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Spatio-Temporal Deep Learning for Predicting the CO_2 Plume Migration in the Quest CCS Project

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Abstract

This study presents a spatiotemporal deep learning framework for forecasting CO_2 injection dynamics at the field scale for the Quest Carbon Capture and Storage (CCS) project in Alberta, Canada. A neural network surrogate is trained to emulate high-fidelity reservoir simulations and predict the temporal evolution of CO_2 plume migration and pressure buildup. The model is evaluated under both interpolation and extrapolation scenarios to assess robustness across geological realizations. Results demonstrate strong predictive accuracy for both saturation and pressure fields, with performance degradation under extrapolation remaining within acceptable limits.

Introduction

Carbon dioxide (CO_2) sequestration in deep saline aquifers represents a key technology for long-term emissions mitigation, involving the capture of CO_2 from point sources and its injection into subsurface geological formations (Chow et al., 2003). Secure storage relies on multiple trapping mechanisms, including structural, residual, solubility, and mineral trapping (Rosenbauer & Thomas, 2010; Blunt, 2010). Accurately simulating CO_2 plume migration and pressure evolution remains challenging due to the strong coupling among diverse physical processes (Kumar et al., 2005), including multiphase flow, temperature- and salinity-dependent phase behavior, geomechanics, geochemical reactions, convective mixing, capillary hysteresis, and permeability heterogeneity. These nonlinear interactions span multiple spatial and temporal scales and require fully coupled numerical simulators that are computationally intensive (Kumar et al., 2005; Qin et al., 2025).

Despite its promise, large-scale deployment of geologic CO_2 storage remains limited, and uncertainties in plume migration and pressure buildup motivate the need for robust monitoring and risk management strategies (Bachu, 2015; Celia et al., 2015; Zheng et al., 2021). Predictive models capable of forecasting plume evolution and pressure response are essential for monitoring, verification, and operational decision-making during both injection and post-injection phases (Ajayi et al., 2019). While physics-based simulators provide high-fidelity predictions, their computational cost limits their repeated use for uncertainty quantification, optimization, and real-time risk assessment.

Recent advances in deep learning (DL) have enabled surrogate models that offer a computationally efficient alternative to traditional simulators (Razak et al., 2021, 2022; Cornelio et al., 2025). Convolutional neural networks (CNNs) have been widely adopted due to their ability to exploit spatial structure in gridded geological data. Early studies demonstrated encoder–decoder CNNs for steady and transient flow prediction (Zhu & Zabaras, 2018; Mo et al., 2019), with subsequent architectural enhancements to address multiphase flow complexity (Wang & Lin, 2020). U-Net-based architectures are particularly effective for subsurface applications due to their multiscale feature extraction via skip connections (Ronneberger et al., 2015; Jiang et al., 2021; Tang et al., 2021; Wen et al., 2021; Yan et al., 2022). However, models that treat time as a static conditioning variable do not explicitly capture temporal dynamics. To address this limitation, recurrent architectures such as ConvLSTM-based Recurrent U-Nets have been developed and successfully applied to multiphase flow and CO_2 storage problems (Tang et al., 2020, 2021, 2022).

This work applies a ConvLSTM-based Recurrent U-Net to the Quest CCS project in Alberta, Canada. Quest is a large-scale saline aquifer storage operation that has been injecting CO_2 since 2015 into the Basal Cambrian Sandstone, a regionally extensive deep saline formation overlain by multiple sealing units. Previous studies have shown that storage performance at Quest is strongly influenced by geological uncertainty and pressure evolution, making it a representative testbed for evaluating data-driven modeling approaches for field-scale CO_2 storage (Wang et al., 2023).

Theory and/or Methods

A schematic of the proposed predictive framework is shown in Figure 1. The model consists of two CNN-based encoders that process static reservoir properties (permeability and porosity) and dynamic state variables (CO_2 saturation and reservoir pressure), respectively. Each encoder extracts spatial features and maps the inputs into a compact latent representation using three-dimensional convolutional layers with nonlinear activation functions and strided down-sampling.

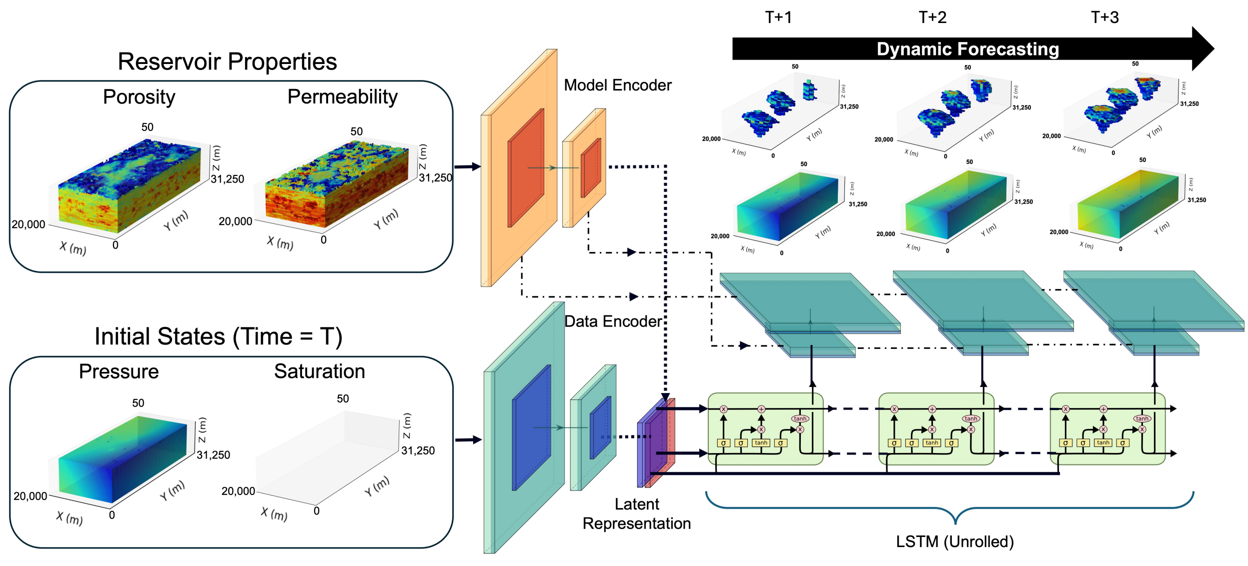

Figure 1: Neural Network Architecture

The latent representations are concatenated and passed to a three-dimensional convolutional long short-term memory (ConvLSTM) module, which introduces temporal recurrence and models the evolution of CO_2 plume migration and pressure buildup over time. The ConvLSTM output is decoded through an upsampling network to predict full-field CO_2 saturation and pressure at the next time step. Decoder parameters are shared across time steps. Skip connections between the static encoder and decoder, along with residual connections at the most compressed latent level, are incorporated to preserve multiscale spatial information and improve training stability (He et al., 2015; Tang et al., 2020, 2021). The resulting architecture constitutes a three-dimensional recurrent residual U-Net (3D R-R-U-Net) for spatiotemporal prediction of CO_2 storage dynamics.

Results

The dataset is generated using a three-dimensional multiphase flow simulation model of the Quest CO_2 storage site constructed from publicly available geological data. The model includes three injection wells and reproduces historical injection rates from 2015 to 2022; thereafter, the final injection rate is held constant to enable long-term forecasting (Wang et al., 2023). A total of 1000 realizations of spatially correlated permeability and porosity fields are generated across 100 distinct facies distribution schemes, with 10 realizations per facies distribution. Each realization is simulated over a 25-year injection period, with CO_2 saturation and reservoir pressure recorded at five-year intervals.

A sliding-window formulation is adopted, in which multiple starting times are extracted from each realization. For each sample, a single input state (e.g., at 0, 5, or 10 years) is used to predict the subsequent three time steps, each corresponding to a five-year forecast interval. This yields a total of 3000 input–output pairs. The dataset is split into training, validation, and test sets at 2400/300/300.

Two evaluation scenarios are considered. In the interpolation case, realizations from each facies distribution are evenly split across training, validation, and test sets. In the extrapolation case, all realizations from selected facies distributions are withheld during training to evaluate generalization to unseen geological patterns.

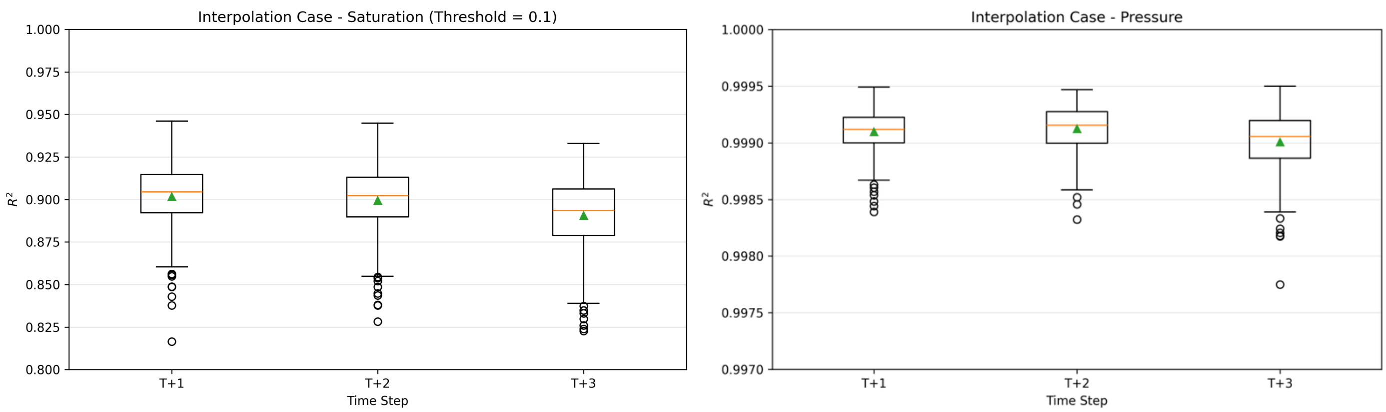

Figure 2: Interpolation-case prediction performance for CO_2 saturation (threshold = 0.1) and reservoir pressure, shown as distributions of sample-wise, spatially averaged R^2

Figure 2 summarizes predictive performance for the interpolation case using the coefficient of determination (R^2). Each data point represents the spatially averaged R^2 for an individual sample. For CO_2 saturation, a threshold of 0.1 is applied to exclude low-saturation regions below practical plume detectability. The model demonstrates strong agreement with reference simulations for both saturation and pressure. Pressure predictions consistently achieve higher R^2 values than saturation, reflecting the smoother spatial structure of pressure fields relative to sharp saturation fronts. Predictive performance decreases gradually with increasing forecast horizon from T+1 to T+3.

Figure 3 presents representative examples of true and predicted CO_2 saturation and reservoir pressure fields, along with corresponding error fields, for multiple forecast horizons in the interpolation case. Prediction errors are concentrated near plume boundaries, where sharp spatial gradients and higher variability pose greater challenges.

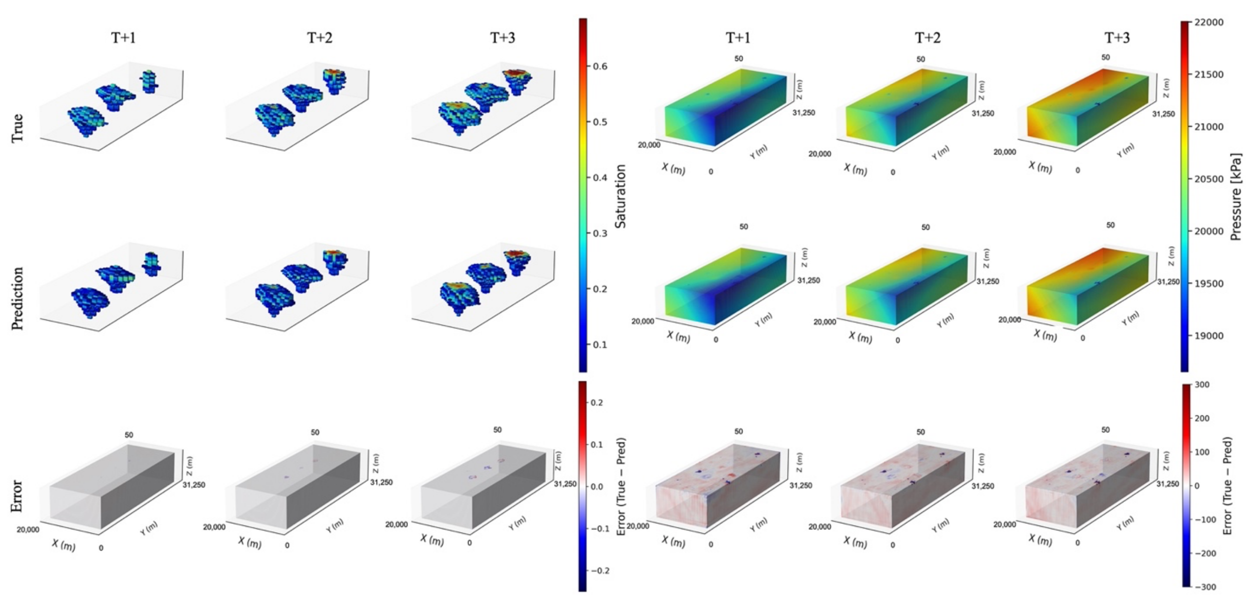

Figure 3:Representative example of true and predicted CO_2 saturation (left) and reservoir pressure (right) fields for increasing prediction horizons (T+1 to T+3), along with the corresponding error fields (true minus prediction) for the interpolation case.

Figure 4 summarizes predictive performance for the extrapolation case using R^2. As expected, performance degrades relative to the interpolation case due to the absence of the corresponding facies distributions during training. Nevertheless, the model maintains robust predictive capability, with R^2 values remaining within an acceptable range across forecast horizons.

Figure 5 presents representative examples of predicted and true CO_2 saturation and pressure fields for the extrapolation case, along with corresponding error fields.

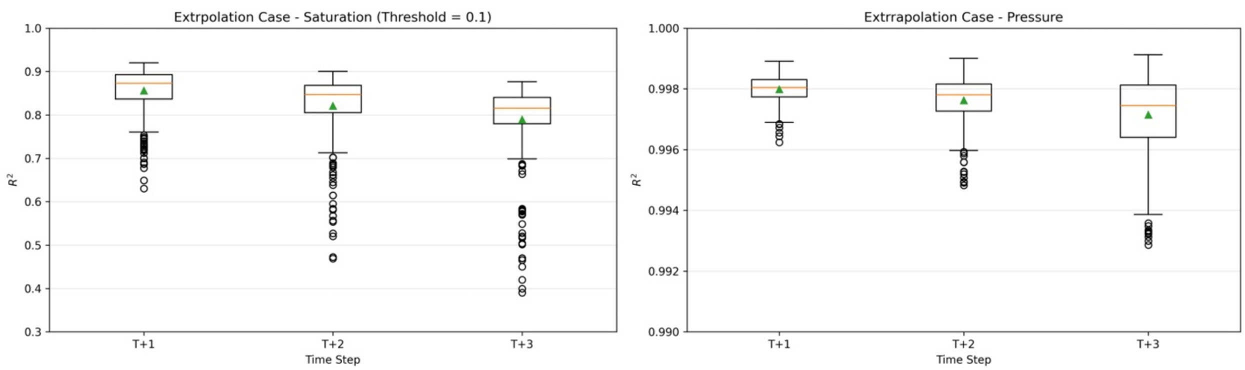

Figure 4: Extrapolation-case prediction performance for CO_2 saturation (threshold = 0.1) and reservoir pressure, shown as distributions of sample-wise, spatially averaged R2.

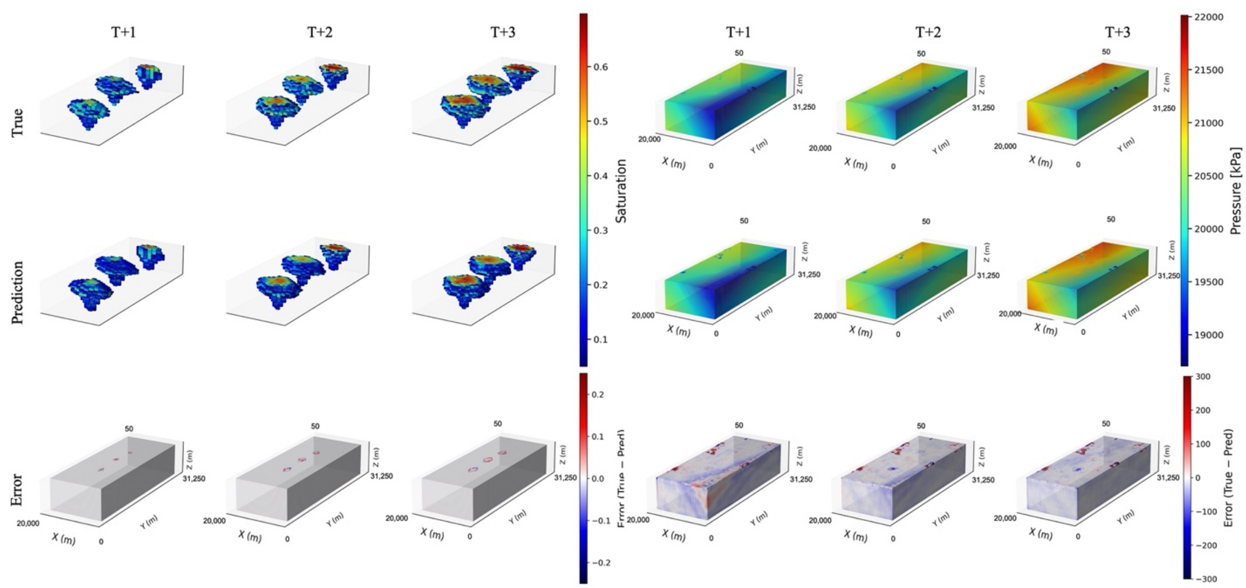

Figure 5: Representative example of true and predicted CO_2 saturation (left) and reservoir pressure (right) fields for increasing prediction horizons (T+1 to T+3), along with the corresponding error fields (true minus prediction) for the extrapolation case.

Conclusions

This study demonstrates that a ConvLSTM-based recurrent residual U-Net can accurately and efficiently predict the spatiotemporal evolution of CO_2 plume migration and reservoir pressure at the field scale for the Quest CCS project. The model achieves strong predictive performance under both interpolation and extrapolation scenarios, indicating robust generalization across geological uncertainty. These results highlight the potential of deep learning surrogate models to complement physics-based simulators for rapid forecasting, uncertainty quantification, and risk-informed decision support in large-scale CO_2 storage operations.

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