



Article Uncertainty Quantification in CO₂ Trapping Mechanisms: A Case Study of PUNQ-S3 Reservoir Model Using Representative Geological Realizations and Unsupervised Machine Learning

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Abstract: Evaluating uncertainty in CO₂ injection projections often requires numerous high-resolution geological realizations (GRs) which, although effective, are computationally demanding. This study proposes the use of representative geological realizations (RGRs) as an efficient approach to capture the uncertainty range of the full set while reducing computational costs. A predetermined number of RGRs is selected using an integrated unsupervised machine learning (UML) framework, which includes Euclidean distance measurement, multidimensional scaling (MDS), and a deterministic K-means (DK-means) clustering algorithm. In the context of the intricate 3D aquifer CO_2 storage model, PUNQ-S3, these algorithms are utilized. The UML methodology selects five RGRs from a pool of 25 possibilities (20% of the total), taking into account the reservoir quality index (RQI) as a static parameter of the reservoir. To determine the credibility of these RGRs, their simulation results are scrutinized through the application of the Kolmogorov-Smirnov (KS) test, which analyzes the distribution of the output. In this assessment, 40 CO_2 injection wells cover the entire reservoir alongside the full set. The end-point simulation results indicate that the CO₂ structural, residual, and solubility trapping within the RGRs and full set follow the same distribution. Simulating five RGRs alongside the full set of 25 GRs over 200 years, involving 10 years of CO₂ injection, reveals consistently similar trapping distribution patterns, with an average value of Dmax of 0.21 remaining lower than Dcritical (0.66). Using this methodology, computational expenses related to scenario testing and development planning for CO₂ storage reservoirs in the presence of geological uncertainties can be substantially reduced.

Keywords: carbon storage; reservoir simulation; uncertainty quantification; geological realizations; unsupervised machine learning; CO₂ trapping mechanisms

1. Introduction

The primary focus of carbon capture and storage (CCS) is the mitigation of humaninduced emissions of CO₂ [1]. This practical strategy entails the capture of CO₂ from the atmosphere, its transport to an underground storage reservoir, and injection into deep formations, where it remains securely stored within the pore spaces of the rock [2]. Various geological formations, such as depleted oil and gas reservoirs and deep saline aquifers, have been identified as suitable sites for storage of CO₂ at depths of several thousand meters [3–5]. The use of geological realizations (GRs) is common in the development and management of these CO₂ storage reservoirs. GRs help to determine long-term trapping of CO₂, plume migration, and the potential for leakage [6–8]. However, due to the limited availability of geological data for each storage site, there is a notable level of uncertainty, affecting estimates of CO₂ storage capacities, leakage risks, and the potential for groundwater contamination [1].



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Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). The evaluation and quantification of geological uncertainties have become increasingly crucial in industries dedicated to decarbonization [2,9,10]. The geological structure of a storage reservoir, coupled with variations in its petrophysical characteristics, constitutes the primary origin of geological uncertainty [11]. Traditional approaches to assessing geological uncertainty involve the generation of numerous potential GRs and the analysis of statistical metrics derived from ensemble objective functions [1]. To encompass the uncertainty space, Monte Carlo sampling is commonly employed to efficiently generate a large number of GRs [12]. However, the computational challenges associated with simulating numerous GRs pose a hurdle, leading to the exploration of methods to expedite this process. These methods can be categorized into two groups: data-driven approaches and physics-based simplifications [13].

Data-driven proxy models for uncertainty quantification rely on simplified fitting procedures, bypassing the flow simulation for CO_2 injections and post-injection [14]. This enables the quick determination of many objective functions but may overlook fluid flow's physical laws, potentially causing errors, especially in high-dimensional input-parameter spaces [15]. On the other hand, physics-based simplifications, such as low-fidelity realizations including up-scaled GRs or reduced ensembles, aim to simplify geological characteristics significantly. Although these methods provide simplicity in implementation, they may limit the representation of sub-grid heterogeneity impacts [14]. Representative geological realizations (RGRs) are a subset of reduced ensembles that aim to represent critical heterogeneity and CO_2 injection phenomena, as long as the model's fidelity is maintained. Their validity relies on the assumption that RGRs closely reflect the uncertainty of the full set. If this approximation fails, predictions about CO_2 storage and migration may be inaccurate. Therefore, it is crucial to assess the representativeness of RGRs and explore optimal selection methods that maximize uncertainty representation. One of the RGR selection methods is the Unsupervised Machine Learning (UML) method [16].

Machine learning and deep learning have recently been explored in many fields to accelerate computationally heavy processes [17–20]. In this area, UML specifically stands out as a widely adopted method to select RGRs, as evidenced in several case studies [21–24]. UML is designed to uncover the underlying structures in unlabeled data, employing techniques such as dimensionality reduction and clustering [25,26]. Dimensionality reduction identifies crucial attributes for distinguishing data samples, while clustering groups similar samples. UML transforms realizations into a reduced-dimensional space and clusters them according to static and/or dynamic features [26]. For instance, UML is applied to discover similar realizations using 3D facies models [27], assess similarity based on generalized travel time (GTT) differences [28], and evaluate various properties for RGR selection [21,29]. In experiments with a 2D aquifer CO₂ model, ref. [30] demonstrated that an effective UML framework for RGR selection involves utilizing Euclidean distance for dissimilarity, multidimensional scaling (MDS) for dimensionality reduction, and deterministic K-means (DK-means) for clustering realizations.

In our investigation, we try not only to select RGRs for a 3D synthetic aquifer CO_2 storage model but also to delve into the efficacy of the optimal UML framework derived from the study by Mahjour and Faroughi [30]. Our objective is to explore the UML framework's ability to maintain the inherent uncertainty found in the full set represented by the RGRs. To gauge the method's performance, we conduct a series of statistical experiments, assessing the outcomes within the context of the PUNQ-S3 benchmark model [31]. This model, designed to mimic a folded geologic formation forming an anticline, serves as an excellent testing ground for examining the robustness and reliability of the UML-based RGR selection method under diverse geological scenarios. Through comprehensive analyses and assessments within this model, we aim to highlight the method's strengths and limitations, offering insights into its practical applicability in capturing and preserving uncertainty within complex subsurface systems. This exploration is crucial for enhancing the efficiency and reliability of RGR selection processes in the context of CO_2 storage initiatives.

2. Methodology

In this work, the RGR selection process is based on the optimal UML algorithm detailed by Mahjour and Faroughi [30], encompassing the measurement of the Euclidean distance, MDS, and the DK-means clustering. As shown in Figure 1, the workflow begins with the generation of numerous GRs while considering uncertainties. To evaluate the UML framework's effectiveness, both the full and RGR sets undergo examination using CMG-GEM (Canada Modeling Group-Generalized Equation of State Model). Consequently, we compare the distributions of simulation outputs obtained from the RGRs with those originating from the full set.



Figure 1. RGR selection and validation workflow including (i) the selection of RGRs by measuring Euclidean distance, applying Multidimensional Scaling (MDS), and implementing Deterministic K-means (DK-means) clustering and (ii) the validation of the RGRs' representativeness through the simulation of both the full and RGR sets using a numerical simulator.

2.1. Generate Multiple Geological Realizations (GRs)

In the initial phase, a set of GRs is generated to capture geological uncertainties. While there are various sampling techniques to create multiple GRs, this study specifically adopts Latin Hypercube Sampling (LHS). LHS serves as a probabilistic geostatistical approach tailored for uncertainty quantification, drawing from diverse data sources [32]. This method ensures comprehensive sampling across the entire parameter range, minimizing the number of simulations required while preserving the statistical integrity of the outcomes [33]. It is essential to emphasize that this particular step, while integral to the overall workflow, is not the primary focus of this study and operates independently of the technique used for scenario reduction. Following this initial stage, the main focus of the study is on the application of UML for the selection of RGRs.

2.2. Euclidean Distance Measurement Between Realizations

Within the UML process, a crucial step involves constructing a matrix based on distance indicators, denoted as δ , calculated between each pair of realizations. This distance metric, δ_{ij} , quantifies the similarity between realization 'i' and realization 'j' [34]. The selection of a specific reservoir attribute and an appropriate distance measurement method significantly impact the evaluation of these distance indicators [35]. Concerning geological distributions, multiple generated geological realizations may exhibit similarities at certain distances, resulting in comparable flow responses. The ability to distinguish these realizations enables the generation of simulation outputs based on a reduced subset of realizations, each representing diverse flow responses [24].

This study employs the Reservoir Quality Index (RQI) as a static reservoir attribute to measure the distance between pairs of realizations. RQI finds widespread applications in various reservoir-related domains, including permeability estimation, stratigraphy, and reservoir modeling [36–40]. Porosity and permeability, integral petrophysical properties

within the RQI formulation, hold particular significance in the context of fluid flow modeling in heterogeneous porous media [41,42], especially in the modeling of CO₂ storage and plume migration [43,44]. Studies by [16,24] have explored the effectiveness of RQI in identifying realizations with similar flow behaviors, which yield promising results. The mathematical definition of RQI is given by,

$$RQI = 0.0314 \sqrt{\frac{K}{\phi}},\tag{1}$$

where *K* represents permeability in milli-darcy (*mD*), and ϕ is the porosity as a fraction. The constant 0.0314 serves as the conversion factor from permeability in μ m² to mD [45]. The RQI is derived from the Kozeny–Carman equation, defined as,

$$K = 1014 \frac{\phi^3}{(1-\phi)^2} \left(\frac{1}{F_s \tau^2 S_{gv}^2}\right),$$
(2)

where F_s represents the shape factor, τ indicates tortuosity, and S_{gv} is the specific surface area per unit grain volume. Each grid cell within the GRs possesses spatial coordinates and a set of geological attributes, including porosity and permeability. To create RQI maps, the RQI value is computed for each grid cell. Subsequently, a distance indicator between these RQI maps is measured using the Euclidean distance metric.

The measurement of the distance between two 3D samples, denoted as 'X' and 'Y', characterizes the degree of similarity between these samples [35]. In this study, we employ the Euclidean distance as the chosen measurement, given its widespread use and familiarity in similarity assessments [46]. After this step, we generate an 'n × n' distance matrix, D, based on the 'n' RQI models, which serve as input for the subsequent step.

2.3. Multidimensional Scaling (MDS)

MDS is used to represent the similarity measurements among objects as distances between points in a low-dimensional space, where each point corresponds to one object [47]. The fundamental concept behind MDS is to construct a map or configuration of points in a lower-dimensional space that accurately reflects the similarities between objects [48]. The outcomes of MDS are visualized by plotting the points in the *k*-dimensional space. As highlighted by Scheidt and Caers [35], using high-dimensional Euclidean spaces may not significantly enhance correlation, thereby suggesting that a 2D space (k = 2) can be appropriate in such cases. Each point in this 2D space represents an individual realization, and the Euclidean distance between two points serves as the measure of similarity between these realizations.

2.4. Deterministic K-Means (DK-Means) Clustering

After the transformation of data from a high-dimensional initial space to a lowerdimensional one, clustering techniques are employed to categorize models into distinct clusters [23]. Realizations within the same cluster exhibit similarity to each other. This study employs DK-means for clustering similar realizations, representing a modification of the conventional K-means clustering algorithm [49]. The objective is to address K-means' non-deterministic behavior resulting from its random choice of initial centroids. The DKmeans algorithm incorporates a deterministic initialization approach by either exploring a range of potential centers through constrained bi-partitioning or implementing a novel systematic method to select initial centroids. The primary goal of DK-means is to enhance the reliability and consistency of clustering outcomes compared to the traditional K-means algorithm [50].

Upon grouping the realizations through clustering, a representative realization from each group is selected using centroid-based sampling. This method targets the model closest to the center of the cluster for selection [23]. To determine a representative, the

Euclidean distance between a model and the center of its corresponding cluster is calculated, indicating the model's closeness to that center. Determining the optimal number of RGRs poses a challenge, necessitating careful consideration of factors such as geological realization complexity, the number and types of uncertain parameters, desired accuracy levels, and available computational resources [16]. The chosen sample size aims to strike a balance between computational efficiency and comprehensive coverage of the entire uncertainty space.

2.5. Numerical Simulation and Uncertainty Evaluation

In this phase, we conduct a comparative analysis of simulation outputs from an injection plan (IP) for both RGRs and the full set to assess how well the RGRs capture the characteristics of the entire set. Initially, the simulation outputs for each set are processed using a commercial flow simulator. Throughout the simulation, numerical realizations are specified to define objectives over time. Focusing on trapping mechanisms, we explore the physics governing CO₂ migration, resulting in three specific simulation outputs: (i) CO₂ structural trapping, (ii) CO₂ residual trapping, and (iii) CO₂ solubility trapping, using CMG-GEM. Simulation outputs are employed to assess and compare uncertainty between the full set and the RGRs. The methodology for quantifying uncertainty plays a crucial role in evaluating the representativeness of the RGRs. In this study, we analyze the distribution of the simulation outputs at the end of the simulation process to provide insights for decision-making under uncertainty [14]. To compare the uncertainty ranges, we examine CDF curves [51] derived from the simulation results of the RGR set and the entire ensemble. The proximity of their uncertainty ranges is assessed by measuring the maximum vertical difference, denoted as D_{max} , between the CDFs of the two datasets, F(x)RGR, m and G(x)full. This analysis is carried out using the Kolmogorov–Smirnov (KS) test [52]. The D_{max} value is determined by,

$$D_{\max} = \max \forall x \left| F(x) R G R, m - G(x)_{full,n} \right|.$$
(3)

Here, the number of realizations in the RGR set (m) and the whole set (n) is predetermined based on the budget and simulation time. If D_{max} is lower than the critical $D_{critical}$, defined as,

$$D_{\text{critical},0.5} = 1.36\sqrt{\frac{n+m}{nm}}.$$
(4)

Thus, if D_{max} from the RGR and full-set samples is less than D_{critical} , we ensure that the RGR set adequately represents the full ensemble.

3. Model Description

3.1. Geometric Model

This study validates the effectiveness of the UML framework in selecting RGRs using the synthetic reservoir model PUNQ-S3. Specific details of the PUNQ-S3 model, adapted by Juanes et al. [31] to represent a storage aquifer, are documented by Floris et al. [53]. PUNQ-S3 consists of five layers of sand and shale, typical sedimentary phases commonly found in geological formations [54]. This configuration results in a grid layout of $19 \times 28 \times 5$ grid blocks, totaling 1761 active blocks. The top formation is positioned at a depth of 2340 m with an average thickness of 15 m. Each grid's length spans 180 m in the horizontal direction. The average horizontal permeability and porosity are 100 mD and 0.2, respectively. The initial pressure and the fixed temperature are set at 23,446 kPa and $32.2 \,^{\circ}$ C, respectively. The rock compressibility is measured at 5.5×10^{-7} kPa⁻¹, and the water compressibility is 4.3×10^{-7} kPa⁻¹. Furthermore, the relative permeability curves, adapted from Juanes et al. [31], incorporate the Killough hysteresis model [55] for the non-wetting phase (CO₂). The relative permeability curves for CO₂ and brine are shown in Figure 2. This study relies on Land's trapping models [56] for the residual CO₂ trapping mechanism. Hence, during the simulation process, computations for drainage and imbibi-



Figure 2. Relative permeability curves used in the CO₂ storage simulation (Killough's model is used for hysteresis [55]).

3.2. Well Control Configurations

We implement an extensive injection plan (IP) specifically designed to elicit a comprehensive and varied response from the reservoir's behavior, facilitating RGR selection. The IP includes forty vertical injection wells strategically positioned to cover the entire reservoir without restrictions in the injection system. The objective behind choosing this well configuration is to ensure unbiased coverage of the reservoir model and to address its inherent heterogeneity. Figure 3a,b shows the top view of the reference porosity map and the placement of these wells within the IP, respectively. Within IP, the surface gas rate (STG) is set at 10,000 m³/day, and the bottom hole pressure (BHP) is maintained at 44,500 kPa for each well. The wells are fully perforated from the top to the bottom of the reservoir.



Figure 3. Reference PUNQ-S3 model. Panel (**a**) shows the 3D porosity map. Panel (**b**) represents the well locations including forty wells, spanning the whole reservoir. Panel (**c**) shows the simulation outputs structural (i) CO_2 trapping, (ii) residual CO_2 trapping, and (iii) solubility CO_2 trapping during 200 years with ten years of injection.

We delve into the physics underlying CO_2 migration and extract three simulation outputs—(i) structural CO_2 trapping, (ii) residual CO_2 trapping, and (iii) solubility CO_2 trapping—using CMG-GEM. In the solubility trapping simulation, we take into account the chemical interactions between the gaseous and aqueous phases [57]. However, mineral trapping is excluded from our study, as it predominantly occurs after 1000 years, whereas our simulation duration spans 200 years with 10 years of injection. The simulation output of the reference model is depicted in Figure 3c.

4. Results

We generated N = 25 realizations using LH sampling, considering diverse variations in porosity and permeability models to ensure comprehensive spatial sampling. The array of 25 porosity models (top views) is illustrated in Figure 4. Subsequently, we generated RQI models using porosity and permeability properties. The RQI for each grid cell was calculated to create the RQI map and determine the distances between pairwise GRs. In this study, we specifically chose five predetermined numbers of RGRs, amounting to 20% of the full set, using UML. This selection enables a reasonable reduction in both realizations and computational expenses while maintaining the full set's uncertainty domain.



Figure 4. Top views of the 25 3D porosity models generated through LH sampling, showing diverse variations in porosity and permeability.

Figure 5 displays a 2D map showing all the realizations obtained through the Euclidean/MDS/DK-means approach with five clusters. The MDS algorithm positions these realizations on a 2D map while preserving their distances based on Euclidean measurements in a distance matrix. Subsequently, the DK-means algorithm groups the realizations into multiple clusters. Using the centroid sampling method, one realization is selected as a representative of each cluster. The black points on the 2D map represent these five



representative realizations. Upon visual examination, it is evident that the representative realizations are evenly distributed across all the models.

Figure 5. A 2D map displaying all realizations generated through the Euclidean/MDS/DK-means framework employing five clusters. The X-axis corresponds to Dimension 1 (D1), and the Y-axis represents Dimension 2 (D2). Five RGRs, marked as black points, are selected through clustering and centroid-based sampling. These RGRs exhibit an even distribution across all models, effectively representing the full uncertain domain.

Next, we proceed with simulating the chosen five RGRs alongside the full set of 25 GRs to evaluate their simulation outputs over 200 years. This includes assessing CO₂ trapping, residual CO₂ trapping, and solubility CO₂ trapping, taking into account the essential inputs for the simulation process. In Figure 6, we compared the CDFs based on the endpoint simulation results of both the RGRs and the entire set. The *D*max values for CO₂ trapping, residual CO₂ trapping, and solubility CO₂ trapping are 0.20, 0.24, and 0.16, respectively. These values are lower than *D*critical, 0.66. Additionally, we compute the total trapping, representing cumulative trapping at the endpoint simulation, generating CDF curves for both RGRs and the full set. The resulting *D*max value is 0.24, also lower than *D*critical. Thus, the CDFs reveal that the simulation outputs from RGRs, selected through the Euclidean/MDS/DK-means framework, stem from the same distribution as the full set.

Figure 7a displays the average CO₂ trapping for different mechanisms from both the RGRs and the full set. The values obtained from the RGRs closely reflect those derived from the complete set of 25 GRs. The values obtained from the RGRs— 6.9×10^9 for CO₂ residual trapping, 1.9×10^{10} for CO₂ structural trapping, 8.9×10^9 for CO₂ solubility trapping, and 3.5×10^{10} for total CO₂ trapping—closely align with those derived from the complete set (6.9×10^9 , 1.9×10^{10} , 8.8×10^9 , and 3.5×10^{10} , respectively). This alignment is evident across various trapping mechanisms, highlighting the effectiveness of the selected RGRs in representing the full set. The proximity in the averages indicates a consistent trend, emphasizing the reliability of the RGRs in simulating CO₂ trapping mechanisms. Additionally, for visual validation, time series curves of the simulation outputs for both RGRs and the full set are depicted in Figure 7b–d. The figure clearly shows that the RGRs properly capture the entire uncertainty domain, confirming their ability to represent the full-set results.

Furthermore, evaluating the UML framework involves a computational efficiency analysis to gauge its effectiveness. We compare the simulation time for the full set against the utilization of five RGRs chosen from Euclidean/MDS/DK means to quantify uncertainty. The results show a significant reduction in time, decreasing from approximately 16 min for the full set to only 3 min for the five RGRs, indicating an 80% time reduction for the simulation. While simulating all 25 GRs is not overly time-consuming at this stage, executing robust optimizations to maximize CO_2 storage can be notably time-intensive with the full set. This highlights that the use of RGRs can significantly reduce the time required for CO_2 storage reservoir development and management compared to employing the full set.



Figure 6. Comparison of CDFs between RGRs and the full set for CO_2 trapping mechanisms. The *D*max values for (**a**) structural, (**b**) residual, (**c**) solubility, and (**d**) total CO_2 trapping are 0.20, 0.24, 0.16, and 0.24, respectively. The average *D*max is 0.21, which is lower than *D*critical, 0.66, indicating a close similarity in the distribution patterns of trapping mechanisms between the RGRs and the entire set of 25 GRs.



Figure 7. Statistical analysis of CO₂ trapping mechanisms between RGRs and the full set. Panel (**a**) compares the average of CO₂ trapping mechanisms between RGRs and the full set. The average values obtained from the RGRs— 6.9×10^9 for CO₂ residual trapping, 1.9×10^{10} for CO₂ structural trapping, 8.9×10^9 for CO₂ solubility trapping, and 3.5×10^{10} for total CO₂ trapping—closely align with those derived from the full set (6.9×10^9 , 1.9×10^{10} , 8.8×10^9 , and 3.5×10^{10} , respectively). Panels (**b**–**d**) show the time series curves of structural, residual, and solubility CO₂ trapping, respectively, for both RGRs and the full set. The comparison validates the RGRs' representation of the full-set results, confirming their reliability in simulating CO₂ trapping mechanisms.

Our findings suggest that the UML framework, using static models for RGR selection without requiring forward numerical simulations, effectively identifies a smaller subset, capturing the uncertainty of the full set within a 3D model characterized by high heterogeneity. Subsequently, these selected RGRs can be employed for rapid scenario testing and development planning at CO_2 storage locations under geological uncertainties. To enhance the efficacy and precision of these outcomes, we recommend further research and evaluation of the employed UML framework, including (i) implementing robust optimization on both the full set and RGRs, comparing results regarding CO_2 storage maximization and computational costs, (ii) analyzing the optimal quantity of RGRs within the UML framework and assessing the trade-off between computational efficiency and accuracy, and (iii) investigating the spatial distribution and plume footprint of the CO_2 plume across both the full set and the RGRs.

5. Conclusions

In this study, the efficacy of employing unsupervised machine learning (UML) to select representative geological realizations (RGRs) within a complex 3D aquifer CO₂ storage model, PUNQ-S3 was investigated. To address the inherent geological uncertainty, a workflow generated 25 geological realizations (GRs) through Latin hypercube sampling (LHS) for uncertainty quantification. Subsequently, an integrated UML framework, including Euclidean distance measurement, multidimensional scaling (MDS), and deterministic K-means (DK-means) clustering, selected five RGRs (20% of the full set). The Kolmogorov-Smirnov (KS) test was used to evaluate the UML framework, comparing absolute distances (Dmax) between the cumulative distribution functions (CDFs) of simulation outputs from the RGR sets and the full set. The findings demonstrated that the selected RGRs properly captured the uncertainty domain of the full set, evident through similar trapping distribution patterns, with an average Dmax value of 0.21, remaining lower than Dcritical (0.66). Furthermore, the average CO_2 trapping for different mechanisms from the RGRs was aligned with those derived from the full set of 25 GRs, highlighting the effectiveness of the selected RGRs in representing the full set. Computational time significantly decreased from around 16 min for the full set to only 3 min for the five RGRs, indicating an 80% reduction in simulation time. Extending verification to the synthetic reservoir model PUNQ-S3 showed the robustness of the UML-based RGR selection method, especially in scenarios with high heterogeneity. These results emphasized the potential of this approach for expediting scenario testing, decision-making, and development planning in CO₂ storage locations faced with geological uncertainties.

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Abbreviations

The following abbreviations are used in this manuscript:

BHP	Bottom Hole Pressure
CCS	Carbon Capture and Storage
CDF	Cumulative Distribution Function
CMG-GEM	Canada Modeling Group-Generalized Equation of State Model
DK-means	Deterministic K-means
GR	Geological Realization
GTT	Generalized Travel Time
IP	Injection Plan
KS	Kolmogorov–Smirnov
LHS	Latin Hypercube Sampling
MDS	Multidimensional Scaling
RGR	Representative Geological Realization
RQI	Reservoir Quality Index
STG	Surface Gas Rate
UML	Unsupervised Machine Learning

References

- Tadjer, A.; Bratvold, R.B. Managing Uncertainty in Geological CO₂ Storage Using Bayesian Evidential Learning. *Energies* 2021, 14, 1557. [CrossRef]
- Wilkinson, M.; Polson, D. Uncertainty in regional estimates of capacity for carbon capture and storage. Solid Earth 2019, 10, 1707–1715. [CrossRef]
- Harp, D.R.; Stauffer, P.H.; O'Malley, D.; Jiao, Z.; Egenolf, E.P.; Miller, T.A.; Martinez, D.; Hunter, K.A.; Middleton, R.S.; Bielicki, J.M.; et al. Development of robust pressure management strategies for geologic CO₂ sequestration. *Int. J. Greenh. Gas Control* 2017, 64, 43–59. [CrossRef]
- Jin, L.; Hawthorne, S.; Sorensen, J.; Pekot, L.; Kurz, B.; Smith, S.; Heebink, L.; Herdegen, V.; Bosshart, N.; Torres, J.; et al. Advancing CO₂ enhanced oil recovery and storage in unconventional oil play—Experimental studies on Bakken shales. *Appl. Energy* 2017, 208, 171–183. [CrossRef]
- Nilsen, H.M.; Lie, K.A.; Andersen, O. Analysis of CO₂ trapping capacities and long-term migration for geological formations in the Norwegian North Sea using MRST-co2lab. *Comput. Geosci.* 2015, 79, 15–26. [CrossRef]
- 6. Diao, Y.; Zhu, G.; Li, X.; Bai, B.; Li, J.; Wang, Y.; Zhao, X.; Zhang, B. Characterizing CO₂ plume migration in multi-layer reservoirs with strong heterogeneity and low permeability using time-lapse 2D VSP technology and numerical simulation. *Int. J. Greenh. Gas Control.* **2020**, *92*, 102880. [CrossRef]
- Langhi, L.; Strand, J.; Ricard, L. Flow modelling to quantify structural control on CO₂ migration and containment, CCS South West Hub, Australia. *Pet. Geosci.* 2021, 27, petgeo2020-094. [CrossRef]
- 8. Shepherd, A.; Martin, M.; Hastings, A. Uncertainty of modelled bioenergy with carbon capture and storage due to variability of input data. *GCB Bioenergy* **2021**, *13*, 691–707. [CrossRef]
- 9. Jia, W.; McPherson, B.; Pan, F.; Dai, Z.; Xiao, T. Uncertainty quantification of CO₂ storage using Bayesian model averaging and polynomial chaos expansion. *Int. J. Greenh. Gas Control* **2018**, *71*, 104–115. [CrossRef]
- 10. Sun, W.; Durlofsky, L.J. Data-space approaches for uncertainty quantification of CO₂ plume location in geological carbon storage. *Adv. Water Resour.* **2019**, *123*, 234–255. [CrossRef]
- 11. Mahjour, S.K.; Faroughi, S.A. Risks and uncertainties in carbon capture, transport, and storage projects: A comprehensive review. *Gas Sci. Eng.* **2023**, *119*, 205117. [CrossRef]
- 12. Bueno, J.F.; Drummond, R.D.; Vidal, A.C.; Sancevero, S.S. Constraining uncertainty in volumetric estimation: A case study from Namorado Field, Brazil. *J. Pet. Sci. Eng.* 2011, 77, 200–208. [CrossRef]
- Mahjour, S.K.; Santos, A.A.S.; Correia, M.G.; Schiozer, D.J. Scenario reduction methodologies under uncertainties for reservoir development purposes: Distance-based clustering and metaheuristic algorithm. *J. Pet. Explor. Prod. Technol.* 2021, *11*, 3079–3102. [CrossRef]
- 14. Schiozer, D.J.; dos Santos, A.A.d.S.; de Graça Santos, S.M.; von Hohendorff Filho, J.C. Model-based decision analysis applied to petroleum field development and management. *Oil Gas Sci. Technol. Rev. D'Ifp Energies Nouv.* **2019**, *74*, 46. [CrossRef]
- 15. Trehan, S.; Carlberg, K.T.; Durlofsky, L.J. Error modeling for surrogates of dynamical systems using machine learning. *Int. J. Numer. Methods Eng.* **2017**, *112*, 1801–1827. [CrossRef]
- Mahjour, S.K.; da Silva, L.O.M.; Meira, L.A.A.; Coelho, G.P.; dos Santos, A.A.d.S.; Schiozer, D.J. Evaluation of unsupervised machine learning frameworks to select representative geological realizations for uncertainty quantification. *J. Pet. Sci. Eng.* 2022, 209, 109822. [CrossRef]
- 17. Faroughi, S.A.; Soltanmohammadi, R.; Datta, P.; Mahjour, S.K.; Faroughi, S. Physics-informed neural networks with periodic activation functions for solute transport in heterogeneous porous media. *Mathematics* **2023**, *12*, 63. [CrossRef]

- Faroughi, S.A.; Pawar, N.M.; Fernandes, C.; Raissi, M.; Das, S.; Kalantari, N.K.; Mahjour, S.K. Physics-Guided, Physics-Informed, and Physics-Encoded Neural Networks and Operators in Scientific Computing: Fluid and Solid Mechanics. *J. Comput. Inf. Sci. Eng.* 2024, 24, 040802. [CrossRef]
- Datta, P.; Faroughi, S.A. A multihead LSTM technique for prognostic prediction of soil moisture. *Geoderma* 2023, 433, 116452. [CrossRef]
- 20. Vaziri, P.; Sedaee, B. A machine learning-based approach to the multiobjective optimization of CO₂ injection and water production during CCS in a saline aquifer based on field data. *Energy Sci. Eng.* **2023**, *11*, 1671–1687. [CrossRef]
- Shirangi, M.G.; Durlofsky, L.J. A general method to select representative models for decision making and optimization under uncertainty. *Comput. Geosci.* 2016, 96, 109–123. [CrossRef]
- 22. Lee, K.; Jung, S.; Lee, T.; Choe, J. Use of clustered covariance and selective measurement data in ensemble smoother for three-dimensional reservoir characterization. *J. Energy Resour. Technol.* **2017**, *139*. [CrossRef]
- Mahjour, S.K.; Correia, M.G.; Santos, A.A.d.S.d.; Schiozer, D.J. Using an integrated multidimensional scaling and clustering method to reduce the number of scenarios based on flow-unit models under geological uncertainties. *J. Energy Resour. Technol.* 2020, 142, 063005. [CrossRef]
- 24. Haddadpour, H.; Niri, M.E. Uncertainty assessment in reservoir performance prediction using a two-stage clustering approach: Proof of concept and field application. *J. Pet. Sci. Eng.* **2021**, 204, 108765. [CrossRef]
- 25. Hinton, G.; Sejnowski, T.J. Unsupervised Learning: Foundations of Neural Computation; MIT Press: Cambridge, MA, USA, 1999. [CrossRef]
- 26. Liu, Z.; Forouzanfar, F. Ensemble clustering for efficient robust optimization of naturally fractured reservoirs. *Comput. Geosci.* **2018**, 22, 283–296. [CrossRef]
- 27. Lee, K.; Jung, S.; Choe, J. Ensemble smoother with clustered covariance for 3D channelized reservoirs with geological uncertainty. *J. Pet. Sci. Eng.* **2016**, *145*, 423–435. [CrossRef]
- 28. Park, J.; Jin, J.; Choe, J. Uncertainty quantification using streamline based inversion and distance based clustering. *J. Energy Resour. Technol.* **2016**, 138, 012906. [CrossRef]
- 29. Pinheiro, M.; Emery, X.; Miranda, T.; Lamas, L.; Espada, M. Modelling geotechnical heterogeneities using geostatistical simulation and finite differences analysis. *Minerals* **2018**, *8*, 52. [CrossRef]
- Mahjour, S.K.; Faroughi, S.A. Selecting representative geological realizations to model subsurface CO₂ storage under uncertainty. Int. J. Greenh. Gas Control. 2023, 127, 103920. [CrossRef]
- Juanes, R.; Spiteri, E.; Orr Jr, F.; Blunt, M. Impact of relative permeability hysteresis on geological CO₂ storage. *Water Resour. Res.* 2006, 42, 2005WR004806. [CrossRef]
- 32. Pilger, G.; Costa, J.; Koppe, J. The benefits of Latin Hypercube Sampling in sequential simulation algorithms for geostatistical applications. *Appl. Earth Sci.* 2008, *117*, 160–174. [CrossRef]
- Damblin, G.; Couplet, M.; Iooss, B. Numerical studies of space-filling designs: Optimization of Latin Hypercube Samples and subprojection properties. J. Simul. 2013, 7, 276–289. [CrossRef]
- 34. Suzuki, S.; Caers, J.K. History matching with an uncertain geological scenario. In Proceedings of the SPE Annual Technical Conference and Exhibition, San Antonio, TX, USA, 24–27 September 2006. [CrossRef]
- 35. Scheidt, C.; Caers, J. Representing spatial uncertainty using distances and kernels. Math. Geosci. 2009, 41, 397–419. [CrossRef]
- 36. Mahjour, S.K.; Al-Askari, M.K.G.; Masihi, M. Identification of flow units using methods of Testerman statistical zonation, flow zone index, and cluster analysis in Tabnaak gas field. *J. Pet. Explor. Prod. Technol.* **2016**, *6*, 577–592. [CrossRef]
- 37. Shan, L.; Cao, L.; Guo, B. Identification of flow units using the joint of WT and LSSVM based on FZI in a heterogeneous carbonate reservoir. *J. Pet. Sci. Eng.* 2018, 161, 219–230. [CrossRef]
- Oliveira, G.; Santos, M.; Roque, W. Constrained clustering approaches to identify hydraulic flow units in petroleum reservoirs. J. Pet. Sci. Eng. 2020, 186, 106732. [CrossRef]
- Yu, P. Hydraulic unit classification of un-cored intervals/wells and its influence on the productivity performance. J. Pet. Sci. Eng. 2021, 197, 107980. [CrossRef]
- 40. Belhouchet, H.; Benzagouta, M.; Dobbi, A.; Alquraishi, A.; Duplay, J. A new empirical model for enhancing well log permeability prediction, using nonlinear regression method: Case study from Hassi-Berkine oil field reservoir–Algeria. *J. King Saud Univ. Eng. Sci.* **2021**, *33*, 136–145. [CrossRef]
- 41. Faroughi, S.A.; Faroughi, S.; McAdams, J. A prompt sequential method for subsurface flow modeling using the modified multi-scale finite volume and streamline methods. *Int. J. Num. Anal. Model.* **2013**, *4*, 129–150.
- 42. Bordbar, A.; Faroughi, S.; Faroughi, S.A. A pseudo-TOF based streamline tracing for streamline simulation method in heterogeneous hydrocarbon reservoirs. *Am. J. Eng. Res.* **2018**, *7*, 23–31.
- Soong, Y.; Crandall, D.; Howard, B.H.; Haljasmaa, I.; Dalton, L.E.; Zhang, L.; Lin, R.; Dilmore, R.M.; Zhang, W.; Shi, F.; et al. Permeability and mineral composition evolution of primary seal and reservoir rocks in geologic carbon storage conditions. *Environ. Eng. Sci.* 2018, 35, 391–400. [CrossRef]
- 44. Xu, R.; Li, R.; Ma, J.; He, D.; Jiang, P. Effect of mineral dissolution/precipitation and CO₂ exsolution on CO₂ transport in geological carbon storage. *Accounts Chem. Res.* 2017, *50*, 2056–2066. [CrossRef]

- George, N.J.; Ekanem, A.M.; Ibanga, J.I.; Udosen, N.I. Hydrodynamic implications of aquifer quality index (AQI) and flow zone indicator (FZI) in groundwater abstraction: A case study of coastal hydro-lithofacies in South-eastern Nigeria. *J. Coast. Conserv.* 2017, 21, 759–776. [CrossRef]
- 46. Ontañón, S. An overview of distance and similarity functions for structured data. Artif. Intell. Rev. 2020, 53, 5309–5351. [CrossRef]
- Fouedjio, F. Multidimensional Scaling. In *Encyclopedia of Mathematical Geosciences*; Springer: Cham, Switzerland, 2023; pp. 938–945. [CrossRef]
- 48. Borg, I.; Groenen, P.J. Modern Multidimensional Scaling: Theory and Applications; Springer: New York, NY, USA, 2005. [CrossRef]
- 49. Jothi, R.; Mohanty, S.K.; Ojha, A. DK-means: A deterministic k-means clustering algorithm for gene expression analysis. *Pattern Anal. Appl.* **2019**, *22*, 649–667. [CrossRef]
- 50. Nidheesh, N.; Nazeer, K.A.; Ameer, P. An enhanced deterministic K-Means clustering algorithm for cancer subtype prediction from gene expression data. *Comput. Biol. Med.* 2017, *91*, 213–221. [CrossRef] [PubMed]
- 51. Xue, B.; Oldfield, C.J.; Dunker, A.K.; Uversky, V.N. CDF it all: Consensus prediction of intrinsically disordered proteins based on various cumulative distribution functions. *FEBS Lett.* **2009**, *583*, 1469–1474. [CrossRef] [PubMed]
- Ferreira, C.J.; Davolio, A.; Schiozer, D.J. Evaluation of the Discrete Latin Hypercube with Geostatistical Realizations Sampling for History Matching Under Uncertainties for the Norne Benchmark Case. In Proceedings of the OTC Brasil, Rio de Janeiro, Brazil, 24–26 October 2017. [CrossRef]
- 53. Floris, F.J.; Bush, M.; Cuypers, M.; Roggero, F.; Syversveen, A.R. Methods for quantifying the uncertainty of production forecasts: A comparative study. *Pet. Geosci.* 2001, *7*, S87–S96. [CrossRef]
- 54. Pan, B.; Liu, K.; Ren, B.; Zhang, M.; Ju, Y.; Gu, J.; Zhang, X.; Clarkson, C.R.; Edlmann, K.; Zhu, W.; et al. Impacts of relative permeability hysteresis, wettability, and injection/withdrawal schemes on underground hydrogen storage in saline aquifers. *Fuel* **2023**, *333*, 126516. [CrossRef]
- 55. Killough, J. Reservoir simulation with history-dependent saturation functions. Soc. Pet. Eng. J. 1976, 16, 37–48. [CrossRef]
- 56. Land, C.S. Calculation of imbibition relative permeability for two-and three-phase flow from rock properties. *Soc. Pet. Eng. J.* **1968**, *8*, 149–156. [CrossRef]
- 57. Maalim, A.A.; Mahmud, H.B.; Seyyedi, M. Assessing roles of geochemical reactions on CO₂ plume, injectivity and residual trapping. *Energy Geosci.* **2021**, *2*, 327–336. [CrossRef]

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