significant thermodynamic cycling effects, requires extension beyond isothermal, single-component flow formulations toward fully coupled thermal-flow-geomechanical representations, a substantial architectural and computational extension of current single-physics PINN approaches.

8. Future Directions

Future research should prioritize the development of physics-informed AI architectures explicitly designed for cyclic, bidirectional displacement scenarios characteristic of natural gas

storage operations, building on the foundational shock-capturing insights established for single-direction Buckley-Leverett problems (Fraces & Tchelepi, 2021; Fuks & Tchelepi, 2020). Extending domain decomposition strategies (Han et al., 2023) to accommodate the spatially heterogeneous, sparse-data conditions characteristic of real-world natural gas storage complexes such as the Evetts site represents a further important direction for improving the practical deployability of physics-informed surrogate models.

Integration of high-resolution petrophysical characterization workflows—such as those demonstrated for the Three Forks geothermal reservoir—directly into physics-informed model parameterization pipelines represents a promising avenue for improving site-specific predictive fidelity, while extending coupled thermal-geochemical process modeling principles developed for reactive heat exchanger engineering toward physics-informed natural gas storage applications could support more comprehensive multiphysics representations relevant to salt cavern and other thermally sensitive storage settings. Finally, adopting governance and validation frameworks informed by constraint-consistent AI deployment in public health and healthcare administration and economics (Nguyen, 2026a, 2026b, 2026c) may help establish the auditability and regulatory trust required for physics-informed AI systems to transition from research demonstration toward routine use in commercial-scale natural gas storage management as the field continues to mature in 2026 and beyond.

9. Conclusion

Physics-informed artificial intelligence represents a critical methodological advance for subsurface natural gas storage modeling, resolving the tension between the computational efficiency of data-driven surrogate models and the physical fidelity required for reliable, safety-relevant subsurface flow prediction. Foundational research on Buckley-Leverett benchmark problems, documented limitations of naive physics-informed formulations for shock-forming flow, extensions toward general porous media fluid flow prediction, and domain decomposition strategies for sparse-data reservoir simulation collectively demonstrate that embedding governing physical laws into neural network architectures substantially improves physical consistency relative to purely data-driven approaches, while retaining meaningful computational advantages over full-physics simulation alone. Cross-domain lessons from constraint-consistent AI deployment in public health and healthcare administration and economics further suggest a pathway toward the governance and validation frameworks

necessary for physics-informed AI to achieve regulatory trust and operational adoption in the natural gas storage industry. Realizing the full potential of physics-informed AI in this domain will require sustained investment in shock-capturing model formulations, training stability, sparse-data domain decomposition strategies, and multiphysics coupling—investments essential to ensuring that subsurface natural gas storage can be modeled, planned, and managed safely and efficiently as the field continues to mature through 2026 and beyond.

References

1. Almajid, M. M., & Abu-Al-Saud, M. O. (2022). Prediction of porous media fluid flow using physics informed neural networks. *Journal of Petroleum Science and Engineering*, 208, Article 109205. <https://doi.org/10.1016/j.petrol.2021.109205>
2. Fraces, C. G., & Tchelepi, H. (2021, October). Physics informed deep learning for flow and transport in porous media. Paper presented at the SPE Reservoir Simulation Conference (p. D011S006R002). SPE. <https://doi.org/10.2118/203934-MS>
3. Fuks, O., & Tchelepi, H. A. (2020). Limitations of physics informed machine learning for nonlinear two-phase transport in porous media. *Journal of Machine Learning for Modeling and Computing*, 1(1), 19–37. <https://doi.org/10.1615/JMachLearnModelComput.2020033905>
4. Han, J.-X., Xue, L., Wei, Y.-S., Qi, Y.-D., Wang, J.-L., Liu, Y.-T., & Zhang, Y.-Q. (2023). Physics-informed neural network-based petroleum reservoir simulation with sparse data using domain decomposition. *Petroleum Science*, 20(6), 3450–3460. <https://doi.org/10.1016/j.petsci.2023.10.019>
5. Nguyen, T. T. (2026a). AI-powered precision public health: A national framework for targeting chronic disease prevention and early intervention. *International Journal of Emerging Trends in Computer Science and Information Technology*, 7(3), 10–20.
6. Nguyen, T. T. (2026b). Transforming prior authorization through artificial intelligence: A national framework for reducing administrative burden and improving patient access. *International Journal of AI, BigData, Computational and Management Studies*, 7(3), 17–27.
7. Nguyen, T. T. (2026c). The economic impact of AI adoption in healthcare: Estimating national cost savings, productivity gains, and long-term health outcomes. *International Journal of Artificial Intelligence, Data Science, and Machine Learning*, 7(3), 1–11.