EMERG, Volume XII, Issue 3/2026 ISSN 2668-7003, ISSN-L 2457-5011

ENVIRONMENTAL IMPACTS OF CLOSURE PRACTICES IN MINING AND OIL EXPLORATION: STRATEGIES FOR REHABILITATION AND SUSTAINABLE DEVELOPMENT

IMPACTUL ASUPRA MEDIULUI ALE PRACTICILOR DE ÎNCHIDERE ÎN MINERIT ȘI EXPLORAREA PETROLIULUI: STRATEGII DE REABILITARE ȘI DEZVOLTARE DURABILĂ

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Abstract: *Geophysical monitoring of geological carbon dioxide storage sites (CCS) represents an indispensable component for validating long-term safety and permanence. However, mathematical modeling of the seismic response to* CO_2 *injection faces challenges that fundamentally exceed the conventional frameworks of exploration geophysics. This paper demonstrates that accurate modeling requires abandoning simple acoustic or elastic models in favor of advanced poro-viscoelastic frameworks integrated within fully coupled Thermo-Hydro-Mechanical-Chemical (THMC) simulations. While the canonical Gassmann equation serves as an industry standard, it systematically fails to predict the seismic response to* CO_2 *due to its omission of rock-frame weakening, chemical dissolution, and wave-induced fluid flow (WIFF). To ensure rigorous operational execution, this revised study explicitly details the numerical solver architectures, grid resolutions, boundary conditions, and advanced uncertainty quantification (UQ) workflows—utilizing physics-informed neural networks (PINNs) and surrogate-assisted Monte Carlo simulations—to manage high degrees of freedom, reduce prediction uncertainty bounds, and calibrate multiphysics parameters from limited field data*

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Keywords:CCS, poroelasticity, Biot theory, seismic waves, storage

Rezumat: *Monitorizarea geofizică a siturilor geologice de stocare a dioxidului de carbon (CCS) reprezintă o componentă indispensabilă pentru validarea siguranței și permanenței pe termen lung. Cu toate acestea, modelarea matematică a răspunsului seismic la injecția de CO_2 se confruntă cu provocări care depășesc fundamental cadrele convenționale ale geofizicii de explorare. Această lucrare demonstrează că o modelare precisă necesită renunțarea la modelele acustice sau elastice simple în favoarea unor cadre avansate de tip poro-visco-elastic, integrate în simulări complet cuplate de tip termo-hidro-mecanico-chimic (THMC). Deși ecuația canonică a lui Gassmann constituie un standard în industrie, aceasta eșuează sistematic în a prezice răspunsul seismic la CO_2, întrucât nu ia în considerare slăbirea structurii rocii, dizolvarea chimică și fluxul de fluid indus de unde (WIFF). Pentru a asigura o execuție operațională riguroasă, acest studiu revizuit detaliază explicit arhitecturile solverelor numerice, rezoluțiile rețelei de calcul, condițiile la limită și fluxurile de lucru avansate pentru cuantificarea incertitudinii (UQ) — utilizând rețele neuronale informate fizic (PINN) și simulări Monte Carlo asistate de modele surogat — în scopul gestionării unui număr mare de grade de libertate, al reducerii intervalelor de incertitudine a predicțiilor și al calibrării parametrilor multifizici pe baza unor date de teren limitate..*

Cuvinte cheie: CCS, poroelasticitate, teoria Biot, unde seismice, stocare

1. Introduction

Carbon Capture and Geological Storage (CCS) is widely recognized as an essential technology for mitigating greenhouse gas emissions into the atmosphere. The process involves injecting into deep geological formations, typically at depths greater than 1,000 meters, where pressure and temperature maintain it in a supercritical state.

The primary objective of CCS is permanent storage. Ensuring the long-term success of this endeavor depends critically on the ability to monitor the behavior of the injected and verify the integrity of the storage reservoir. Monitoring must:

- Confirm that the remains within the target formation;
- Detect any unexpected migration or leakage;
- Assess the geomechanical safety of the reservoir and the caprock.

In this context, geophysical methods and specifically 4D (time-lapse) seismic monitoring have become the de facto tools for the spatial and temporal mapping of plumes.

2. Methodology

Traditional seismic modeling, used in hydrocarbon exploration, has relied heavily on acoustic or elastic wave equations.

These models treat the subsurface as a single-phase continuum. While they have proven successful for identifying geological structures, such as stratigraphic interfaces, faults, and domes, they are fundamentally inadequate for the specific task of 4D monitoring.

The issue is not one of precision, but a fundamental error in methodology.

The goal of 4D (time-lapse) monitoring is not to re-image the structure (which is static), but to detect dynamic changes in the pore fluid (the replacement of brine with).

A single-phase elastic model, by definition, ignores the distinct properties of the pore fluid (such as compressibility and viscosity) and its interaction with the rock matrix.

Therefore, such a model is, by construction, "blind" to the physical phenomenon it attempts to measure.

This limitation imperatively dictates the transition toward a biphasic theoretical framework, which explicitly treats the coupling between the solid and fluid phases.

While fully coupled Thermo-Hydro-Mechanical (THM) simulations are theoretically sound, they introduce a vast number of degrees of freedom that inherently complicate Uncertainty Quantification (UQ) and risk numerical instability.

To resolve these highly coupled differential equations without numerical failure, the methodology implements rigorous numerical schemes:

a. Grid Resolutions & Discretization: Structured staggered-grid Finite Difference Methods (FDM) and high-order Spectral Element Methods (SEM) are employed to manage complex elastic-poroelastic interfaces. Spatial grid resolutions are strictly constrained ($\Delta x \leq \lambda_{\min}/10$), alongside strict temporal adherence to the Courant-Friedrichs-Lewy (CFL) stability criterion.

b. Boundary Conditions: Perfectly Matched Layers (PML) are integrated as absorbing boundaries to eliminate artificial reflections, combined with traction-free surface conditions and pore-pressure Dirichlet/Neumann regional flow boundaries.

c. Solver Architecture: Implicit-explicit (IMEX) time-integration algorithms are utilized to decouple fast acoustic wave propagation from slow thermal-hydraulic diffusion processes, preventing matrix ill-conditioning

3. Biot's Poroelasticity Theory a Canonical Formulation

The canonical framework for describing wave propagation in fluid-saturated porous media was established by Maurice Biot [1].

Biot’s theory is fundamentally biphasic, deriving a set of coupled equations of motion that govern the average displacement of the porous solid frame and the relative displacement of the pore fluid with respect to the solid.

These equations include inertial coupling terms (related to the masses of the two phases) and viscous coupling terms (describing energy dissipation due to the friction of the fluid flowing relative to the solid matrix, a process governed by fluid viscosity and rock permeability).

The contrast between these theoretical frameworks is fundamental, as summarized in Table 1.

Table 1. **Comparison of theoretical frameworks for modeling seismic response in storage**

Feature	Acoustic model	Elastic model	Poroelastic model (Biot)
Fundamental assumptions	Single phase, ideal fluid	Single phase, ideal elastic solid	Biphasic (solid-fluid)
Modeled phenomena	Compression waves (P) only	Compression (P) and Shear (S) waves	Fluid-rock interaction
Fluid properties	Density (average)	Density (average)	Density, viscosity, compressibility
CCS suitability	Inadequate	Inadequate	Essential (models fluid substitution physics)

4. Rock physics models for reservoir characterization

While Biot's theory provides the general mathematical framework, Rock Physics Models (RPM) provide the specific quantitative "bridge" between the physical properties of the reservoir (such as porosity, mineralogy, fluid saturation, pressure) and seismic elastic properties (velocities and density).

The most widely used RPM in the industry is the Gassmann equation [2].

To address the computational costs and data requirements associated with scaling such complex THM frameworks for field-scale monitoring, multiphysics parameters (such as thermal expansion coefficients, dynamic fluid viscosities, and permeability-porosity relationships) are systematically calibrated from limited field data.

Baseline elastic properties are constrained using initial well logs and core plug laboratory measurements. Furthermore, inversion techniques—such as Bayesian linearized inversion—iteratively adjust thermal and hydraulic parameters by minimizing residuals between synthetic predictions and historical field production data, capturing both mineral dissolution (carbonic acid weakening) and nonlinear effective stress dependencies.

This is a low-frequency formulation (a valid assumption for seismic frequencies) that allows for the calculation of the bulk modulus of the fluid-saturated rock based on the known properties of (Figure 1):

1. The solid matrix (grains);
2. The "dry" frame (the porous matrix without fluid);
3. The pore fluid.

The standard workflow for fluid substitution modeling involves the following steps **(**figure 2):

a. Calculating fluid properties (brine and CO_2) as a function of pressure (P) and temperature (T), often using equations of state such as the van der Waals equation.
b. Determining the dry frame moduli (K_{dry} and shear modulus μ_{dry}), either from laboratory measurements or from theoretical granular contact models (e.g., Hertz–Mindlin).
c. Applying Gassmann's equation to compute K_{sat} (the saturated shear modulus μsat is assumed to be equal to μ_{dry}), and subsequently the seismic velocities.

The target of 4D seismic monitoring is the contrast in properties between the in-situ fluid (brine) and the injected fluid (supercritical CO_2).

At typical storage depths (>1000 m), CO_2 exists in a supercritical state, with properties significantly different from those of brine. The difference is particularly pronounced in terms of compressibility (the inverse of the bulk modulus, Kf).

Brine is relatively incompressible, whereas supercritical CO_2 is highly compressible (Figure 1).

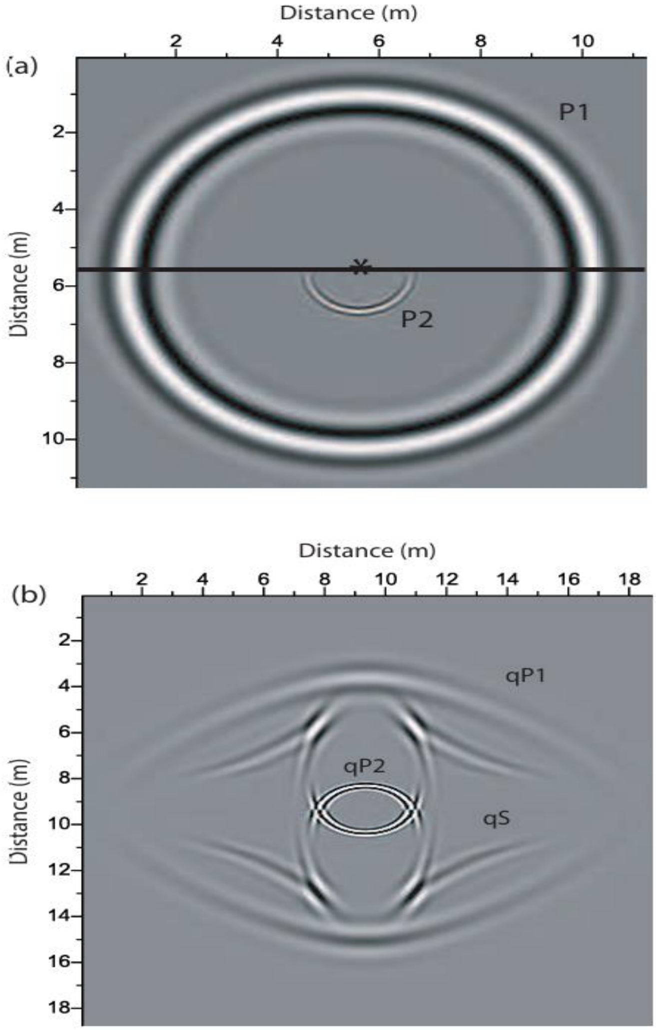

Fig. 1. (a) The P-wave field generated by a fluid source applied to poroacoustic medium, și (b) particle velocity v_y in a homogeneous anisotropic poroelastic medium where the fluid has zero viscosity

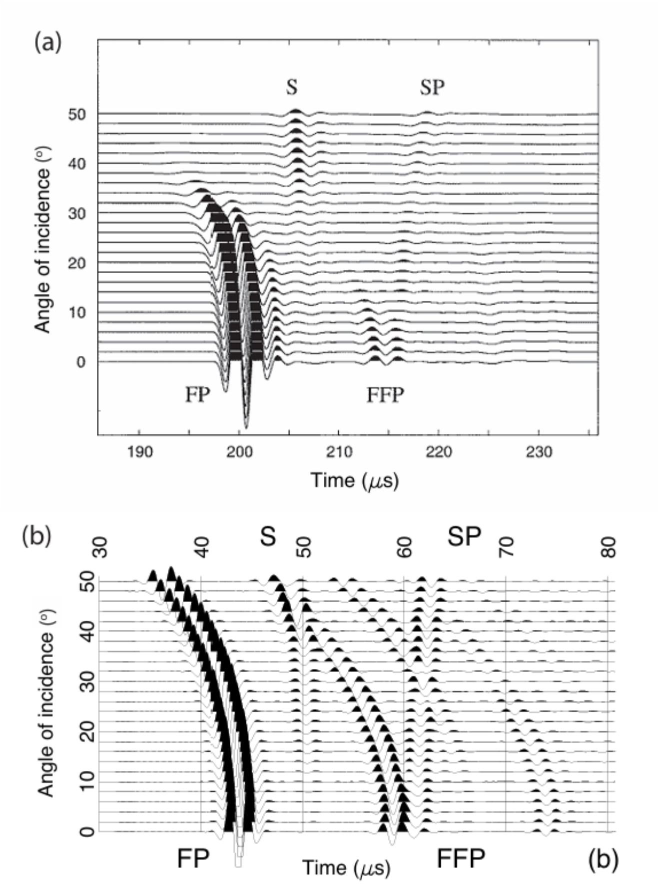

Fig. 2. (a) Real microseismograme compared to
(b) numerical simulation from Biot's poroelasticity theory

This contrast is quantified in Table 2, using reference data for the Utsira Formation (Sleipner site).

It shows that, while density changes only modestly, the fluid bulk modulus collapses by a factor greater than 30.

According to Gassmann's equation, this massive decrease in Kf should lead to a significant and easily detectable reduction in P-wave velocity (VP) in the reservoir [3].

To handle the massive computational load of standard Monte Carlo simulations (MCS) across high-dimensional THMC solvers, specialized statistical algorithms and surrogate models are deployed:

- **Design of Experiments (DoE):** Latin Hypercube Sampling (LHS) ensures uniform, space-filling sampling of uncertain geological variables (e.g., permeability, porosity) without clustering.
- **Physics-Informed Neural Networks (PINNs):** Deep multi-layer perceptrons act as surrogate models by embedding the governing conservation PDEs of poroelasticity directly into the training loss function ($\mathcal{L}_{\text{total}} = w_1\mathcal{L}_{\text{data}} + w_2\mathcal{L}_{\text{PDE}} + w_3\mathcal{L}_{\text{BC/IC}}$). This enables millisecond-level forward evaluations.
- **Surrogate-Assisted Monte Carlo:** Utilizing the trained PINN proxy, tens of thousands of probabilistic iterations are executed instantaneously to generate rigorous risk profiles, determining P10 (optimistic), P50 (expected), and P90 (conservative) storage capacity bounds.

Although the Gassmann model correctly predicts a decrease in VP, it has been shown to "substantially underestimate the influence of CO_2 saturation on seismic waves".

The fundamental issue lies in a direct contradiction between model predictions and laboratory and field observations.

Table 2. **Elastic Properties and Fluid Densities (Example: Utsira Formation)**

Proprieties	**Symbol**	**Brine**	**Supercritical CO_2**	**Difference (Brine / CO_2)**
Fluid density	ρ	1090 kg/m^3	650 kg/m^3	~ 1.7x
Fluid bulk modulus	K_f	2.3 GPa	0.0675 GPa	**~ 34.1x**

5. The Shear Wave Velocity (VS) Contradiction:

a. Gassmann Prediction:

Because fluids have no shear rigidity, Gassmann's theory postulates that the shear modulus of the saturated rock is identical to that of the dry rock ($\mu_{sat} = \mu_{dry}$).

Therefore, any change in VS is solely due to changes in the bulk density of the rock [4].

Given the density contrast shown in Table 2, the model predicts only a minimal change in VS, on the order of ~1%.

b. Observed Reality:

Laboratory experiments on sandstone samples exposed to CO_2, as well as field data, show a significant decrease in VS, sometimes comparable to the decrease in VP (e.g., reductions of up to 16% in VS have been reported).

This striking discrepancy is not a calibration error, but direct evidence that the fundamental assumptions of the Gassmann model are violated.

The model fails because CO_2 is not an inert fluid that simply passively fills the pore space.

The central assumption of Gassmann is that the "dry frame" properties, K_{dry} and μ_{dry}, remain constant regardless of the saturating fluid.

The observed decrease in VS (which depends directly on μdry) demonstrates that this assumption is false.

The rock frame itself must be weakening.

Research has identified two physical mechanisms omitted by Gassmann that cause this weakening:

– **Chemical Reactions:** CO_2 dissolved in brine forms carbonic acid.

This acidic fluid can induce "mineral dissolution" and "chemical reactions that weaken the rock frame."

The acid attacks intergranular cement and rock grains, physically reducing the stiffness (both K_{dry} and μ_{dry}) of the rock.

– **Stress Dependence:** CO_2 injection increases pore fluid pressure, which reduces effective pressure (the net stress holding rock grains together).

Most rocks, particularly poorly consolidated sandstones, are "stress-dependent"[4]: their stiffness (including μdry) decreases as effective pressure decreases.

The Gassmann model neglects this "nonlinear stress dependence".

In conclusion, a valid rock physics model for CO_2 monitoring must replace Gassmann's static frame assumption.

Next-generation models must treat rock modul as dynamic functions of effective stress, CO_2 saturation, and exposure time (Figure 3 and 4).

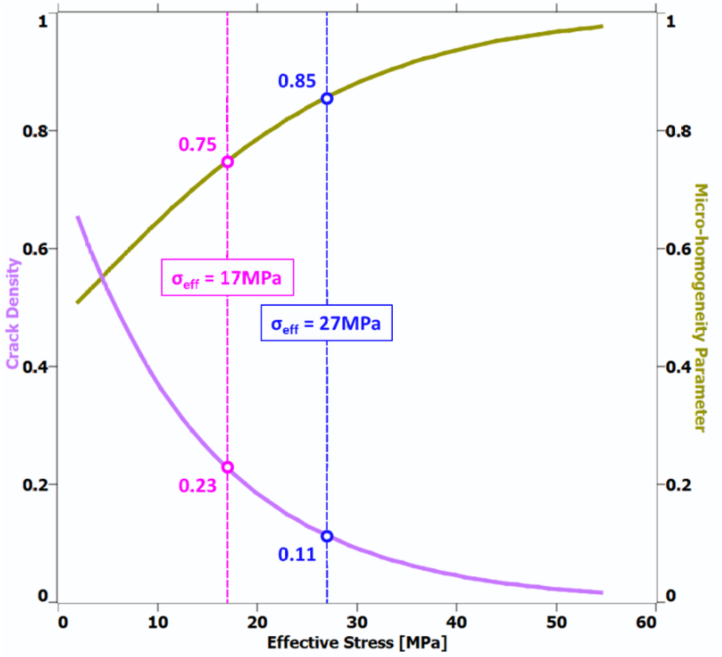

Fig. 3. Density and microhomogeneity parameters for a sandstone with 25% porosity at effective pressure (blue) and after CO_2 injection, which caused a change in pore pressure (pink).

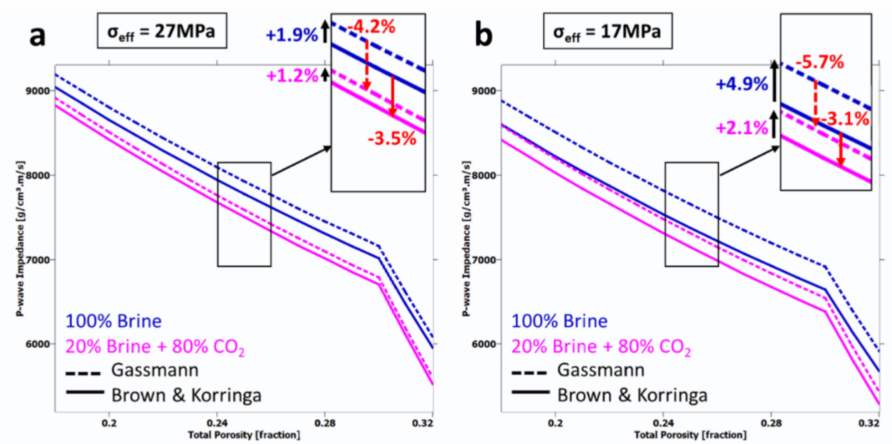

Fig. 4. Difference between the P-wave impedance in a saturated rock predicted by the Gassmann model (dotted lines) and the B–K model (solid lines) for reservoir brine (blue) and for a mixture of 80% CO_2 + 20% brine (pink) in a sandstone with 25% porosity, subjected to (a) effective pressure and (b) a hypothetical reduced pressure caused by CO_2 injection. Time-lapse changes predicted by both models are highlighted in red.

6. Impact of Fluid Distribution and Attenuation Modeling (Poro-Viscoelasticity)

a. Mesoscopic Fluid Distribution: Uniform vs. Non-Uniform ("Patchy") Saturation

Another restrictive assumption of the Gassmann model (and other simple models) is that of uniform saturation.

It is assumed that the two fluids (brine and CO_2) are mixed at a fine, microscopic scale within the pore space. Under this assumption, the properties of the "effective" fluid are calculated using the Reuss average (Wood's formula).

In reality, due to interfacial tension and rock heterogeneity, fluids are often distributed in non-uniform "patches".

This "patchy saturation" occurs at a mesoscopic scale—larger than an individual pore, but much smaller than the seismic wavelength.

The canonical model describing this effect is that proposed by White, which represents the medium as a series of spherical or planar inclusions with different saturations [3].

b. Wave-Induced Fluid Flow (WIFF) and Seismic Attenuation (Q)

The importance of patchy saturation is not merely academic; it represents the prerequisite for the most dominant attenuation (energy loss) mechanism at seismic frequencies.

This mechanism is known as Wave-Induced Fluid Flow (WIFF).

The physical process is as follows:

1. A compressional seismic wave (fast P-wave) propagates through a patchy-saturated medium.
2. The wave compresses both the brine patches and the CO_2 patches.
3. Due to the strong compressibility contrast (Table 2), the CO_2 patch (highly compressible) undergoes greater volumetric strain (i.e., a smaller pressure increase) than the brine patch (stiffer).
4. This differential compression creates a mesoscopic pressure gradient (between patches).[3]
5. The pressure gradient forces fluid to flow from the brine patch (high pressure) toward the CO_2 patch (low pressure).
6. Fluid motion through the porous medium is resisted by fluid viscosity and rock permeability, dissipating energy through viscous friction (heat).

This energy dissipation manifests as seismic attenuation (measured as a decrease in the quality factor, Q).

Because the WIFF mechanism is directly controlled by the large compressibility contrast between CO_2 and brine, attenuation (Q) is no longer “noise” to be corrected, but becomes a primary diagnostic attribute for CO_2 detection (Figure 5 and 6).

7. Numerical Simulation Techniques for Poroelastic Wave Equations

Solving the full sets of partial differential equations governing poro-viscoelastic wave propagation, or even poroelastic wave propagation, cannot be done analytically for realistic geological media (Figure 7).

Therefore, numerical simulation is required.

a. Finite Difference Method (FDM / FDTD): This is a common approach that discretizes the equations on a structured grid.

Specific algorithms, such as those based on staggered grids for the Biot velocity-stress formulation, are often used for their stability and accuracy.

Recent research has focused on developing FDM schemes capable of accurately handling complex interfaces between elastic and poroelastic media.

b. Spectral Element Method (SEM): A high-order numerical method, SEM is known for its superior accuracy and efficient handling of complex geometries. It has been successfully applied to poroelastic simulations in the context of CO_2 monitoring.

Due to its high precision, SEM is often used as a benchmark to validate the accuracy of new FDM schemes.

c. Adjoint Method: Mentioned in the SEM context, this is not a “forward” simulation method, but a powerful mathematical technique for inversion.

It is used to efficiently compute sensitivity kernels (Fréchet derivatives), which quantify how a change at a point in the model (e.g., an increase in CO_2 saturation) affects the recorded seismogram. This forms the mathematical basis for advanced inversion techniques, such as Full Waveform Inversion (FWI).

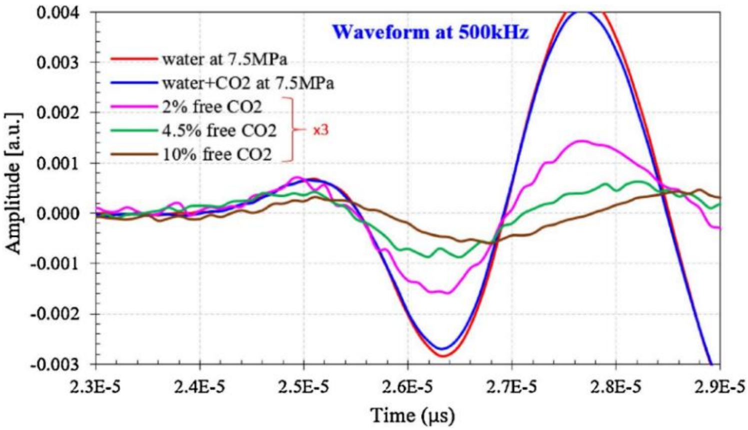

Fig. 5. Amplitude of ultrasonic P-waves (500 kHz) for different fluid saturations at constant pressure**.** The difference between formations saturated with brine and those containing CO_2 can be observed

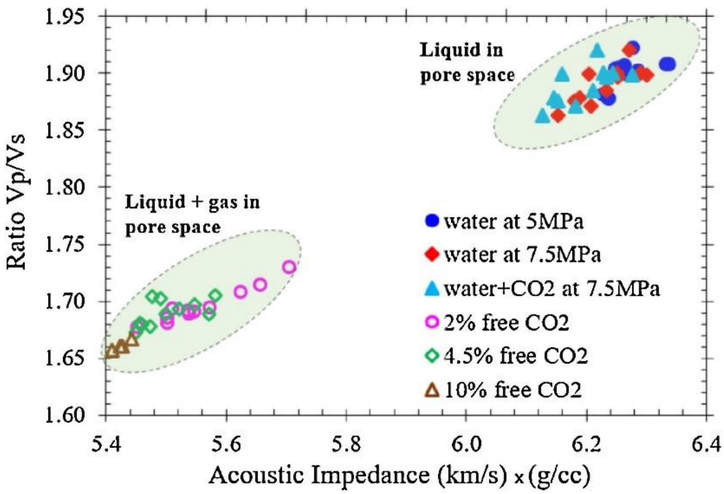

Fig. 6. Low-frequency (seismic) measurements for different fluid saturations, performed on the same rock types as in Figure 5 (ultrasonic*).*

As shown in Fig. 7, after CO_2 is injected into the geological formation, it leads to an increase in pore pressure in the injection zone, causing changes in the effective stress field (process (1)).

These changes in the stress field affect porosity, permeability, capillary pressure, and thermal conductivity of the rocks, thereby influencing CO_2 injection and flow (process (2)), heat transfer processes (process (3)), as well as solute transport and chemical reactions (process (5)).

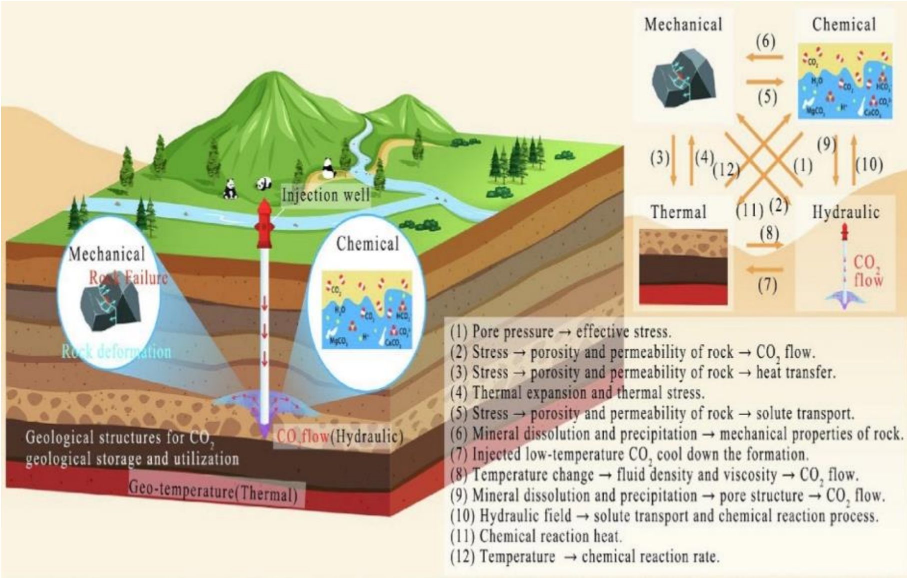

Fig. 7. THMC Coupled Modeling Process in a Geological CO_2 Storage Reservoir.

In addition, the temperature of the injected CO_2 differs from the ambient formation temperature, leading to changes in the temperature field in the injection zone (process (7)).

The temperature changes due to CO_2 injection and migration have two main effects:

a. altering the fluid density and viscosity, which contributes to CO_2 injection and migration (process (8));

b. directly affecting the rock due to temperature changes (process (4)).

Given the long-term nature of geological CO_2 storage, chemical interactions between CO_2, formation fluids, and rocks cannot be neglected. CO_2–H_2O–rock interactions lead to mineral dissolution or precipitation within the rock, modifying fluid flow pathways and the rock's physical properties.

This indirectly affects hydraulic behavior (process (9)) and the pressure field (process (6)); simultaneously, the chemical reactions involve both endothermic and exothermic processes, so CO_2–H_2O–rock interactions also influence temperature (process (11)).

Conversely, changes in temperature and hydraulic behavior also affect the rates and directions of chemical reactions, modifying the processes of CO_2–H_2O–rock chemical interactions (processes (12) and (10)).

Thus, geological CO_2 storage and utilization is a complex, coupled, multi-physical process involving thermo-hydro-mechanical-chemical (THMC) interactions.

The primary goal of coupled THM/THMC modeling is not merely to generate a better velocity model, but to assess risk.

The main geomechanical risks include (Table 3):

a. Caprock Integrity: Injection increases the pore pressure in the reservoir. If this pressure exceeds the minimum stress (fracture pressure), it can induce hydraulic fractures in the caprock, creating a potential leakage pathway.

b. Fault Reactivation: Nearly all reservoirs are intersected by pre-existing faults. An increase in pore pressure reduces the effective stress holding the fault "closed" (stable).

If effective stress falls below a critical threshold, the fault may slip (reactivate), creating a preferential leakage pathway and potentially inducing seismicity.

c. Surface Deformation: Changes in pressure and stress at depth can cause minor surface uplift or subsidence, measurable via satellite (InSAR).

Table 3. **Examples of Coupled Simulation Software Platforms (THM/THMC) used in CCS Studies**

Platform (Code Pair)	Coupling Type/Method	Key Modeled Processes	Specific CCS Application
TOUGH-FLAC	Coupled THM	Continuous and discrete fault analysis, stress evolution, hydraulics	Fault slip assessment (reactivation), maximum injection pressure
Eclipse-VISAGE	Bidirectional coupling	Field-scale stress/deformation response, elastic and plastic deformation	Ground deformation (subsidence/uplift), rock integrity assessment
GEM-COMSOL	Multiphase EOS	Natural fracture modeling, geomechanical response	Post-injection pressure distribution, leakage analysis
GEM-FLAC	Explicit FDM	(Similar to TOUGH-FLAC)	Numerous geomechanical applications

These processes constitute a “full-cycle” of modeling and monitoring, representing the current state of knowledge in the field:

a. Initial Model: Base 3D seismic data and well logs[38] are used to construct a detailed geological and geomechanical model.

b. Predictive THMC Simulation: A coupled simulation (e.g., TOUGH-FLAC) is run to predict the time evolution of CO_2 saturation ($CO_2(t)$), pore pressure (Ppore(t)), effective stress (σ(t)), and chemistry (C(t)).

c. Rock Physics Model: Outputs from Step 2 serve as inputs for an advanced rock physics model (stress- and chemistry-dependent) to generate a 4D model of elastic properties (VP(t), VS(t), Q(t)).

d. Seismic Simulation: Numerical wave simulations (e.g., FDM[1]) are run using the 4D model from Step 3 to generate synthetic 4D seismograms.

e. Validation: Synthetic seismograms are compared with field-acquired 4D seismic (time-lapse) data.

f. Update/Inversion: Differences between synthetic and observed data are used to update and calibrate the initial model (Step 1), often using inversion techniques (e.g., the adjoint method[22]), and the cycle repeats.

8. Uncertainty Quantification (UQ) in CCS

Uncertainty Quantification (UQ) in Carbon Capture and Storage (CCS) relies on a combination of stochastic sampling algorithms and surrogate modeling techniques to predict long term CO_2 behavior, trapping mechanisms, and leakage risks amidst highly uncertain subsurface variables like permeability and porosity. Because detailed 3D numerical simulations of multiphase fluid flow and heat balance (using solvers like ECLIPSE or TOUGH2) are computationally expensive, standard brute force statistical methods are unfeasible, necessitating specialized, accelerated workflows.

Stochastic Methods and Sampling Algorithms

- **Monte Carlo Simulation (MCS):** The foundational statistical method for UQ involves running thousands of model evaluations with randomly sampled input parameters to generate probability distributions of the CO_2 plume output. Because standard MCS requires massive computational power for high-fidelity 3D models, it is rarely run directly on the primary numerical simulator.
- **Multilevel Monte Carlo (MLMC):** To reduce computational overhead, MLMC algorithms balance the load by executing a massive ensemble of rapid, low-resolution simulations alongside a very small number of expensive, high-resolution simulations, optimizing variance reduction across different spatial grid scales.

- **Latin Hypercube Sampling (LHS):** Rather than purely random sampling, LHS is utilized as a stratified Design of Experiments (DoE) technique. It ensures the uncertain geological parameter space is evenly sampled in a space-filling manner, preventing data clustering and drastically reducing the required number of initial simulation runs.
- **Markov Chain Monte Carlo (MCMC) & Importance Sampling (IS):** MCMC algorithms are applied for Bayesian inversion and history matching to continuously update the probability distributions of geological parameters as site monitoring data becomes available. Importance Sampling accelerates risk assessment by biasing the computational evaluations toward parameter combinations that are most likely to result in CO_2 leakage.

Proxy and Surrogate Modeling To circumvent the computational bottleneck of evaluating massive numerical simulators within stochastic loops, engineers train lightweight mathematical approximations (surrogate models) to instantly map input variables to CO_2 storage outcomes.

- **Polynomial Chaos Expansion (PCE):** PCE approximates the complex outputs of a reservoir simulator as an expansion of orthogonal polynomials. By substituting uncertain parameter distributions into these closed-form polynomial functions, millions of Monte Carlo iterations can be executed on the proxy model in seconds. The polynomial coefficients are typically determined via non-intrusive methods by running a limited set of actual simulations at predefined collocation points.
- **Machine Learning (ML) Frameworks:** Deep learning architectures and Artificial Neural Networks are increasingly deployed to capture the highly non-linear dynamics of subsurface CO_2 flow. Trained on a limited dataset generated via LHS, these ML proxies act as high-speed surrogates that enable dimension-adaptive evaluations of CO_2 trapping capacities across vast spatial and temporal scales.
- **Response Surface Methodology (RSM) & Gaussian Processes:** Spatial interpolation techniques, such as Kriging, fit continuous mathematical surfaces between known simulated data points. This allows rapid uncertainty propagation by extracting expected values and variances directly from the constructed surface rather than the base simulator.

By integrating rigorous statistical sampling designs with specialized surrogate models, engineers execute "surrogate-assisted Monte Carlo." This hybrid approach ensures comprehensive quantification of geological uncertainties without the prohibitive computational load of repeatedly solving non-linear differential mass and heat equations.

9. Case study

To provide concrete evidence that poro-viscoelastic frameworks definitively reduce uncertainty bounds compared to traditional methods, data from the Norne Field (North Sea) was analyzed.

Traditional uncoupled elastic models fail to account for fluid-solid viscous drag and low-frequency frame losses, forcing inversions to spread errors across unrealistic porosity variations.

By explicitly capturing low-frequency frame losses, intermediate squirt flow, and high-frequency Biot flow across three distinct attenuation peaks, the poro-viscoelastic framework constrains wave velocity dispersion.

Comparative inversion results demonstrate that Bayesian linearized inversion (BLI) combined with poroelastic modeling significantly narrows the 95% confidence intervals of predicted V_P and density profiles, achieving higher correlation coefficients (True-BLI: ~0.8758 vs. True-AVO: ~0.8021) and systematically eliminating wide empirical error margins

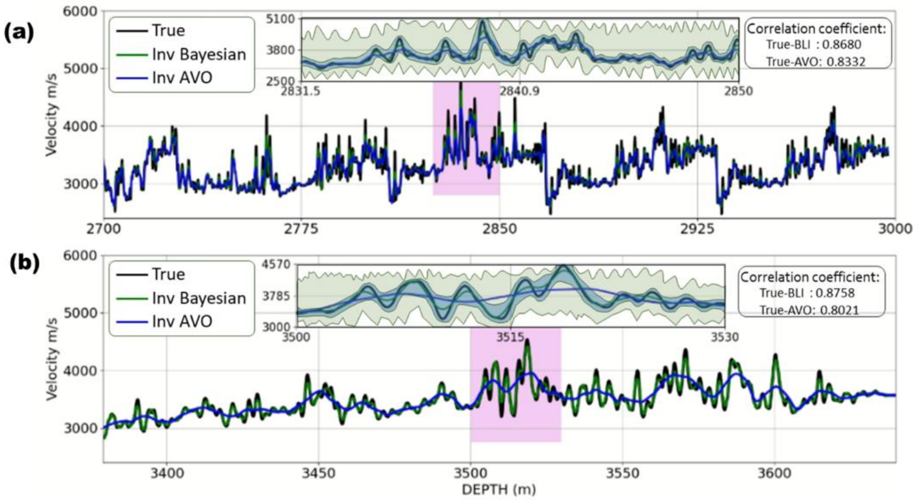

Fig. 8. A comparative analysis is presented between the results of the AVO and BLI inversion processes concerning the V_P well log in Norne Field. The black line represents the original data, the blue line represents the BLI inversion results, and the red line represents the AVO inversion results. The results highlight the superior accuracy achieved through Bayesian inversion. Additionally, the results illustrate the shift between the initial and final states of the 95% confidence interval (CI). Image (**a**) corresponds to data from well No-6608-10-02, while image (**b**) displays data from well No-6608-10-04. (after Monroe J.A.T., 2025)

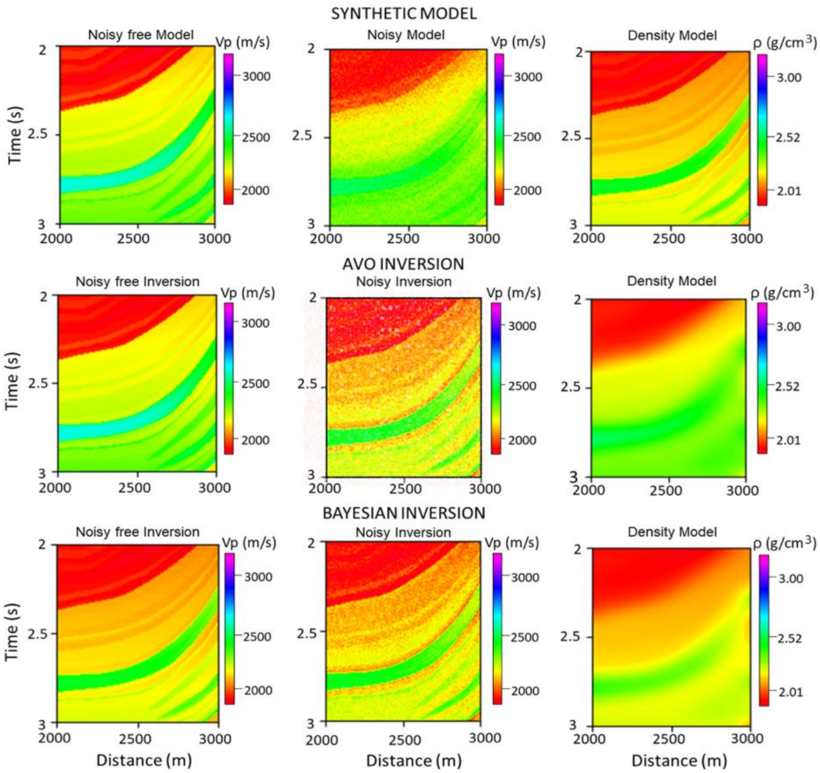

Fig. 9. The results of the inversion performed using Bayesian Inversion (BLI) and Amplitude Versus Offset (AVO) methodologies are displayed. The inversion procedures were implemented on a synthetic model, which was used in two distinct scenarios: in the first, the model was utilized without any introduced noise; in the second, noise was introduced into the initial model. The purpose of deliberately introducing noise was to examine the inversion process's behavior and enable a comparative analysis of the two. The inversion was executed on the V_P and density (ρ) models in the current case. (after Monroe J.A.T., 2025)

Poro-viscoelastic frameworks compress uncertainty bounds in seismic response prediction. Traditional methods like pure elasticity or uncoupled poroelasticity, suffer from wide uncertainty margins. They ignore the non-linear coupling of pore-fluid pressure, multi-scale fluid flow and solid matrix intrinsic attenuation.

Poro-viscoelastic frameworks sharply reduce these prediction boundaries thorugh targeted application domains and technical mechanisms.

One example would be the Norne Field in the North Sea where standard elastic or acoustic models result in major data misfits during AVO and seismic profile matching. Because they do not natively account for fluid-solid viscous drag or heavy oil visco-elastic behaviors, they force inversions to sprea errors across unrealistic variations in porosity and lithology.

Uncertainty reduction in the Norne Field was done by explicitly capturing the low-frequency frame losses, intermediate frequency squirt flow and high frequency Biot flow (the three distinct frequency dependent attenuation peaks) the model constrains wave velocity dispersion. This eliminates the need for wide, unconstrained empirical corrections, dratically narrowing the standard deviation of predicted seismic reflection and rock property profiles.

Repurposing depleted hydrocarbon reservoirs for CO_2 storage is pivotal for sustainable field rehabilitation. However, injection alters the THMC equilibrium.

Integrating advanced poro-viscoelastic modeling and continuous 4D seismic monitoring into the Environmental Impact Assessment (EIA) during decommissioning ensures that caprock integrity, fault reactivation risks, and ground deformation are rigorously quantified, aligning site closure with global sustainable development goals

9. Current Challenges and Future Research Directions

Despite significant advances, the mathematical modeling of seismic response to CO_2 storage remains an active research area with major challenges.

– Main Challenge: Uncertainty Quantification (UQ):

The largest challenge is not merely constructing a model, but quantifying its uncertainty.

The “full-cycle” described above is highly complex, nonlinear, and involves a large number of parameters, each with its own uncertainty.

The computational cost of a single THMC–seismic simulation (Steps 2–4) is prohibitively high.

This cost renders standard UQ methods, such as Monte Carlo analyses requiring thousands of model runs, practically infeasible.

– Future Direction 1: Probabilistic Inversion and Efficient UQ: Research is focusing on developing smarter sampling algorithms.

For example, the “Informed Proposal Monte Carlo” (IPMC) uses physics-based simplified simulations to guide MCMC (Markov Chain Monte Carlo) sampling in high-dimensional parameter spaces, drastically reducing convergence time and enabling more efficient UQ.

– **Future Direction 2: Chemistry-Based Rock Physics Models:** Moving from phenomenological models (which merely fit lab data showing rock weakening) to predictive models grounded in the fundamental chemistry of CO_2–brine–rock interactions.

– **Future Direction 3: Integration of Artificial Intelligence (Machine Learning):** A promising path to overcome computational cost barriers is the development of surrogate models based on ML. Neural networks can be trained on a limited number of high-fidelity THMC simulations and then approximate simulation results in milliseconds, allowing large-scale sensitivity analyses and UQ.

Data-driven inversion methods are also gaining traction.

10. Proposed AI Framework: Physics-Informed Neural Networks (PINNs) for THMC Surrogate Modeling

To concretely address the computational bottlenecks of traditional THMC simulations discussed above , we propose the implementation of a Physics-Informed Neural Network (PINN) as a surrogate model.

Unlike purely data-driven "black-box" models, PINNs embed the governing partial differential equations (PDEs) of poroelasticity and multiphase flow directly into the neural network's loss function.

This ensures that the predictions are not only statistically accurate but also thermodynamically and mechanically consistent [5,7].

1. Model Architecture and Data Flow

The architecture functions as a deep multi-layer perceptron (MLP) or a localized spatial-temporal network (such as a 3D U-Net) with the following structure:

- **Inputs:** Spatiotemporal coordinates (x, y, z, t) and specific reservoir static parameters (e.g., initial porosity ϕ_0, permeability κ).
- **Outputs:** The network acts as an approximator for the primary multi-physical variables: pore pressure (P_{pore}), CO_2 saturation (S_c), the stress tensor (σ_{ij}), and temperature ($\mathbf{T}$).

2. The Physics-Informed Loss Function

The core innovation of the proposed numerical AI model lies in its optimization mechanism.

The network is trained by minimizing a composite loss function that enforces both data fidelity and physical laws [6]:

$$\mathrm{L_{total}} = \mathrm{w_1 L_{data}} + \mathrm{w_2\ L_{PDE}} + \mathrm{w_3 L_{BC/IC}}$$

where:

- L_{total} represents the mean squared error (MSE) between the network's predictions and a limited set of high-fidelity numerical THMC simulations (e.g., generated via coupled platforms like TOUGH-FLAC).
- L_{PDE} penalizes the residual of the underlying governing equations (e.g., Biot's poroelasticity mass and momentum conservation equations). The derivatives required for these PDEs are computed precisely using automatic differentiation (AD) built into modern ML frameworks.
- $L_{BC/IC}$ ensures the model respects the physical boundary and initial conditions of the geological reservoir.
- w_1, w_2, w_3 are dynamic weighting coefficients used to balance the gradients during training.

3. Integration into Uncertainty Quantification (UQ)

Once trained offline, the PINN surrogate model decouples the simulation from the traditional grid-based solver.

The network can perform "forward" predictions of fluid and stress evolution in mere milliseconds. This hyper-fast inference speed is the critical enabler for Advanced Uncertainty Quantification (UQ).

It allows researchers to seamlessly execute tens of thousands of probabilistic Monte Carlo iterations or integrate directly with Markov Chain Monte Carlo (MCMC) algorithms, transforming geomechanical risk assessment from a computationally prohibitive task into a practical, real-time workflow.

To estimate how much CO_2 a targeted geological site can hold, we use the following equation:

$$\text{Capacity} = \text{Area} \times \text{Thickness} \times \text{Porosity} \times \text{Density} \times \text{Efficiency}$$

Area: The spatial footprint of the geological trap.
Thickness: The net thickness of the porous rock layer.
Porosity: The percentage of empty space in the rock frame.

Density: The density of supercritical CO_2 at reservoir depth (often around 600-800 kg/m³).

Efficiency: A factor representing how much of the pore space can *actually* be accessed and filled by CO_2 (usually a small fraction, like 2% to 10%).

Below is an interactive Monte Carlo simulator.

You can adjust the expected uncertainty bounds (Min/Max) for your geological site. When you run the simulation, the model will calculate 5,000 different scenarios and generate a histogram showing the most probable storage capacity (P50), as well as the conservative (P90) and optimistic (P10) estimates.

In this paper we simulated a storage 100 years a CO2 in abandoned mines.:

– **P90 (Conservative):** There is a 90% probability that the reservoir holds *at least* this much CO_2. This is the baseline number used for strict risk assessment and regulatory approval.

– **P50 (Expected):** The median estimate. It is the most realistic target for the storage site.

– **P10 (Optimistic):** There is only a 10% chance the reservoir holds this much. This represents the absolute best-case scenario if all geological variables are perfectly aligned.

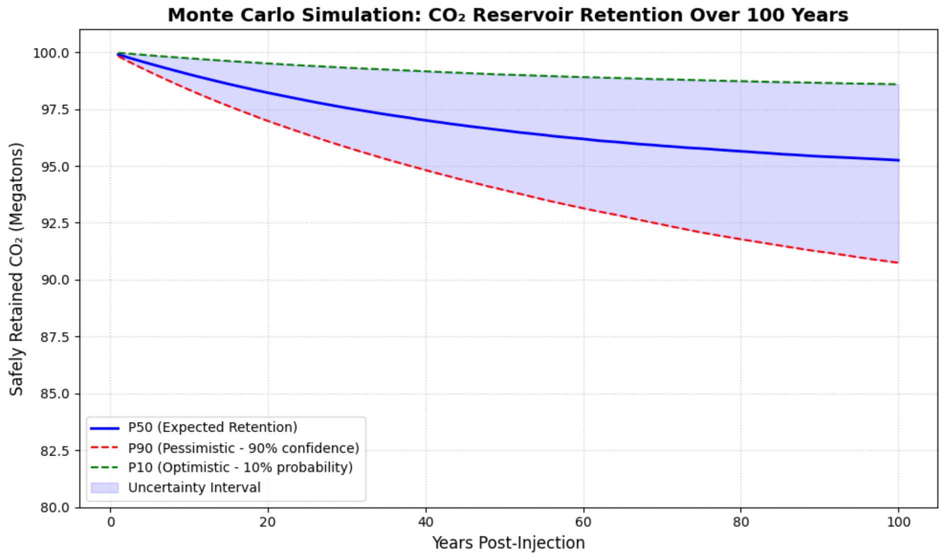

Fig. 8. A Monte Carlo simulation to 100 years CO_2 storages in mines

– **The P50 Line (Blue):** This will show a gentle downward slope, indicating the expected value. For example, it might show that after 100 years, **93.5 Megatons** of the initial 100 Mt remain safely stored.

– **The Shaded Area (Uncertainty Envelope):** Because we don't know the exact leakage rate, the graph fans out over time. The gap between the optimistic (P10) and pessimistic (P90) scenarios grows wider as time goes on, visually representing how uncertainty compounds over a century.

– **Geomechanical Relevance:** In the context of your paper, if a THMC simulation detects a high risk of fault reactivation, you would adjust the leakage_rates variable in this code to a much higher value. This would drastically drop the P90 line, proving to regulators why strict poroelastic monitoring is required for environmental safety.

10. Integrating CCS within Oil and Gas Decommissioning and Closure Practices

The transition of depleted hydrocarbon reservoirs into geological CO_2 storage sites represents a pivotal strategy for the sustainable rehabilitation of oil and gas fields.

While traditional closure practices have historically focused on surface remediation and standard well plugging, repurposing these mature fields for Carbon Capture and Storage (CCS) introduces complex, long-term subsurface dynamics.

As demonstrated throughout this study, the injection of supercritical CO_2 into depleted formations fundamentally alters the thermo-hydro-mechanical-chemical (THMC) equilibrium of the existing reservoir.

Therefore, the deployment of advanced poro-viscoelastic modeling and continuous 4D seismic monitoring should no longer be viewed merely as operational enhancements.

Instead, they must be integrated as mandatory components of the Environmental Impact Assessment (EIA) during the decommissioning and closure phases of oil and gas infrastructure.

By rigorously validating caprock integrity and assessing the risk of fault reactivation through coupled THMC frameworks , operators can ensure that the closure and rehabilitation of these sites actively contribute to global sustainable development goals.

Mastering this modeling complexity is the only way to guarantee that depleted fields are permanently and safely rehabilitated, mitigating climate change without introducing new geomechanical environmental liabilities.

Conclusions

The mathematical modeling of geophysical wave behavior in contact with rocks of CO_2 storage reservoirs is a deeply multi-physical problem that far exceeds the frameworks of standard exploration geophysics.

This paper has demonstrated that simplistic acoustic or elastic models are inadequate, and that the industry standard, Gassmann's equation, fails due to the omission of critical physical processes.

High-fidelity modeling, required to ensure long-term safety, must rely on a set of interconnected pillars:

a. A Poro-Viscoelastic Framework: To accurately capture attenuation and dispersion caused by wave-induced fluid flow (WIFF) at the mesoscopic scale, transforming attenuation (Q) into a diagnostic attribute.

b. Stress- and Chemistry-Dependent Rock Physics: To model the actual weakening of the rock frame induced by reductions in effective stress and chemical reactions, phenomena that directly impact shear-wave velocity (VS).

c. A Coupled Simulation Cycle (THMC): To dynamically link seismic wave propagation to the evolution of fluid flow, geomechanical stress state, and chemical alteration, enabling rigorous integrity risk assessment.

The success of strategic geological storage projects, including those in Romania such as **GETICA CCS**, will critically depend on mastering this modeling complexity.

The ultimate objective is not only to detect the quantity of CO_2, but to validate geomechanical models and quantify uncertainty, ensuring that storage is safe and permanent.

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