Abstract
The potential for large-scale storage of carbon dioxide (CO₂) through Geological Carbon Sequestration (GCS) in deep geological formations such as saline aquifers and depleted oil and gas reservoirs is significant. Effectively implementing GCS requires evaluating the risk of plume confinement and storage capacity at each site through a thorough assessment. To assess the stability of the caprock after CO₂ injection, efficient tools are needed to evaluate the safe duration of CO₂ injection. This study used Particle Swarm Optimization (PSO) evolutionary algorithm to optimize the maximum CO₂ storage capacity in saline aquifers without risking the integrity of the caprock. A deep learning (DL) model, fully connected neural networks, was trained to predict the safe injection duration. The movement of CO₂ was simulated for 170 years following a 30-year injection period into a deep saline aquifer using a physics-based numerical reservoir simulator. The simulation took into consideration uncertainty variables such as petrophysical properties and reservoir physical parameters, as well as operational decisions like injection rate and perforation depth. Sampling the reservoir model with the Latin-Hypercube approach accounted for a range of parameters. Over 720 reservoir simulations were performed to generate training, testing, and validation datasets, and the best DNN model was selected after multiple executions. The three-layer FCNN model with 30 neurons in each layer showed excellent prediction efficiency with a coefficient of determination factor over 0.98 and an average absolute Percentage Error (AAPE) less than 1%. The trained models showed a good match between simulated and predicted results and were 300 times more computationally efficient. PSO was utilized to optimize the operational parameters in the DL models to achieve maximum CO₂ storage with minimum damage to the caprock. The results suggest that the DNN-based model can serve as a reliable alternative to numerical simulation for estimating CO₂ performance in the subsurface and monitoring storage potential in GCS projects.

Keywords: Geological Carbon Sequestration (GCS); Geomechanics; Deep Learning (DL); CO₂ injection well monitoring; Well bottom-hole pressure prediction

1. Introduction
Underground storage of carbon-dioxide (CO₂) is considered as the one of the most imperative need of the current era to reduce the release of anthropogenic greenhouse gases emission into the atmosphere
[1,2]. Reducing the emission of the greenhouse gases to the atmosphere and the initiatives towards net zero carbon neutral energy options have attracted significant attention over the past many years across the globe [3,4]. The world population continually increases which consequently results in increase on energy demand and subsequently the world will not peak on utilizing energy in the near future [4–6]. This has triggered collaborative discussions among hydrocarbon peers to address the risks of climate action on business sustainability as the greenhouse gases are the primary concerns for global warming and climate change [7–15]. Geological Carbon Sequestration (GCS) into a deep subterranean formations, like saline aquifers, unminable coal seams, and depleted hydrocarbon reservoirs, brings huge potential for large-scale storage of carbon dioxide [16–20]. Among all the storage sites, saline aquifers are the most attractive one because of large room for the storage, but it requires high capital investment in terms of drilling new wells and conducting seismic surveys for the long term storage assessments [21]. The successful implementation of GCS requires comprehensive risk assessment of the confinement of plumes at each potential storage site [21–24]. The accurate prediction of the flow, geochemical, and geochemistry responses of the formation is essential for the better management of the overall GCS project in long-term operations [25–34].

Modeling of the reservoir during GCS is traditionally conducted by physics-based numerical simulators in which a set of partial differential equations describing the subsurface processes are solved considering initial and boundary conditions for a quantity such as reservoir pressure and CO2 saturation [33–35]. In other words, the main aim of the simulation process is to solve the spatial-temporal evolution of the response of interest in the domain after the governing equations are discretized. Kumar et al. [36] analyzed important CO2 storage mechanisms in a deep saline aquifer by using a compositional reservoir simulator. They concluded from their study that the effect of residual trapping on carbon dioxide storage can be more critical than solubility and mineral trapping. However, the impact of the mineralization process is significant in immobilizing carbon dioxide over tens of thousands of years. Ranganathan et al. [37] have performed the simulation study of three different CO2 trapping mechanisms to evaluate the feasibility of a potential storage site. They confirmed that during the injection period the most dominant mechanism is mobility trapping while mineral and solubility trapping mechanisms effects became dominant at later times while mobility trapping diminishes.

Solving the modeling equations can be computationally expensive especially in large-scale problems using conventional reservoir simulators [35–38]. Deep learning models have proven to be faster alternatives to physics-driven models. They can be used as proxy models, also known as surrogate models, to reduce the computational time of the simulation [39–44]. Deep learning and Machine learning are making great progress in the oil and gas industry, with various researchers investigating advance applications pertaining to complex/heterogeneous systems [45–52]. A wide range of AI algorithms have been employed to develop models/correlations for estimating various parameters related to hydrocarbons development [53–65]. Kalam et al. [66] and Artun [67] have utilized artificial neural network to determine the performance of water-flooding in a five spot pattern. They have found that the proxy model developed from ANN performed much faster compared to the conventional numerical simulator. In the area of subsurface flow and transport simulation, various applications have been implemented using convolutional neural networks (CNN). These models act like finite-dimensional operators which, using simulation data, can learn mappings from the input space (e.g. permeability, porosity, injection rate) to output space (e.g. saturation, pressure). Zhu and Zabaras [68] utilized deep convolutional encoder-decoder networks in the image-to-image regression task to predict velocity and pressure fields. Omosebi et al. [69] investigated deep-learning-based surrogate models developed with different algorithms to predict the pressure plume and CO2 saturation plume during displacement of water by CO2. Zhong et al. [70] formulated a conditional generative adversarial network (GAN) to learn the dynamic functional mapping in heterogeneous reservoirs. They demonstrated the performance of the surrogate model for predicting the migration of CO2 plume in both spatial and temporal domains. Wen et al [71] utilized a deep convolutional neural network based on U-Net architecture [72] for an image-to-image regression task. They used the permeability, injection duration, and injection rate fields as input and CO2 saturation field as output of the
network. Moreover, ML and DL have extensively been utilized in reservoir characterization and petrophysical properties determination from the well logs utilizing neural networks [73,74].

In this study, Particle Swarm Optimization (PSO) was used to optimize the storage capacity of CO$_2$ into saline aquifers. The optimization problem involves finding the optimal CO$_2$ injection rate and perforation thickness zone for a vertical well drilled at the center of the target reservoir. In the first part of the study, we built a machine Learning (ML) workflow to effectively infer the reservoir characterization and petrophysical properties determination from the well logs utilizing neural networks [73,74].

2. Methodology

2.1 Simulation Model

Figure 1 shows the physical model created to run multiple simulations to capture the flow, transport, and fate of long-term storage of injected CO$_2$ in a saline aquifer. The physical model was comprised of a single well located at the center of a cylindrical reservoir. The classical carbonate reservoir is considered to establish the ML workflow in this study. Table 1 shows the reservoir model parameters used in numerical modeling. Table 2 shows the critical parameters properties of the H$_2$O and CO$_2$. To capture the fluid flow dynamics, logarithmic grid refinement were used nearby the wellbore in the radial direction. The reservoir has no-flow boundaries on the top and bottom. We have used a vertical grid dimension of 4 meters to capture the vertical heterogeneity of the reservoir. The outer edge boundary is closed but is sufficiently distant away from the injection well that it behaves like an infinite-acting reservoir. The initial reservoir pressure is 25888.4 KPa.

Figure 1. The radial cross-sectional view of the reservoir at different times.
Table 1. Reservoir simulation inputs for the base case model.

<table>
<thead>
<tr>
<th>Reservoir Parameters</th>
<th>Values</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid System</td>
<td>Radial</td>
<td></td>
</tr>
<tr>
<td>Total Reservoir Grids</td>
<td>2500 (50 × 1 × 50)</td>
<td></td>
</tr>
<tr>
<td>Grid Sizes in r - Direction</td>
<td>varying</td>
<td>m</td>
</tr>
<tr>
<td>Grid Sizes in Theta - Direction</td>
<td>360</td>
<td>Degrees</td>
</tr>
<tr>
<td>Grid Sizes in z - Direction</td>
<td>4</td>
<td>m</td>
</tr>
<tr>
<td>Reservoir Thickness</td>
<td>200</td>
<td>m</td>
</tr>
<tr>
<td>Reservoir Depth at the top of the formation</td>
<td>2400</td>
<td>m.</td>
</tr>
<tr>
<td>Initial Reservoir pressure</td>
<td>25888</td>
<td>KPa</td>
</tr>
<tr>
<td>Radial Length</td>
<td>5000</td>
<td>m</td>
</tr>
<tr>
<td>Reservoir Lithology</td>
<td>Limestone</td>
<td></td>
</tr>
<tr>
<td>Rock Compressibility</td>
<td>3x10^6</td>
<td>psi^1</td>
</tr>
<tr>
<td>Porosity</td>
<td>25</td>
<td>%</td>
</tr>
<tr>
<td>Initial Reservoir Temperature</td>
<td>80</td>
<td>°C</td>
</tr>
<tr>
<td>Aquifer Salinity</td>
<td>57000</td>
<td>ppm</td>
</tr>
<tr>
<td>Residual gas saturation</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Residual water saturation</td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>Dykstra-Parsons Coefficient</td>
<td>0.6</td>
<td></td>
</tr>
<tr>
<td>Average Horizontal Permeability kh</td>
<td>220</td>
<td>mD</td>
</tr>
<tr>
<td>Vertical Permeability</td>
<td>0.1 * k_h</td>
<td>mD</td>
</tr>
<tr>
<td>No. of Injection Well</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Well diameter</td>
<td>0.375</td>
<td>ft.</td>
</tr>
<tr>
<td>Aquifer water density</td>
<td>1020</td>
<td>Kg/m^3</td>
</tr>
<tr>
<td>Injection rate</td>
<td>1x10^6</td>
<td>m^3/day</td>
</tr>
</tbody>
</table>

Table 2. Critical Properties of H_2O and CO_2

<table>
<thead>
<tr>
<th>Components</th>
<th>H_2O</th>
<th>CO_2</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical Pressure</td>
<td>220.6</td>
<td>73.8</td>
<td>Bar</td>
</tr>
<tr>
<td>Critical Temperature</td>
<td>373.94</td>
<td>30.98</td>
<td>°C</td>
</tr>
<tr>
<td>Critical Volume</td>
<td>0.056</td>
<td>0.094</td>
<td>liter/g-mol</td>
</tr>
<tr>
<td>Molecular Weight</td>
<td>18.015</td>
<td>44</td>
<td>g/g-mol</td>
</tr>
<tr>
<td>Acentric factor</td>
<td>0.344</td>
<td>0.22394</td>
<td>-</td>
</tr>
<tr>
<td>Parachor</td>
<td>52</td>
<td>78</td>
<td>-</td>
</tr>
</tbody>
</table>

During the GCS project, super-critical phase CO_2 is injected into the deep saline aquifers which were initially saturated with saline water. Therefore, two-phase (aqueous and supercritical phases) relative permeability is a crucial parameter to determine the effective permeability of each phase. In this study, Brooks and Corey's correlation [75] is used for the relative permeability of two-phase super-critical CO_2 and brine system, shown as,

\[ k_{rw} = \frac{S_w^{(3+2/\lambda)}}{S_w} \]  \( (1) \)
\[ k_{rg} = S_g \left( 1 - (1 - S_g)^{1+2/\lambda} \right) \]  

\[ \bar{S}_w = \frac{S_w - S_{wi}}{1 - S_{gi} - S_{wi}} \]  

\[ \bar{S}_g = \frac{S_g - S_{gi}}{1 - S_{gi} - S_{wi}} \]  

\( \lambda \) is the pore size distribution index, where \( k_{rw} \) is the relative permeability of the water phase, \( k_{rg} \) is the relative permeability of the super-critical \( \text{CO}_2 \) phase, \( S_{wi} \) is the irreducible water saturation, \( S_{gi} \) is the irreducible super-critical \( \text{CO}_2 \) saturation.

The mass balance equation for flow and transport equation of \( \text{CO}_2 \) storage is given by Eq. 5

\[
\frac{\partial}{\partial t} \left( \varphi \sum_{\alpha} S_{\alpha} \rho_{\alpha} x_{\alpha,i} \right) - \nabla \left( K \sum_{\alpha} \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{\alpha,i} (\nabla p_{\alpha} + \rho_{\alpha} g \nabla Z) \right) + \sum_{i} \left( \sum_{\alpha} \rho_{\alpha} x_{\alpha,i} q_{\alpha} \right)^l = 0
\]  

where, the first term denotes the fluid accumulation; the second term is the advective flux based on Darcy’s law; the third term is the source or sink term. The subscript \( i \) denotes the primary fluid components, including \( \text{CO}_2 \) and water; \( \alpha \) denotes the fluid phases including water and \( \text{CO}_2 \); \( t \) is the time; \( \varphi \) is the porosity; \( S_{\alpha} \) is the phase saturation; \( \rho_{\alpha} \) is the fluid phase density; \( x_{\alpha,i} \) is the mole fraction of component \( i \) in the fluid phase \( \alpha \); \( k \) is the permeability; \( k_{r\alpha} \) is the phase relative permeability; \( \mu_{\alpha} \) is the phase viscosity; \( p_{\alpha} \) is the pressure of the fluid; \( g \) is the gravity; \( Z \) is the depth; \( q_{\alpha} \) is the denotes the rate for producing or injecting fluid phase through well perforation \( l \).

### 2.3 Workflow Methodology

The methodology of the workflow is shown in Figure 3. The dataset for the DL workflow was created from a compositional numerical simulator, with 722 simulations/realizations being carried out. Each simulation involved varying geological, petrophysical, geomechanical, and operational parameters, such as permeability field, porosity field, Young’s modulus, Poisson’s ratio, Biot’s coefficient, reservoir temperature, aquifer salinity, reservoir thickness, perforation thickness, and \( \text{CO}_2 \) injection rate. The training data was created using a design of experimentation technique, where the Latin-Hypercube method was employed to generate random cases for multiple simulations. The DL model consists of three fully connected feedforward neural networks with 30 neurons in each layer, with a tangent hyperbolic activation function used in the hidden layers and WBHP as the target variable to predict in the output layer. Finally, the safe injection duration time was calculated from the WBHP by taking the time derivative of WBHP.
2.4 Performance Metrics

This study used several graphical and error metrics to evaluate the predictive performances of the model. These metrics include predictive cross-plots, average absolute percentage error (AAPE), coefficient of determination ($R^2$), root mean square error (RMSE), residual errors (RE), and standard deviation (S.D.). The definitions of AAPE, $R^2$, RMSE, RE, and S.D. are given by Eqs. 10 – 14.

$$R^2 = \left( \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum(x_i - \bar{x})^2(y_i - \bar{y})^2}} \right)^2$$

$$AAPE = \frac{1}{n_{samples}} \sum \left| \frac{x_{measured} - x_{pred}}{x_{exp}} \right| \times \frac{100}{x_{exp}}$$
\[ RMSE = \sqrt{\frac{1}{n_{\text{samples}}} \sum_{i=1}^{n_{\text{samples}}} (x_{\text{measured}} - x_{\text{pred}})^2} \]  
\[ RE = x_{\text{measured}} - x_{\text{pred}} \]  
\[ SD = \sqrt{\frac{1}{n_{\text{samples}} - 1} \sum_{i=1}^{n_{\text{samples}}} \left( \frac{x_{\text{measured}} - x_{\text{pred}}}{x_{\text{measured}}} \right)^2} \]

Where \( x_{\text{exp}} \) is the actual value and \( x_{\text{pred}} \) is the predicted value from the model, \( n_{\text{samples}} \) are the total number of data points, \( x \) and \( y \) are the two variables.

3. Results and Discussions

In this study, a dataset with 722 simulations was analyzed. Each simulation involved injecting super-critical \( \text{CO}_2 \) into a vertical well with a radius of 0.076 meters at a corresponding constant rate for 30 years. The well was perforated to a specified depth, and the movement of the \( \text{CO}_2 \) plume was monitored for 170 years. The simulation was carried out in 68 different time steps, with 30 time steps in the injection stage and 38 in the monitoring stage. Figures 3 and 4 show the simulation results of \( \text{CO}_2 \) pressure and saturation plume evolution, respectively.

![Pressure Front (Bar)](image)

**Figure 3.** \( \text{CO}_2 \) Pressure plume movement for first 26 years.
Figure 4. CO₂ saturation front movement for full simulation time.

The goal of the study was to determine the safe injection duration, and so the simulation data corresponding to the first 30 years at injection stage were used for FCNN training, prediction and optimization. During the injection period, annual time steps chosen, while in the monitoring phase, we took time step size at every ten years. Figure 5 displays the profiles of WBHP across all cases over the 200-year simulation time. The trainable dataset consists of 21660 samples (722 runs × 30 timesteps). The dataset was further divided into three parts, training (70%), testing (15%), and validation (15%). Therefore, 505 simulations were used for training, yielding 15150 data samples, while 109 simulations were utilized for testing, resulting in 3270 data samples. The remaining 108 simulations (3240 data samples) were used for validation.
The FFNN model was trained on a set of random data and produced an R2 score of 0.988, AAPE of 0.657%, and RMSE of 4.07 KPa. When tested on a blind dataset, the FFNN model had an R2 score of 0.975, AAPE of 0.855%, and RMSE of 9.22KPa, as shown in Figure 6. The figure also displays the Kernel Density Estimation (KDE) of the residual errors, which primarily ranged from -2000 to 2000 KPa and were mostly concentrated around zero.
Using the trained FFNN model, sensitivity analysis of safe injection duration time with decision parameters, including CO$_2$ injection rate and perforation thickness, was conducted. Figure 7 suggests that by increasing the injection rate, the safe CO$_2$ injection duration decreases: from 25 years (at the CO$_2$ injection rate of $1.5 \times 10^6 \text{ m}^3/\text{day}$) to 6 years (at the CO$_2$ injection rate of $6.0 \times 10^6 \text{ m}^3/\text{day}$).
Figure 7. Sensitivity of the injection rate.

Figure 8. Example of PSO based optimization for the case with permeability heterogeneity in terms of Dykstra parson coefficient is
4. Conclusions
In this study, we have developed the DL model followed by optimization workflow to effectively monitor the CO\textsubscript{2} injection well. The coupled hydro-mechanical approach, in combination with deep learning workflow, resulted in excellent accuracy in predicting the safest injection duration of CO\textsubscript{2}. The DL/optimization workflow can be used as a quick alternative to tedious numerical simulation for maximum CO\textsubscript{2} storage into deep saline aquifers.

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