An Integrated Deep Learning Framework for Predictive CO2 Storage Modeling

Introduction

In recent years, addressing climate change has become a global priority, driving the development of sustainable solutions like carbon capture and storage (CCS). CCS is designed to mitigate CO_2 emissions from industries and power plants by capturing and securely storing carbon dioxide in geological formations (Awan et al., 2021). Traditional modeling approaches often struggle to capture the complexity of subsurface systems, as they often fail to represent intricate linkages and unknown variables effectively (Eidelson, 1997). Additionally, these methods require significant computational resources to solve the Partial Differential Equations (PDEs) governing multiphase flow, such as Darcy's law, further complicating simulations (Ahusborde et al., 2021). Techniques like non-uniform grids have been used to reduce computational costs and enhance efficiency (Shahsavari and Akbari, 2018).

Machine learning (ML) has emerged as a promising tool to overcome the limitations of conventional numerical methods. Techniques such as Logistic Regression (LR) have successfully simulated three-dimensional CO_2 storage systems, offering improved accuracy and efficiency (Lyu et al., 2021). The application of Artificial Intelligence (AI) and ML in numerical simulations has grown significantly, enabling a better understanding and prediction of subsurface phenomena (Samnioti and Gaganis, 2023).

Physics-Informed Neural Networks (PINNs), guided by established scientific principles, have gained traction for solving complex problems in geologic carbon storage. These networks have demonstrated the ability to address key challenges in simulating CO_2 storage and related processes (Wang et al., 2023). PINNs are particularly effective in enhanced oil recovery (EOR) projects, where CO_2 is injected to both boost oil production and enable carbon sequestration (Al-Shargabi et al., 2022).

This research introduces an integrated framework combining Vision Transformers (ViTs) and advanced deep learning techniques to predict CO_2 storage capacity. The framework provides a comprehensive approach to simulating CO_2 movement and storage in geological formations by leveraging neural networks, data integration methods, and geoscientific insights. It addresses critical challenges in accuracy and efficiency, paving the way for improved solutions in carbon storage modeling (Paulvannan Kanmani et al., 2020).

Method

Figure 1 gives a brief overview of the proposed methodology.

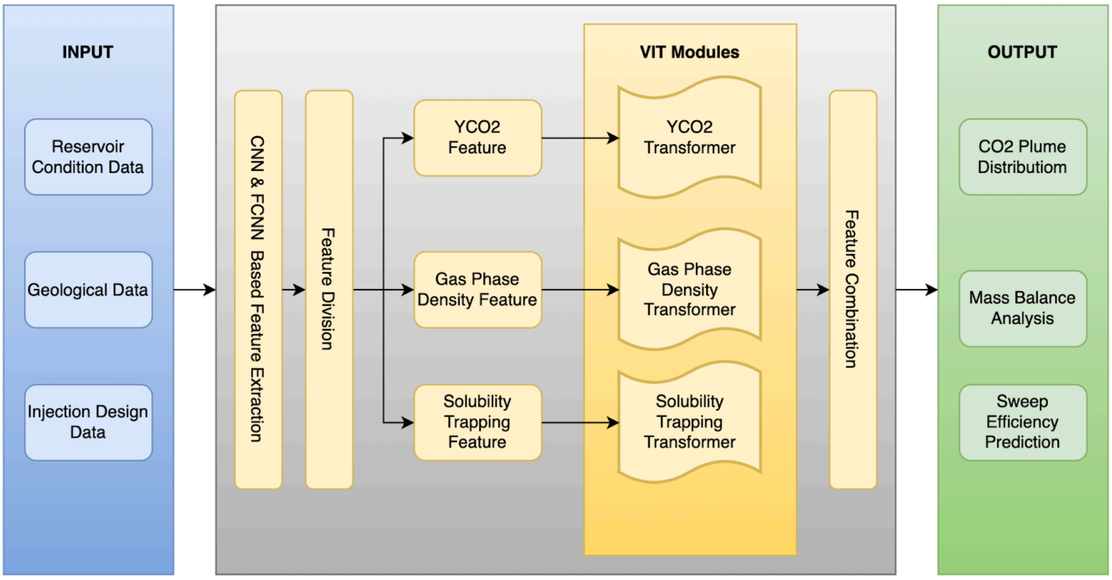

Figure 1: Proposed Methodology

Step 1: Data Collection
Collect data on reservoir conditions, geological characteristics, and injection design.
Step 2: Data Preprocessing

- **Cleaning:** Detect and remove irregularities, missing, or extreme values.
- **Normalization:** Scale data to ensure consistency and improve model performance.

Step 3: Data Splitting
Divide the preprocessed data into training, testing, and validation sets.
Step 4: Feature Extraction
Extract spatial features from the reservoir and geological data using CNN.
Extract temporal features from injection design data using FCNN.
Step 5: Feature Division
Separate features into three streams: CO_2, gas phase density, and solubility trapping.
Step 6: ViT Modules
Process each feature stream using specialized transformers:

- **CO_2 Transformer:** Extract CO_2 solubility and hydrate formation characteristics.
- **Gas Transformer:** Extract features related to porosity, permeability, and rock type.
- **Solubility Transformer:** Extract features tied to injection rate and pressure.

Step 7: Feature Combination
Combine outputs from all transformers into a unified feature vector.
Step 8: VNet Model Evaluation
Feed combined features into the VNet model to predict CO_2 plume distribution and evaluate performance using the validation set.

Dataset Description
The dataset comprises **reservoir condition**, **geological**, and **injection design data**. It includes key parameters related to shale formations, reservoir properties, and injection design. These features cover a range of properties critical for simulating and predicting CO_2 storage and plume behavior. Table 1 lists the fields in the dataset, along with their units and value distributions.

Table 1: Dataset Description

Variable Type	Parameters	Unit	Value Distribution
Field	Shale - Number of horizontal zones	-	5-11
	Shale - Number of vertical subzones	-	50-200
	Shale - Layer thickness	m	2-4
	Shale - Layer permeability	mD	0.001-0.1
	Number of anisotropic materials	-	1-6
	Material anisotropy ratio	-	1-150
	Porosity random perturbation	-	
Reservoir Condition	Initial pressure	bar	100-300
	Reservoir temperature	°C	40-155
	Reservoir thickness	m	12.5-200
Injection Design	Injection rate	MT/y	0.4-2
	Perforation thickness	m	100-200
Rock property	Irreducible water saturation	-	0.1-0.3
	van Genuchten scaling factor	-	0.4-1

Evaluation Metrics

Evaluation metrics are essential for assessing the performance, accuracy, and effectiveness of the models. Below are the metrics used:

1. **Mean Absolute Error (MAE):**
   Measures the average of the absolute differences between predicted and actual values, ignoring the direction of errors.
   $$MAE = \frac{1}{n}\sum_{i=1}^{n} |y_i - \hat{y}_i|$$
2. **Mean Squared Error (MSE):**
   Assesses the average squared differences between predicted and actual values, penalizing larger errors more severely.
   $$MSE = \frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
3. **Root Mean Squared Error (RMSE):**
   Represents the square root of the average squared differences, providing an interpretable metric in the same units as the original data.
   $$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$
   Where n is the number of observations
   y_i is the actual value.
   $\hat{y}_i$ is the predicted value.

Result

Table 2 compares the performance of three machine learning models - ANN, XGBoost, and VNet for a prediction task using two evaluation metrics: RMSE (lower values indicate better accuracy) and R^2 (higher values indicate better fit).

- DNN Model: Introduced by Alqahtani et al. (2023), this method achieved an RMSE of 0.00783 and an R^2 of 0.9988, demonstrating high accuracy.
- XGBoost Model: Proposed by Hamadi et al. (2023), this model reported an RMSE of 0.22710 and an R^2 of 0.9985, indicating strong but slightly inferior performance compared to ANN.
- VNet Model: The proposed VNet model outperformed both ANN and XGBoost, achieving the lowest RMSE (0.03042) and the highest R^2 (0.9998), underscoring its superior precision and reliability for the prediction task.

This comparison highlights the remarkable accuracy of the VNet model, making it a promising choice for addressing complex prediction challenges.

Table 2: Comparative Analysis of Error Rate

Authors	RMSE	R^2
Alqahtani et al. (2023)	0.00783	0.9988
Hamadi et al. (2023)	0.22710	0.9985
Proposed Method	0.03042	0.9998

Conclusion and Future Scope

The computational system leverages advanced deep learning (DL) algorithms to predict the behavior and outcomes of carbon capture and storage (CCS) operations, significantly improving the accuracy and efficiency of CO_2 storage evaluations. By integrating a cutting-edge deep learning framework, the system has demonstrated remarkable performance.

On the primary dataset, the ViT model achieved training and validation losses of 0.0945 and 0.0840, respectively, while the VNet model achieved training and validation losses of 0.1164 and 0.1103, respectively. Further analysis revealed that the VNet model excelled in predictive metrics, achieving a root mean square error (RMSE) of 0.03042 and an R^2 value of 0.9998. These results underscore the framework's ability to deliver precise forecasts of CO_2 plume dynamics and reservoir responses under diverse operational scenarios. These findings highlight the potential of this approach to revolutionize CCS strategies by providing actionable insights to mitigate greenhouse gas emissions and address climate change effectively.

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