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Review Article

ARTIFICIAL INTELLIGENCE IN SUBSURFACE ENERGY SYSTEMS: A COMPREHENSIVE REVIEW OF CO_2 STORAGE, HYDROGEN STORAGE, AND GEOTHERMAL ENERGY

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ABSTRACT

The global shift toward clean energy is turning deep underground rock layers into a vital infrastructure for storing energy and cutting carbon emissions. This paper examines how computer models and smart data tools are being used to improve three major areas: capturing and burying carbon dioxide, storing hydrogen underground for later use, and tapping into volcanic heat for geothermal energy. By analyzing 46 relevant peer-reviewed studies in this field, this review shows how these smart computer models can quickly assess underground sites, monitor for gas leaks, handle the stress of repeatedly refilling and emptying storage zones, and prevent small earthquakes. The paper also looks at the big picture by comparing the pros, cons, and real-world readiness of these different technologies. Finally, we address current hurdles, such as data gaps and the difficulty of understanding how these 'black box' computers make decisions, while exploring future trends, such as secure data sharing and automated safety systems. Ultimately, bringing computer data science and earth sciences together creates a reliable digital foundation for managing our future clean energy networks.

Keywords: Carbon Storage, Geothermal Energy, Hydrogen Storage, Machine Learning, Risk Mitigation.

INTRODUCTION

The global energy transition is reshaping the subsurface from a hydrocarbon province into infrastructure for decarbonization and energy storage. Carbon capture and storage (CCS) remains central to net-zero strategies; recent reviews show that deployment must increase dramatically from current levels, and that scaling to 2050 will require sustained expansion of subsurface storage capacity (Mitterrutzner *et al.*, 2026). Underground Hydrogen Storage (UHS) is emerging as a key buffer for variable renewables. However, recent reviews emphasize that full-scale implementation still requires resolving obstacles in regulations, geology, technology and economics, as well as a better understanding of reservoir geomechanics under cyclic loading (Taiwo, Tomomewo and Oni, 2024; Ghafouri, Younes and Grasselli, 2026). Enhanced geothermal systems offer firm, low-carbon power. However, their broader deployment continues to be constrained by technical issues and concerns over induced seismicity, as well as by drilling and wellbore failures that have delayed or terminated multiple projects (Pollack, Horne and Mukerji, 2020; Horne *et al.*, 2025). Taken together, these pathways show that the subsurface is becoming an integrated energy system, one in which geomechanics will play a key role across storage, containment, and heat extraction.

Subsurface operations remain highly uncertain because geological formations are heterogeneous, direct well measurements are sparse, and tightly coupled thermo-hydro-mechanical-chemical processes govern reservoir behavior. Recent work notes that laboratory rock property tests are often minimal, that empirical correlations depend on limited core data, and that heterogeneity makes it difficult to predict porosity and permeability away from wells (Davies *et al.*, 2022; Ray *et al.*, 2022). At the same time, fully resolving coupled Thermo-Hydro-Mechanical-Chemical (THMC) behavior is computationally demanding, which limits the practical value of traditional forward simulations for operational decisions (Huang *et al.*, 2023). For this reason, the field is moving toward uncertainty-aware digital twins and machine-learning surrogates that assimilate multimodal data and update forecasts more rapidly. Recent studies show that uncertainty-aware digital shadows can track CO2 plume state from seismic and well data, that machine-learning workflows can detect leakage from pressure signals, and that other models can forecast induced seismicity from injection parameters, offering earlier risk mitigation for CO2 storage and geothermal operations (Sinha *et al.*, 2020; Cuvier *et al.*, 2025; Gahlot *et al.*, 2025).

Artificial intelligence is increasingly bridging classical physics and data-driven inference in subsurface engineering. Recent reviews show that physics-informed machine learning improves generalization, interpretability, and adherence to governing laws, while supporting seismic applications, reservoir simulation, and decision-making across carbon, hydrogen, and geothermal systems (Latrach *et al.*, 2024). In parallel, deep learning has become central to seismic data processing and subsurface characterization, with demonstrated gains in interpretation, inversion, and uncertainty-aware prediction (Mousavi *et al.*, 2024). Together, these methods are moving the field beyond purely black-box models toward hybrid workflows that are faster, more robust, and better suited to operational risk reduction, especially where well data are limited and conditions evolve rapidly.

This review systematically evaluates the integration of Artificial Intelligence (AI) across three critical subsurface domains: CO_2 storage, hydrogen storage, and geothermal energy. The objective is to synthesise current advancements in Machine Learning (ML) and Deep Learning (DL) architectures while identifying specific knowledge gaps in operational integrity and long-term site monitoring. By examining the convergence of data science and geosciences, this paper provides a roadmap for de-risking the subsurface energy systems essential for a sustainable future.

While existing reviews focus heavily on isolated applications, such as pure carbon storage monitoring or geothermal resource mapping, they often treat these geological media as distinct domains. This review uniquely addresses the cross-cutting algorithmic foundations that bind these technologies into co-located Subsurface Energy Hubs. Furthermore, we provide a unified evaluation framework that maps algorithmic computational loads directly to technical risks such as microbial hydrogen loss and induced seismicity.

METHODOLOGY OF THE REVIEW

This review follows a systematic approach to identify and synthesise high-impact research at the intersection of geoscience and computer science. The literature shows a clear shift from purely data-driven models toward physics-informed machine learning, which improves generalization, interpretability, and adherence to governing physical laws; this is especially relevant for subsurface problems where data are sparse and the physics are strongly coupled. In geophysics, deep learning has also become central to seismic processing, interpretation, and inversion, making it a natural companion to traditional numerical simulation rather than a replacement for it. Literature was systematically aggregated from three primary databases: Scopus, Web of Science, and Google Scholar.

The search string utilized Boolean operators: (“machine learning (ML)” OR “Artificial Intelligence (AI)” OR “Physics-Informed Neural Network (PINN)”) AND (“carbon storage” OR “underground hydrogen storage” OR “geothermal energy”). Inclusion criteria restricted the scope to English-language peer-reviewed journal articles and high-impact conference proceedings published between 2019 and 2026. A total of 78 records were initially screened, resulting in 46 peer-reviewed publications undergoing full-text critical synthesis after removing duplicates, irrelevant engineering baselines, and papers lacking validated field/synthetic data.

Foundations of AI in Subsurface Engineering

The application of Artificial Intelligence (AI) in subsurface engineering represents a shift from purely deterministic models to hybrid, data-driven frameworks capable of handling high-dimensional geological data. The core of this transition lies in a suite of machine learning algorithms tailored for classification, regression, and spatial analysis. Traditional algorithms such as Support Vector Machines (SVMs) and Random Forests (RFs) remain prevalent for petrophysical property prediction and lithology classification due to their robustness on small datasets (Lin *et al.*, 2025). However, the industry is increasingly adopting Deep Learning (DL) architectures for more complex tasks. Convolutional Neural Networks (CNNs) have become the gold standard for automated seismic interpretation and fracture characterization. In contrast, Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks are vital for time-series forecasting, such as predicting pressure depletion or thermal breakthrough in geothermal reservoirs (Mojtahedi *et al.*, 2025).

Despite the power of pure ML, black-box models often fail to provide geologically consistent results because they lack an inherent understanding of physical laws. To bridge this gap, Physics-Informed Neural Networks (PINNs) have emerged as a critical innovation. PINNs integrate governing partial differential equations (PDEs), such as Darcy’s Law for fluid flow or heat diffusion equations, directly into the neural network's loss function. This ensures that the AI’s predictions respect the fundamental conservation laws of mass, momentum, and energy (Meng *et al.*, 2025). In subsurface energy systems, where data is often sparse or noisy, PINNs provide a physical regularization that improves model generalizability and reduces the risk of physically impossible predictions during CO_2 injection or hydrogen withdrawal (Nagao & Datta-Gupta, 2026).

The success of these algorithms is contingent upon the quality of data acquisition and the rigor of pre-processing. Subsurface data is uniquely challenging; it is collected across vastly different scales, from micro-scale pore imaging and well logs to macro-scale seismic surveys. Real-time monitoring now increasingly relies on Internet of Things sensors and Fiber Optic Sensing (e.g., Distributed Acoustic Sensing), which generate massive, high-frequency data streams (Delpisheh *et al.*, 2024). Pre-processing these inputs involves complex denoising, imputation of missing well-log intervals, and synchronization of static geological models with dynamic sensor data. Furthermore, the high level of noise in seismic data requires advanced AI-driven filtering techniques to improve signal-to-noise ratios prior to feature extraction. As the industry moves toward automated operations, integrating edge computing with these AI foundations is becoming essential for handling time delays in real-time subsurface management (Ramírez-Rojas *et al.*, 2026).

AI in CO_2 Capture and Storage (CCS)

The deployment of Carbon Capture and Storage (CCS) at the gigatonne scale is a cornerstone of global decarbonization strategies. However, the geological sequestration of CO_2 involves complex multi-phase flow, geomechanical risks, and long-term containment uncertainties. Artificial Intelligence (AI) has transitioned from a research curiosity to a critical operational tool, enhancing the safety and economic viability of storage in saline aquifers and depleted oil and gas reservoirs (Yan *et al.*, 2022).

Site Characterization and Reservoir Selection

Selecting a sequestration site requires a detailed understanding of porosity, permeability, and seal integrity. Traditionally, this involved years of manual seismic interpretation and static modeling. AI accelerates this by automating the identification of structural traps and stratigraphic features. Convolutional Neural Networks (CNNs) are now routinely deployed to process massive 3D seismic volumes, identifying faults and salt domes with accuracy surpassing human interpreters (Liang *et al.*, 2026). In depleted reservoirs, Machine Learning models use historical production data to characterize spatial heterogeneity, enabling operators to distinguish high-permeability thief zones from secure storage compartments. Furthermore, Random Forest and Gradient Boosting algorithms are being used to screen thousands of potential saline aquifers globally, ranking them based on geomechanical stability and proximity to emission hubs (Al-Ali, Stephen and Shams, 2019).

Figure 1 illustrates how Artificial Intelligence (AI) enhances site characterization and reservoir selection by integrating geological, petrophysical, and production data into a faster and more reliable

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decision-making framework.

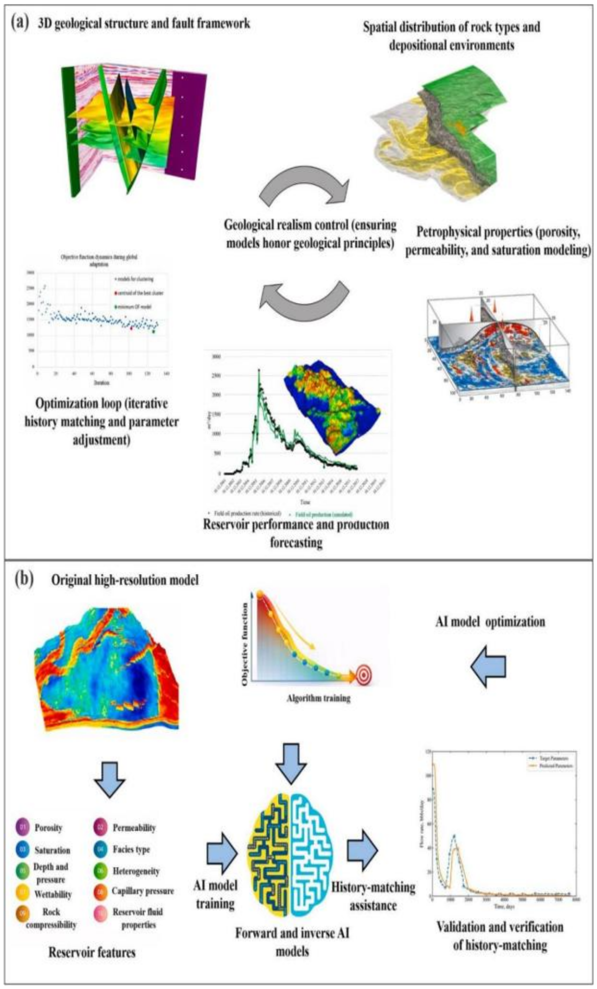

Figure 1. AI-based framework for reservoir site characterization, modeling, and production optimization (Davoodi *et al.*, 2026b).

In part (a), the workflow begins with the development of a 3D geological model and fault framework, which defines the structural architecture of the subsurface reservoir. AI assists by processing large geological datasets to identify spatial relationships between rock layers, faults, and depositional environments. This improves the understanding of reservoir heterogeneity and supports the prediction of critical petrophysical properties such as porosity, permeability, and fluid saturation. The diagram also highlights the concept of geological realism control, where AI-driven models are constrained to remain consistent with geological principles and historical production data. Through iterative optimization and history matching, machine learning algorithms continuously adjust model parameters until simulated reservoir behavior closely matches actual field performance. This enables more accurate forecasting of reservoir productivity and long-term recovery potential.

Part (b) demonstrates the role of AI in transforming traditional high-resolution reservoir models into efficient predictive systems. Reservoir features such as porosity, saturation, pressure, facies type, permeability, and capillary pressure are used to train forward and inverse AI models. During training, optimization algorithms minimize prediction errors and improve model accuracy. AI-based history-matching techniques accelerate the calibration process by rapidly comparing simulated and observed production responses, significantly reducing computational time compared to conventional reservoir simulation methods. Validation and verification steps ensure that the AI model reliably reproduces reservoir performance trends before deployment.

Monitoring and Leakage Detection

The long-term success of Carbon Capture and Storage (CCS) depends on ensuring that injected CO_2 remains within the target complex. Traditional monitoring, such as repeat 4D seismic surveys, is intermittent and expensive. AI enables a shift toward continuous, autonomous surveillance. By integrating data from Distributed Acoustic Sensing (DAS) and downhole pressure sensors, Deep Learning models can detect subtle signatures of CO_2 leakage into overlying formations or through abandoned wellbores in real time (Zheng *et al.*, 2022).

Anomaly detection algorithms, particularly Autoencoders, are trained on normal reservoir behavior to identify deviations that might signal a seal breach or an unexpected pressure spike. These AI-driven systems significantly reduce false alarms and provide early warning signals, allowing for immediate remedial actions such as injection rate adjustments or pressure relief (Vijai and P, 2025).

Storage Capacity Estimation and Plume Migration

Accurately predicting how much CO_2 a reservoir can hold and where it will move over centuries is a significant computational challenge. Conventional numerical simulators (e.g., ECLIPSE or CMG) solve complex partial differential equations that can take days to run. AI-based surrogate models, or reduced-order models (ROMs), can replicate these simulations in milliseconds (de la Cruz-Azuara, Hamzaoui and Sanchez, 2026).

Physics-Informed Neural Networks (PINNs) are particularly effective here, as they incorporate fluid-flow physics to predict CO_2 plume migration while maintaining mass balance. These models enable researchers to run thousands of Monte Carlo simulations to account for geological uncertainty, yielding a range of likely storage-capacity outcomes rather than a single, potentially flawed estimate (Paltsev *et al.*, 2022). This predictive power is essential for determining long-term trapping mechanisms, including structural, residual, and solubility trapping, ensuring the CO_2 eventually mineralizes and remains permanently sequestered.

Optimization of Injection Strategies

Managing CO_2 injection is a delicate balancing act: injection rates must be maximized to meet climate targets, yet remain below the caprock's fracture pressure to avoid induced seismicity or leakage. Reinforcement Learning (RL) has emerged as a powerful tool for this dynamic optimization. Unlike static plans, RL agents can learn from real-time pressure and flow data to adjust injection parameters automatically (Jo *et al.*, 2025).

These systems optimize well-to-well interactions in large-scale storage hubs, ensuring that pressure build-up from one well does not compromise the capacity of another. AI-driven optimization has been shown to increase effective storage efficiency by up to 15% while significantly lowering the risk of geomechanical failure (Algburi *et al.*, 2025). By automating these complex decisions, AI ensures that CCS operations are not only safe but also cost-effective, facilitating the rapid scaling required by the Paris

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Table I. Applications of AI techniques in CCUS for improved characterization, monitoring, storage capacity prediction, and injection optimization.

Domain	Primary AI Technique	Key Benefit
Characterization	CNNs, Random Forest	Faster site screening; 90% reduction in interpretation time.
Monitoring	Autoencoders, LSTMs	Real-time leakage detection; reduced monitoring costs.
Capacity	PINNs, Surrogate Models	Instantaneous plume prediction; uncertainty quantification.
Injection	Reinforcement Learning	Pressure management; maximized storage efficiency.

Table I confirms that AI serves as the digital backbone of modern CCS. By transforming sparse, noisy subsurface data into actionable insights, it de-risks the sequestration process and provides the regulatory and public confidence necessary for large-scale carbon management.

AI in Underground Hydrogen Storage (UHS)
Underground Hydrogen Storage (UHS) in salt caverns, depleted reservoirs, and aquifers is essential for balancing the intermittency of renewable energy. However, hydrogen's unique physical properties- low viscosity, high diffusivity, and chemical reactivity- present significant technical hurdles (Leng *et al.*, 2025). AI is increasingly utilised to manage these complexities, ensuring that UHS can function as a reliable geological battery.

Operational Integrity and Rapid Cycling
Unlike natural gas storage, which typically follows seasonal cycles, UHS for grid balancing requires high-frequency injections and withdrawals (on daily or weekly cycles). This rapid cycling induces significant thermomechanical stress on the reservoir and wellbore components. Machine Learning models, specifically Long Short-Term Memory (LSTM) networks, are being deployed to predict the geomechanical response of storage sites to these fluctuations. By training on historical pressure and temperature data, AI can forecast potential fatigue in the caprock or cement sheath integrity, allowing operators to define safe operating windows that prevent fracture propagation (Davoodi *et al.*, 2026a).
Figure 2 illustrates how AI improves the operational integrity and rapid cycling performance of underground hydrogen storage systems. AI-driven models enable real-time monitoring of hydrogen injection, withdrawal, pressure variations, and leakage risks, ensuring safer and more stable storage operations. Machine learning algorithms also optimize rapid charge–discharge cycling by predicting reservoir behavior, minimizing efficiency losses, and enhancing storage reliability during fluctuating energy demand.

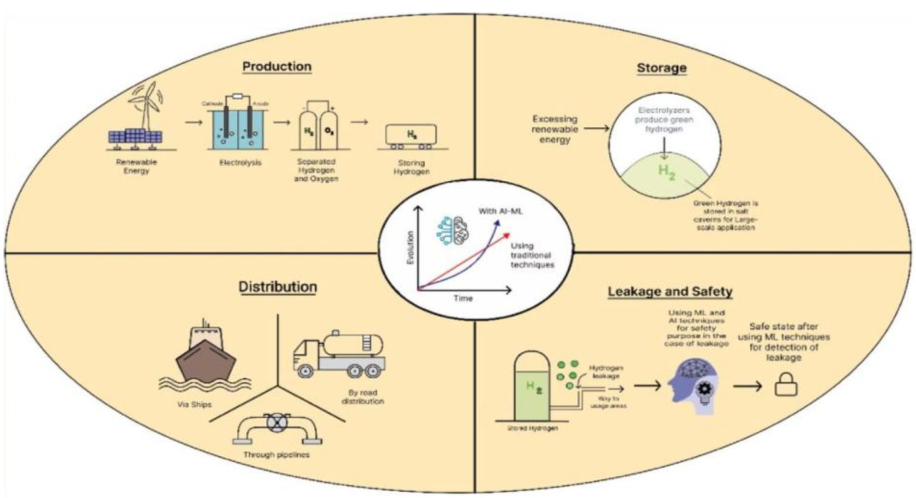

Figure 2. AI-enabled hydrogen production, storage, distribution, and safety management for underground hydrogen storage systems (Motiramani *et al.*, 2025).

Biogeochemical Prediction and Gas Loss
One of the most critical challenges unique to UHS is hydrogen loss caused by subsurface microorganisms (e.g., sulphate-reducing bacteria) and abiotic chemical reactions. These processes not only reduce the volume of stored energy but also produce unwanted by-products such as hydrogen sulphide (H_2S), which can corrode infrastructure and sour the gas. AI-driven predictive modelling is now used to map the risk of microbial activity based on reservoir temperature, salinity, and mineralogy. Random Forest and XGBoost algorithms have proven effective in predicting hydrogen consumption rates by correlating sparse geochemical samples with spatial reservoir data, yielding a more accurate energy recovery factor than traditional metabolic models (Yu, Mao and Mehana, 2024).

Cushion Gas Management and Mixing Dynamics
To maintain reservoir pressure and ensure high delivery rates, a cushion gas (such as CO_2, N_2, or CH_4) is required. A major operational risk is the mixing of the high-purity hydrogen working gas with the cushion gas at the interface. AI-based surrogate models are replacing computationally intensive CFD

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(Computational Fluid Dynamics) simulations to predict the movement of this mixing zone in real time. Physics-Informed Neural Networks (PINNs) are particularly valuable here, as they can model the high diffusivity of hydrogen while adhering to the laws of multi-phase flow in porous media (Chang *et al.*, 2024). These models enable operators to optimize the cushion gas volume, maximizing storage efficiency while ensuring that the withdrawn hydrogen meets the purity standards required for fuel cells.

Supply Chain Integration and Logistics

Underground Hydrogen Storage (UHS) does not operate in isolation; it serves as a link between renewable energy production (e.g., electrolysis) and end users. AI facilitates the integration of UHS into the broader Hydrogen Economy by optimizing the timing of storage operations. Reinforcement Learning (RL) agents can process weather forecasts, electricity market prices, and grid demand to decide when to store hydrogen (during surplus renewable production) and when to release it (during peak demand). This AI-driven orchestration ensures that the subsurface asset is utilized to maximize both grid stability and financial returns (Mwakipunda *et al.*, 2026).

Table II highlights how AI and machine learning improve the safety, reliability, and efficiency of underground hydrogen storage operations. Advanced predictive models help detect mechanical failures, monitor hydrogen purity, optimize gas management, and coordinate storage operations with renewable energy supply and demand.

Table II. AI approaches for operational integrity and optimization in UHS.

Operational Challenge	AI/ML Approach	Impact on Project
Mechanical Fatigue	LSTMs / Deep Learning	Extends wellbore life; prevents caprock failure.
Microbial Loss	Gradient Boosting	Predicts gas purity; quantifies energy loss.
Gas Mixing	PINNs / Surrogate Models	Optimizes cushion gas ratio; maintains H_2 purity.
Logistics	Reinforcement Learning	Synchronizes storage with renewable energy markets.

AI in Geothermal Energy Systems

Geothermal energy offers a unique advantage in the renewable portfolio: it provides constant, baseload power regardless of weather conditions. However, the high upfront costs of drilling and the technical challenges of managing high-temperature, high-pressure reservoirs have historically limited its expansion. Artificial Intelligence (AI) is now being leveraged to reduce these financial and operational risks, transforming geothermal projects into data-driven enterprises.

Resource Exploration and Automatic Drilling

The exploration phase of a geothermal project is fraught with resource risk, the possibility that a drilled well will not yield sufficient heat or flow. AI enhances exploration by integrating disparate datasets, including gravity, magnetic, and hyperspectral satellite imagery, to identify blind geothermal systems that lack surface expressions like geysers. Deep Learning (DL) models can fuse these multi-physics data layers to produce high-probability maps of subsurface heat anomalies (Parsa & Pour, 2021).

Once a site is selected, drilling accounts for up to 50% of total project costs. AI-driven drilling optimization systems are used to mitigate expensive non-productive time (NPT). For instance, Random Forest and Support Vector Machines (SVMs) are trained on real-time sensor data from the drill string (e.g., torque, weight-on-bit, and rate of penetration) to predict stuck-pipe incidents or bit wear before they occur. These predictive maintenance models allow for proactive adjustments, significantly reducing the likelihood of catastrophic mechanical failures in harsh, abrasive geothermal environments (Panico & Boccarusso, 2025).

The implementation of Enhanced Geothermal Systems (NetRegs), as illustrated in Figure 3, provides a path to continuous baseload clean energy by accessing deep, hot, dry rock formations typically located at depths of 3 to 5 kilometers. However, unlocking these resources poses significant economic and technical challenges, primarily due to the high upfront costs of drilling in harsh, abrasive subsurface environments.

Artificial Intelligence is proving to be an essential tool in de-risking this exploration and development phase. During resource exploration, AI enhances exploration by integrating different types of data, including gravity, magnetic, and hyperspectral satellite imagery, to accurately map subsurface heat anomalies and identify viable blind geothermal systems before a single well is drilled.

Once drilling commences, AI systems significantly lower costs by reducing non-productive time (NPT). By analyzing real-time sensor streams from the drill string (such as torque, weight-on-bit, and penetration rates), machine learning algorithms like Random Forest and Support Vector Machines can predict equipment degradation or stuck-pipe incidents well before they occur. This predictive capability allows operators to make proactive adjustments, protecting expensive assets and fundamentally shifting geothermal drilling from a reactive process to an automated, data-driven operation.

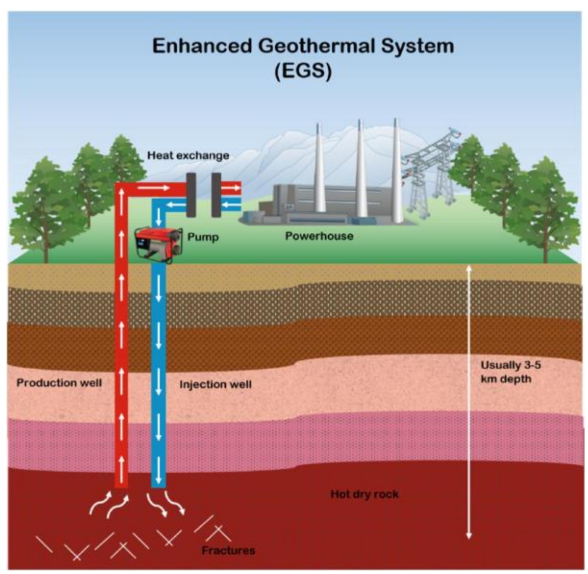

Figure 3. Enhanced Geothermal System (NetRegs) framework where AI optimizes deep resource exploration and automates

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drilling to reduce costs (Shan *et al.*, 2026).

Reservoir Characterization and Thermal Prediction

Managing a geothermal reservoir requires maintaining a delicate balance between water injection and heat extraction. A major risk is thermal breakthrough, where the injected cold water reaches the production well too quickly, prematurely cooling the reservoir. Physics-Informed Neural Networks (PINNs) are now used to characterize complex fracture networks, the primary pathways for fluid flow in Enhanced Geothermal Systems (NetRegs).

By constraining AI with the laws of thermodynamics, these models can predict the thermal front migration with high precision. Unlike traditional simulators that require extensive manual grid tuning, AI-based surrogate models can rapidly simulate thousands of scenarios to determine the optimal spacing between injection and production wells, ensuring the field's long-term thermal stability (Sheini Dashtgoli *et al.*, 2026).

Production Optimization and Heat Recovery

Once a plant is operational, AI serves as the brain of the facility, optimizing flow rates and injection temperatures in real time. Reinforcement Learning (RL) agents are particularly suited for this task. An RL agent can monitor fluctuating surface power demands and adjust subsurface pump speeds to maximize heat recovery while minimizing parasitic power consumption (Ali *et al.*, 2026).

Furthermore, AI-driven Digital Twins of the geothermal field allow operators to run what-if scenarios. For example, if a specific production well shows a temperature decline, the AI can automatically suggest redistributing injection volumes across other wells to reheat the depleted zone. This level of autonomous management has been shown to increase the net energy output of geothermal plants by 10–15% (Mastoi *et al.*, 2026)

Induced Seismicity Monitoring and Risk Mitigation

Perhaps the most sensitive challenge in geothermal development, particularly in EGS, is the risk of induced seismicity (small earthquakes caused by fluid injection). Public and regulatory acceptance of geothermal energy often hinges on effective seismic risk management. Machine Learning has revolutionized this area by providing traffic light systems that are far more sophisticated than traditional threshold-based models (He *et al.*, 2025).

Convolutional Neural Networks (CNNs) are used to process seismic waveforms in real time, distinguishing natural background noise from microseismic events caused by fracturing. More importantly, AI models can predict the probability of a larger seismic event by analyzing foreshock patterns that are too subtle for human analysts to detect. These early warning systems allow operators to throttle back injection pressures immediately, de-risking the project and ensuring community safety (Lurka, 2024).

Table III. AI applications in geothermal energy exploration and reservoir management.

Challenge	AI Technique	Operational Impact
Exploration Risk	Multi-modal Deep Learning	Identifies blind resources; reduces dry-hole risk.
Drilling Costs	Random Forest / SVM	Predicts equipment failure; reduces NPT by 20%.
Thermal Breakthrough	PINNs / Surrogate Models	Optimizes fracture utilization; extends reservoir life.
Induced Seismicity	CNNs / RNNs	Real-time risk assessment provides early warning

Table III shows how AI supports geothermal energy systems by reducing exploration uncertainty, lowering drilling risks and costs, improving reservoir performance, and enabling real-time monitoring of induced seismicity, thereby supporting safer, more efficient operations.

Integrated Systems & Cross-Cutting Synergies

The transition to a decentralized energy landscape is driving the move toward Subsurface Energy Hubs, where CO_2, Hydrogen, and Geothermal systems are co-located to maximize efficiency. AI serves as the primary orchestrator of these synergies, managing the complex multiphysics interactions that arise when different fluids and thermal regimes share the same geological space. A prominent example is the use of Multi-Objective Reinforcement Learning (MORL) to manage CO_2-Enhanced Geothermal Systems (CO_2-EGS). In these setups, captured CO_2 is used as the heat-exchange fluid instead of water; AI optimizes injection rates to ensure simultaneous carbon sequestration and maximum heat extraction, balancing two distinct environmental goals in real time (Fentaw *et al.*, 2026).

Furthermore, the rise of Digital Twins, high-fidelity virtual replicas of subsurface assets, enables a holistic view of the energy lifecycle. These twins integrate real-time data from Fiber-Optic Sensors and IoT-enabled wellheads across domains. For instance, an AI-driven Digital Twin can simulate how the pressure plume from a CO_2 injection site might affect a nearby Hydrogen storage cavern. By utilizing Surrogate Modeling, operators can run thousands of what-if scenarios in seconds to prevent cross-contamination or geomechanical interference between different energy assets (Agho *et al.*, 2024).

Finally, AI facilitates the integration of these subsurface systems with the surface grid. By processing weather patterns and market volatility, AI determines when to divert excess renewable power to hydrogen electrolysis for storage or when to ramp up geothermal production to stabilize the grid. This surface-to-subsurface optimization ensures that these geological assets function as a unified, flexible energy battery, reducing the need for fossil-fuel-based backup power.

Table IV. Cross-Domain Comparative Matrix of Subsurface AI Implementations

Subsurface Domain	Primary AI Method	Advantages	Disadvantages	Computational Needs	Est. TRL
CCUS	PINNs & Autoencoders	-Real-time plume tracking. -Physics-compliant results.	-High initial training time (AI in SSS. -Out-of-distribution errors.	High (GPU clustering for training)	TRL 5–6 (Pilot field validated)
UHS Storage	LSTMs & Gradient Boosting	-Exceptional time-series forecasting - Captures rapid cyclic fatigue	-Poor physical law constraints. -Requires dense sensor inputs.	Medium (Standard cloud computing)	TRL 3–4 (Laboratory & simulated)
Geothermal Systems	CNNs & Reinforcement Learning	-Automated anomaly detection - Dynamic pump/flow adjustments	-Extreme black-box opacity. -Vulnerable to noisy sensor data.	High (Real-time edge execution)	TRL 4–5 (Field demonstration)

Challenges and Future Perspectives

The forward trajectory of AI in subsurface energy systems is rapidly shifting away from isolated, site-specific models toward highly integrated, next-generation computational architectures. A primary paradigm shift is the development of Geoscience Foundation Models. These large-scale models are pre-trained on massive, globally aggregated datasets of seismic surveys, well-log parameters, and core sample analyses, allowing them to capture universal geological patterns. Once established, these models can be fine-tuned with minimal local data to predict site-specific behaviors in carbon storage, hydrogen containment, or geothermal flow, drastically reducing the data scarcity bottleneck.

Closely aligned with this is the emergence of advanced Generative AI and Generative Adversarial Networks (GANs). Instead of relying strictly on traditional, computationally demanding stochastic simulators, generative architectures can instantly synthesize high-fidelity, physically conditioned 3D static reservoir realizations that honor complex underlying petrophysical properties. To circumvent the deep-seated challenge of proprietary data silos, where competitive commercial operators and state agencies are hesitant to share sensitive geological assets, Federated Learning presents a viable path forward. This decentralized training methodology enables machine learning algorithms to train locally on individual wellsite or corporate servers, sending only updated model weights to a centralized framework rather than the raw data itself.

However, as subsurface operations increasingly rely on these automated AI-driven digital twins and automated wellhead routing mechanisms, the industrial attack surface expands significantly. This automation necessitates the immediate integration of rigorous cybersecurity protocols and strict AI governance frameworks. Future deployments must incorporate automated physics-constrained sanity checks directly into the edge-computing control loops, ensuring that immutable thermodynamic boundaries block any rogue data injection or adversarial algorithmic override before physical wellbore integrity is compromised.

Conclusion

Artificial Intelligence has transitioned from a supporting tool to an essential architect of subsurface energy systems. By de-risking CO_2 sequestration, managing the complex biogeochemistry of hydrogen, and optimizing the thermal efficiency of geothermal reservoirs, AI provides the technical certainty required for large-scale investment. While challenges in data standardization and model transparency persist, the convergence of physics-informed algorithms and real-time monitoring offers a clear roadmap to a sustainable, Net-Zero future.

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