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Weiwei	Zhu	King Abdullah University of Science and Technology
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Abstract

Geological CO₂ sequestration (GCS) has been a practical approach used to mitigate global climate change. Uncertainty and sensitivity analysis of CO₂ storage capacity prediction are essential aspects for large-scale CO₂ sequestration. This work presents a rigorous machine learning-assisted workflow for the uncertainty and global sensitivity analysis of CO₂ storage capacity prediction in deep saline aquifers. The proposed workflow comprises three main steps: 1) dataset generation – we first identify the uncertainty parameters that impact CO₂ storage in deep saline aquifers and then determine their corresponding ranges and distributions. We generate the required data samples by combining the Latin Hypercube Sampling (LHS) technique with high-resolution simulations. 2) surrogate development – a data-driven surrogate is developed to map the nonlinear relationship between the input parameters and corresponding output interests from the previous step. The implementation of Bayesian optimization accelerates the tuning process of hyper-parameters instead of traditional trial-error analysis. 3) uncertainty and global sensitivity analysis – Monte Carlo simulations based on the optimized surrogate are performed to explore the time-dependent uncertainty propagation of model outputs. Then the key contributors are identified by calculating the Sobol indices based on the global sensitivity analysis. The proposed workflow is accurate and efficient and could be readily implemented in field-scale CO₂ sequestration in deep saline aquifers.

Introduction

Geological CO₂ sequestration (GCS) is recognized as one of the most effective approaches to reduce global CO₂ emissions. Generally, the geological structure used to store CO₂ mainly includes depleted oil and gas formations, coalbed reservoirs, geothermal formations, and saline aquifers (Hoteit et al., 2019; Omar et al., 2021). The first four geological sites are distributed in specific areas, therefore with limited applicability. Saline aquifers, however, are easily found and widely distributed worldwide. Deep saline aquifers honor the great potential of storing CO₂ with a maximum of 10,000 Gt (Javaheri et al., 2009). Thus, investigating CO₂ storage capacity in deep saline aquifers becomes essential.

Extensive researches have been done in the literature to investigate the storage capacity in deep saline aquifers, including (semi-) analytical and numerical measures. For example, Ahmadi & Chen (2019) presented an analytical model to quantify pressure response and leakage rates in CO₂ sequestration in deep

saline aquifers. Qiao et al. (2021) developed a semi-analytical model for predicting CO₂ leakage in the subsurface through the abandoned wells. Pasala et al. (2003) analyze the impact of faults on the CO₂ sequestration in a saline aquifer by using a simulation study. Kumar et al. (2004) conducted reservoir simulations to explore the significant CO₂ storage mechanisms with actual physical conditions. Hesse et al. (2006) performed a sensitivity analysis of aquifer dimension, formation angles, capillarity, and residual trapping on CO₂ sequestration in saline aquifers and further optimized the injected CO₂ rates. Lee (2009) applied compositional simulations to investigate the feasibility of injecting CO₂ into deep saline aquifers and explore the possible leakage amount to the surface. In summary, all analytical models are derived under ideal assumptions and work well for specific cases. On the other hand, numerical simulations suffer from extensive computational costs, making them unpractical for field-scale applications, especially for Monte Carlo runs. Moreover, a comprehensive study of uncertainty and sensitivity analysis of time-series CO₂ storage capacity is rarely reported in the literature.

Recent years have seen many advanced applications based on machine learning in geoscience and petroleum disciplines. Examples include fracture recognition from actual outcrop (Santoso et al., 2019; Zhu et al., 2020), equivalent continuum model construction from discrete-fracture characterization (He et al., 2020), oil recovery factor forecasting in gas-injected reservoirs (He, Qiao, et al., 2021) multi-component flash calculations (Li et al., 2019; Zhang et al., 2020) and history matching in reservoir simulations (Santoso et al., 2021). These applications demonstrate with appropriate datasets and suitable network architecture, machine learning offers a competitive approach in terms of accuracy and efficiency compared with traditional methods. These successful implementations motivate us to perform the uncertainty and global sensitivity analysis based on machine learning instead of expensive high-fidelity simulations.

This paper, therefore, provides a rigorous machine learning-based work for developing a data-driven, physics-featuring surrogate for CO₂ storage capacity prediction and further explores the uncertainty propagation using Monte Carlo simulations, and eventually conducts global sensitivity analysis by calculating the Sobol indices. This workflow integrates the knowledge of sampling techniques, machine learning (coupled with Bayesian optimization), uncertainty quantification, and global sensitivity analysis. To our best knowledge, the workflow is implemented in CO₂ storage in deep saline aquifers for the first time. The proposed workflow is demonstrated with high accuracy and efficiency and could be readily implemented in the large-scale CO₂ sequestration in deep saline aquifers.

This paper is organized as follows. In section 2, high-fidelity simulations and the base case will be detailed. We provide a sound description of the proposed workflow in section 3. Section 4 will provide the results and discussion. Finally, we will close with the conclusion and highlight some future work.

High-Fidelity Simulations

We consider injecting supercritical CO₂ into the deep saline aquifers as an example. The corresponding physical processes are governed by the conservation equation and the extended Darcy's law. We assume to be incompressible flows for both two phases.

$$\frac{\partial(\phi \rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \vec{u}_\alpha) = Q_\alpha \quad \alpha = CO_2, w \quad (1)$$

$$\vec{u}_\alpha = -\frac{k_{ra}}{\mu_\alpha} \vec{K} (\nabla p_\alpha + \rho_\alpha g \nabla z) \quad (2)$$

Where ϕ is the porosity and t is the time; ρ_α , S_α , $\overline{u}_\alpha$, Q_α , $k_{r\alpha}$, μ_α , and p_α are the density, saturation, velocity, sink/source term, relative permeability, viscosity, and pressure for phase α , respectively; subscription α represents the phases for CO₂ and water, respectively; $\overline{K}$ is the absolute permeability tensor, g is the gravity acceleration, and z is the depth.

The two-phase saturations are constrained by:

$$S_{CO_2} + S_w = 1 \quad (3)$$

We relate the two pressures by capillary pressure (denoted by p_c):

$$p_c(S_w) = p_{CO_2} - p_w \quad (4)$$

The high-fidelity simulations are solved by a two-phase black-oil model within the MRST framework. A detailed description could be found in the reference (Lie & Møyner, 2021).

We take the geological model from (He, Zhu, et al., 2021a), yet with heterogeneous permeability and spatially-distributed porosity, as shown in Figure 2. Figure 1 illustrates the implemented geological model with the well placement. The well is positioned in the flank of the model, with the bottom layer perforated. All outer boundaries (i.e., not in contact with shale layers and thus open to flow) are represented by blue-color faces and assigned with the corresponding hydrostatic boundary conditions. The others are in contact with shale layers with no-flow boundary conditions specified.

Figure 1. The geological model with the well location, in which blue-color faces define all outer boundaries open to flow, and the others are no-flow boundaries.

We consider the base case with a 50-year CO₂ injection and followed by a 450-year migration. The related parameters and corresponding values are summarized in Table 1. Figure 2 illustrates the heterogeneous permeability and spatially-dependent porosity distributions of the base case.

Figure 2. The permeability distribution (left) and porosity distribution (right) for the base case.

Table 1. Related parameters and corresponding values for the base case.

CO ₂ injection rate, Q	8000 m^3/day
Residual CO ₂ saturation, S_{rcO_2}	0.2
Residual water saturation, S_{rw}	0.1
Permeability, K	As shown in Figure 2 (left)
Porosity, ϕ	As shown in Figure 2 (right)
Fluid properties	$\rho_{co_2} = 686.54$ $\rho_w = 975.86$ kg/m^3 $\mu_{co_2} = 0.056641$ $\mu_w = 0.30860$ cp
Phase relative permeabilities at residual saturations	[0.2142 0.85]
Injection period	50 years
Post-Injection (Migration) period	450 years

Figure 3 shows the simulation results for the base case at 50 years (top) and 500 years (bottom), illustrating the migration of CO₂ in the post-injection period and the corresponding evolution of different storage capacities. We observe movable plume is significantly reduced from 71 % to 47 %, and residual increases around 19 %, yet residual plume reduces from 20 % to 14 %. Only around 4 % of the CO₂ is leaked during the migration period.

Figure 3. CO₂ saturation profiles and corresponding trapping inventory diagrams at 50 years (top) and 500 years (bottom), respectively.

Proposed Workflow

High-fidelity simulations are generally computationally expensive and unpractical for cases requiring various runs, such as uncertainty and global sensitivity analysis. This work presents a rigorous machine learning-based workflow as an alternative. Figure 4 shows the proposed workflow, mainly including three steps.

Figure 4. The proposed workflow for performing uncertainty and global sensitivity analysis, including three steps 1) dataset generation, 2) surrogate development, 3) uncertainty quantification and global sensitivity analysis.

Step 1: Dataset Generation

We first identify the uncertainty parameters that impact the final interests (i.e., different storage capacities) and collect their corresponding ranges and distributions from the literature or other sources. The Latin Hypercube Sampling (LHS) technique is implemented to generate various input designs. The implementation of LHS assures the data points are distributed in a space-filling manner instead of the clustering effect (He, Santoso, et al., 2021; He, Zhu, et al., 2021a, 2021b; Santoso et al., 2021). The clustering effect leads to the developed model working well for data samples from the clustered area and poor predictions on the others areas. Table 2 summarizes the identified uncertainty parameters and their corresponding ranges and distributions. We assume each parameter to be uniform distribution and independent of each other. High-resolution numerical simulations based on the two-phase black-oil solver are then used to produce the corresponding output for each input design. We eventually collect the inputs and final outputs to be read for the next step.

Table 2. The identified uncertainty parameters and their corresponding ranges and distributions.

Uncertainty Parameters	Lower Bound	Upper Bound	Distribution
CO ₂ injection rate, Q	8000 m^3/day	14000 m^3/day	Uniform
Residual CO ₂ saturation, S_{rcO_2}	0.1	0.4	Uniform
Residual water saturation, S_{rw}	0.1	0.4	Uniform
Permeability coefficient, α_K	0.8	1.4	Uniform
Porosity coefficient, α_ϕ	0.8	1.4	Uniform

Step 2: Surrogate Development

This step is to develop a data-driven, physics-featuring surrogate model to map the nonlinear relationship between these identified uncertainty parameters and CO₂ storage capacity (herein, refers to three types of storage formats – residual, moveable, and leaked). Figure 5, top-right, illustrates the implemented machine learning, called Artificial Neural Network (ANN), including three types of layers input, hidden, and output layers. ANN with time term as input could also describe time series problems compared to Long-Short Term Memory (LSTM), yet honors the simplicity and efficiency (He, Zhu, et al., 2021a; Kim et al., 2017). Figure 5 illustrates the detailed procedures for the coupled ANN building&training with Bayesian optimization. We first determine the hyper-parameters, including the number of hidden layers, the number of neurons in each layer, activation function, and the ratio of the train to validation samples. We then build the neural network based on these assigned hyper-parameters. The training-validation process is conducted until the accuracy for both training and validation samples exceeds 95 %. If not, we go into the Bayesian optimization part, in which we update the Gaussian process model and sample the hyper-parameters using the acquisition function. We then iterate the ANN building and training part with the updated hyper-parameters until the accuracy is reached. The implementation of the Bayesian optimization is to automate the process of tuning hyper-parameters and accelerate the convergence process instead of traditional trial-error analysis. Readers could find the detailed implementation of Bayesian optimization in this link (<https://www.mathworks.com/help/stats/bayesian-optimization-workflow.html>).

Figure 5. Coupled process of ANN building & training with Bayesian optimization.

The metric evaluation parameters are defined as follow:

- 1) **APE**: average of prediction errors (**PE**) between the predicted (denoted by $M^{Predicted}$) and ground-truth (M^{Truth}) at each time step.

$$PE = \left| \frac{M^{Predicted} - M^{Truth}}{M^{Truth}} \right| \times 100\% \quad (5)$$

$$APE = \frac{1}{N} \sum_{i=1}^N PE_i \quad (6)$$

- 2) **PPE**: percentage of prediction errors (**PE**) within an acceptable error margin (10% as a threshold in this study).

$$PPE = \frac{N_{(where, PE \leq 10\%)}}{N} \times 100\% \quad (7)$$

Where N is the number of time steps.

Step 3: Uncertainty Quantification and Global Sensitivity Analysis

Figure 6 shows the flowchart of global sensitivity analysis. We first assign the probabilistic distribution to the uncertain model input parameters in step A. Herein, we keep the uncertainty parameters and their corresponding ranges and distributions the same as in Table 2. We then determine the computational model in step B, in which the optimized surrogate model developed in **Step 2** is employed. We then perform the Monte Carlo simulations based on the optimized surrogate model to explore the uncertainty propagation of time-series model outputs for each storage mechanism. The sampled results are collected to quantify probabilistic percentiles P10, P50, and P90. Eventually, global sensitivity analysis is performed to identify the critical uncertain parameters by calculating the Sobol indices. A detailed implementation of GSA could be found in this link (<https://www.uqlab.com/>).

Figure 6. The workflow for performing the global sensitivity analysis, including four steps -1) identifying uncertainty parameters, 2) determining computational model, 3) uncertainty analysis, 4) global sensitivity analysis.

Results and Discussion

We generate 100 simulation cases, with each case selecting 70 time steps. A total of 7000 data points are, thus, obtained. The coupled process of ANN building & training and Bayesian optimization is conducted until the PPE > 95 % and the APE < 5 % for both the training and validation samples are achieved. The Bayesian-optimized hyper-parameters are summarized in Table 3. The optimized ANN architecture comprises three hidden layers with the optimized neurons of 8, 6, 5, respectively, on each layer. The Sigmoid function is selected as the optimized activation function compared to ReLu and Tanh. The optimized ratio of training to validation is 7:3. We also include the evaluation results in Table 3. Figure 7 illustrates the diagonal plots comparing the normalized ANN predicted and the ground truth solutions for training and validation samples. The optimized model, thus, could be considered as the fully trusted model for Monte Carlo runs and eventually for performing global sensitivity analysis.

Table 3. The optimized hyper-parameters and corresponding evaluation performance on both training and validation datasets.

ANN Structure	[8 6 5] Sigmoid function	
Training	Training Samples	4900 (70 %)
	APE	4.8 %
	PPE	95.6 %
Validation	Validation Samples	2100 (30 %)
	APE	3.5 %
	PPE	96.3 %

Figure 7. The diagonal plots show the comparison of the ANN predicted and ground-truth results in a normalized manner for both training (left) and validation samples (right).

We perform 5,000 Monte Carlo simulations using the fully-trusted model to explore the uncertainty propagation of the time-series output variations for each type of storage format. The 5,000 runs are proven to be stable. We then group the resulting time-series outputs in the way the percentiles of P_{10} , P_{50} , and P_{90} are quantified, as shown in Figure 8. We observe in residual trap (1st row), residual (2nd row), and movable trap (4th row) that CO_2 storage capacity exhibits two-segment characteristics – it doesn't increase during the first 50-year period (i.e., injection period) and significantly increases in the post-injection (i.e., migration) period. In other words, these three types of storage capacities do not dominate storage mechanisms in the injection period yet start showing an increasingly important role in the migration period. The residual plume (3rd row) and movable plume (5th row) show a different trend – increasing to reach the peak at the injection-stop year during the injection period and then decreasing within the migration period. These observed storage trends based on various Monte Carlo runs provide helpful guidance for the importance of each storage capacity in different periods.

Figure 8. Uncertainty analysis based on 5000 Monte Carlo simulations for time-series outputs – residual trap (1st row), residual (2nd row), residual plume (3rd row), and movable trap (4th row), and movable plume (5th row).

We eventually conduct the global sensitivity analysis to determine the most significant uncertain parameters on the investigated outputs by calculating the first-order indices. The sensitivity analysis is performed within the UQLAB framework (Marelli et al., 2019). We take outputs at 50 year and 500 year as examples to illustrate the time-series sensitivity analysis. We observe in Figure 9 in all storage formats, permeability and porosity don't show any influence on the final outputs, which is due to the neglect of the capillary pressure. In the residual trap (1st row), the residual CO₂ saturation significantly influences the storage capacity at both 50 and 500 years. The others two (i.e., injection rate and residual water saturation) start increasing to some extent with the increasing time. However, in the residual (2nd row), the injection rate and residual water saturation show the important impact, and their impacts decrease within the migration period. A reverse trend is observed in residual CO₂ saturation. The others (3rd, 4th, 5th rows) could be observed and summarized from the figure 9 and will not be detailed here.

Figure 9. Global sensitivity analysis by calculating the first-order Sobol indices to determine the key contributors on the time-continuous outputs.

Conclusions and Future Work

This work presents a rigorous machine learning-based workflow for predicting CO₂ storage capacity in deep saline aquifers and further conducting uncertainty and global sensitivity analysis. The main findings are summarized as follows:

- Artificial Neural Network (ANN) with time term as input could also describe time-series problems yet with simplicity and efficiency. In this study, ANN is designed explicitly for time-dependent multiple inputs and outputs problems.

- Latin Hypercube Sampling (LHS) assures space-filling dataset distribution and avoids the generation of unnecessary data samples and the unbalanced performance of the ANN model.
- The quality of datasets significantly impacts the quality of surrogate and further its applications. Herein, we employ the high-resolution simulations solutions as our data samples.
- The coupled process of ANN building & training and Bayesian optimization automates and accelerates the process of tuning hyper-parameters instead of extensive traditional trial-error analysis.
- 5000 Monte Carlo simulations based on the optimized surrogate are performed to explore the uncertainty propagation of time-series model outputs for each storage mechanism. We observe two different trends among these five investigated storage mechanisms. The observed trends offer helpful guidance for each storage mechanism in different periods.
- Global sensitivity analysis is performed to identify the critical model input certain parameters by calculating the first-order Sobol indices. The top three crucial input parameters are injection rate, residual CO₂, and water saturations. Their order of importance could vary and depend on different specific storage mechanisms. The conclusions obtained by the global sensitivity analysis offer us the most key time-series contributors, which could ensure better management during large-scale CO₂ sequestration.

The proposed comprehensive workflow is implemented for the first time in deep saline aquifers regarding CO₂ storage capacity prediction and further uncertainty and global sensitivity analysis. The proposed workflow is demonstrated to be efficient and accurate and could be readily implemented in large-scale CO₂ sequestration in saline aquifers.

Future work will focus on including more complex physics, such as capillary pressure, solubility trapping, and mineral trapping. Also, more complex cases, such as significantly heterogeneous and anisotropic permeability tensor and more uncertain parameters, will be considered.

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Additional Information

Any discussion on this paper is highly encouraged. All codes are developed in a MATLAB environment and are available upon request (xupeng.he@kaust.edu.sa). Citing the paper is required once implementing the original or modified codes.

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