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Prediction/Assessment of CO2 EOR and Storage Efficiency in Residual Oil Zones Using Machine Learning Techniques

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Abstract

Residual oil zones (ROZ) arise due to a wide range of geologic conditions and are located under the oilwater contact of main pay zones. These ROZs have historically been deemed economically unviable for development using conventional primary recovery methods due to the presence of immobile oil. Yet, they represent substantial subsurface volume suitable for CO2 sequestration and storage. However, there is a deficiency of effective techniques for assessing the performance of CO2-EOR in coupled with CCUS in ROZs. This study introduces the use of Machine Learning techniques to assess/predict the potential of oil recovery and CO2 storage capacity in ROZs. Our framework was built upon the concept of supplying the machine learning model with data obtained from several simulation runs involving CO2 injection in ROZs. This dataset includes key geological and operational attributes as inputs (Thickness, Permeability/Kh, Porosity, Sorw, Sorg, Producer BHP, Injection rate, formation water salinity). The objective is to forecast CO2 storage capacity and oil recovery potential, eliminating the necessity for time-consuming and costly reservoir simulations. We have tested this method in both synthetic and field-scale cases. The study results demonstrated a significant positive correlation between the cum-oil production with sorw, CO2 injection rate, reservoir permeability. In contrast, producer BHP and the vertical permeability to horizontal permeability ratio showed negative correlation. Conversely, the cumulative CO2 storage in ROZs exhibited a positive relation with producer BHP, reservoir thickness, and CO2 injection rate, while showing a negative correlation with reservoir permeability. The utilization of our proposed ANN models has proven highly effective accuracy in predicting CO2-EOR and storage performance. Notably, the tested R2 values for Cumulative oil production and CO2 Storage models were in range of 0.9 to 0.98 with low average absolute percentage error less than 10%. Furthermore, these models serve as a valuable tool for improved reservoir management by optimizing operational parameters, such as producer BHP and CO2 injection rates. These findings have been rigorously validated through real field data, affirming a high level of agreement between the model's predictions and actual outcomes. The developed model can be applied as a

fast technical and cost-effective tool for evaluating CO2-EOR and storage in ROZs. Using real ROZs field data demonstrated an excellent agreement between the ANN's forecasts and the actual data, making it well-suited for field applications.

Introduction

Geological CO2 Storage is considered as an important technique to reduce the CO2 gas emissions into the atmosphere that causes climate change challenges. CO2 can be stored in different geological reservoirs such as depleted oil or shale gas reservoirs, deep saline aquifers, coal beds and geothermal reservoirs (Li et al,2006). One of main attractive reservoirs are the depleted oil and gas reservoirs as the CO2 can serve as EOR solvent and as well as for CO2 storage purpose (Bachu,2016). CO2 enhanced oil recovery (CO2-EOR) has been widely used as EOR method for medium and light oil production in conventional and unconventional oil reservoirs for more than decades as when CO2 is injected into the reservoir, the oil swells, oil viscosity reduces, interfacial tension reduces, oil vaporizes, capillary number increases, and both the sweep and displacement efficiencies increase.(Manrique et al,2010),(Johns and Dindoruk, 2013). In addition, the injected CO2 is retained and trapped in reservoir due either structural trapping, residual trapping, solubility, and mineral trapping (Cao et al,2020). Most of previous studies on CO2-EOR and storage focused on the main pay zone (Ettehadtavakkol et al,2014), (Ampomah et al,2017), (Liu et al,2022). Recently, CO2-EOR and storage in Residual Oil Zones (ROZs) has drawn significant attention due to the successful commercial CO2-EOR projects in ROZs. Residual oil Zone can be defined as interval of the reservoir rock that contain immobile oil with respect to the formation water at the level of residual oil saturation typically 40% and less (Sanguinito et al,2020). An ROZ can be categorized as brownfield if it occurs below the producing oil-water contact (OWC) of an associated primary pay zone (MPZ), or greenfield if it occurs without an MPZ. Because the oil saturation in ROZs may be at or near residual levels, ROZs have traditionally been considered commercially undesirable when compared to MPZs. However, as many large oil reservoirs reach depletion and carbon dioxide enhanced oil recovery (CO2-EOR) is implemented, ROZs may become attractive targets for increased oil recovery.CO2-EOR is increasingly used for oil production in areas with documented ROZs, primarily in the Permian Basin (Ren et al,2022) (Kuuskraa et al, 2020). Chen and Pawar (2019), characterized the effect of CO2 storage and EOR in ROZ using Monto Carlo simulations and sensitivity analysis on geological and operational parameters(Chen and Pawar, 2019). Ren and Duncan (2019) used reservoir simulation to investigate the hydrodynamic effects of water flow in aquifer at the base of oil zones and emphasis in the importance of these factors in assessing the EOR and storage capacity in ROZs. David and Ahmed (2022) introduced the use of dimensional analysis and pulser process for quantifying and discerning the production of the MPZ and ROZ due to CO2 flooding without the need of numerical simulations. Recently, machine learning techniques have grown in popularity for developing computationally quick proxy models, surrogate models, and predictive empirical models in subsurface modeling. Several machine learning algorithms have been widely used in prediction of reservoir production and performance assessment (Song et al, 2020), (He et al, 2016). Therefore, as ROZs have emerged as potential reservoirs for CCUS and there is lack of efficient tools for evaluating CO2 EOR performance coupled with CCUS in ROZs. In this paper we will use a 3D reservoir model to simulate the CO2 injection process. The reservoir properties referenced to one of potential ROZ in Permian basin (Goldsmith-Landreth San Andres Unit). The main objectives of this work are the following:

- Evaluate the CO2 injection as EOR and CCUS in ROZs in terms of Cumulative oil Production, Cumulative CO2 injection, Retained CO2 injection in each phase.
- Evaluate the Sensitivity of the uncertainty of the Reservoir Rock Properties (Net Pay Thickness, Permeability, Vertical to Horizontal Permeability Ratio, Porosity, Residual Oil Saturation to water flood, Residual Oil saturation flood, Formation water Salinity) and the Operational parameters including (Producer BHP and Gas injection Rate).

• Develop Proxy predictive model to predict the performance of CO2-EOR-CCUS using machine learning techniques to provide rapid screening and evaluation of the injection performance.

Theory and approach

Residual Oil Zones

A Residual Oil Zone (ROZ) refers to a section of reservoir rock holding immobile oil, with oil saturation levels typically below 40%. ROZs are formed by the movement of water within the reservoir due to natural or production-induced flow, water flooding with injection below the oil-water contact, or water imbibition into an oil-saturated formation caused by buoyant or hydrostatic forces. The upper limit of the ROZ is defined by the conventional oil-water contact, extending down-section from the highest oil saturation to near-zero levels. The upper part may include a transition zone (TZ) if there's an overlying conventional reservoir, but a ROZ can also exist independently. ROZs can be categorized into two primary groups: brownfields and Greenfields, as illustrated in Figure 1. Brownfield ROZs are located beneath a conventional reservoir's main pay zone (MPZ) or the subsurface interval where oil is traditionally extracted using conventional primary and/or enhanced recovery methods. On the other hand, greenfield ROZs are found in regions lacking an overlying conventional oil formation and are frequently identified as hydrodynamic fairways (Melzer, 2006).



Figure 1. Residual Oil Zone types (Greenfield and Brownfield) (Sanguinito et al, 2020)

Governing equations

The mass conservation equation, considering molecular diffusion, for each component i present in the oil, gas, and water phases can be expressed as follows:

$$\frac{\partial}{\partial t} \left(\phi \sum_{l=1}^{Np} \rho_l S_l m_{il} \right) + \nabla \left(\sum_{l=1}^{Np} \rho_l m_{il} v_l - \phi \rho_l S_l D_{il} \nabla m_{il} \right) - qi = 0, i = 1: Nc$$

$$\tag{1}$$

Where, t is the time, \emptyset is the porosity, ρ is the density, S is phase saturation, mi weight fraction for each component i, v is Dracy Velocity, Di is the coefficient of the molecular diffusion of component i in phase 1 and qi is the production mass rate or injection mass rate.

The Darcy's velocity is expressed in terms of Darcy's law:

$$v_l = -\frac{\kappa kr l}{\mu l} (\nabla P l - \rho_l g) \tag{2}$$

.

Where, K is the absolute permeability of the rock, krl is the relative permeability of phase l. Pl is the pressure of the phase 1, μl is the phase viscosity, ρl is the phase density.

The mass rate of production or injection can be expressed as

,

$$qi = \sum_{l=1}^{Np} \rho_l m_{il} P I_l (P_{well}^l - P_{block}^l)$$
(3)

Where Pwell is the wellbore pressure, P block is the grid pressure, PI is the productivity index.

The two-phase water-oil and liquid gas relative permeability are fitted using relative permeability tables. While the three-phase relative permeability is generated using one of the three relative permeability model as Stone's model II (Stone, 1970)

$$k_{ro} = (k_{rog} + k_{rg}) + (k_{row} + k_{rw}) - (k_{rw} + k_{rg})$$
(4)

The mass exchange between the oil and gas phases for each component is modeled using thermodynamic phase equilibrium conditions which is defined by equality of the fugacity of all components

$$f_g^i = f_o^i \tag{5}$$

CO2 Trapping Mechanism

This paper focuses on three main mechanisms of CO2 storage explicitly, solubility and residual trapping.

Solubility Trapping

Depending on the temperature of the reservoir, Minimum Miscibility Pressure (MMP), and the properties CO2 can either stay soluble or become miscible with the oil. The supercritical characteristics of CO2 play a crucial role in penetrating the oil surface, leading to swelling and a reduction in viscosity. In a study by Mosavat and Torabi (2014), they demonstrated how the solubility of CO2 varies with changes in temperature and pressure. Their findings indicated that solubility tends to increase with higher reservoir pressure and API gravity, while it decreases with a reduction in reservoir temperature (Mosavat and Torabi,2014). Also, the water can partition in the water phase, to model the CO2 solubility, in aqueous phase Henry's law is used.

$$f_i^{aq} = y_{iaq} * Hi \tag{6}$$

Where, f_i^{aq} is the fugacity of component i in aqueous phase, yiaq is the mole fraction of component i in aqueous phase and Hi is the Henry's constant of component i.

Henry's law constants are functions of temperature, pressure, and water salinity. They can be estimated using the molar volume at specific pressure and temperature, along with the known Henry's constant at a specific reference pressure and temperature, considering fixed salinity and temperature. However, this approach may not be applicable in thick reservoirs. Therefore, the use of Henry constant correlation provides more flexibility to handle such situations, such as the Harvey 1996 correlation, as shown in equations 7 and 8(Harvey, 1996).

$$\ln Hi^{s} = \ln P_{H20}^{s} + A(T_{rH20})^{-1} + B(1 - T_{rH20})^{0.335} (T_{rH20})^{-1} + C[\exp(1 - T_{rH20})](T_{rH20})^{-0.41}$$
(7)

Where, Hi^{s} is Henry's constant at saturation pressure P_{H20}^{s} , Tr is the reduced temperature. A, B,C are constants and for CO2 are -9.4234,4.0087 and 10.3199 respectively.

The Henry's law Constant at given P ad T is expressed as

$$\ln Hi = \ln Hi^{s} + \frac{1}{RT} \int_{P_{H_{20}}}^{P} v_{i}^{-} dP$$
(8)

The Solubility Trapping efficiency can be calculated using the following formula in equation 9,

Solubility Trapping index =
$$\frac{\text{Total dissolved mass of injected CO2 in brine}}{\text{Total injected CO2 mass}}$$
 (9)

Residual Trapping

Residual trapping is an important CO2 trapping mechanism. Hysteresis phenomena allow capillary pressures and relative permeabilities to vary between imbibition and drainage curves through scanning curves. Capillary pressure follows drainage curves for decreasing wetting-phase saturations and imbibition curves for increasing wetting-phase saturations. In the case of a reversal of saturation directions, capillary pressure follows along the scanning curves. Entrapment of the nonwetting phase occurs when it is bypassed by the wetting phase, thereby making it immobile. Several research has presented several correlations for the modeling of hysteresis. In this paper, the hysteresis in relative permeability is modeled based on land correlation(land,1968) equation 10-11.

$$S_{grh} = \frac{S_{gh} - S_{gic}}{1 + C(S_{gh} - S_{gic})} \tag{10}$$

$$C = \frac{1}{S_{grmax} - S_{gcrit}} - \frac{1}{S_{gmax} - S_{gcrit}}$$
(11)

Where Sgrh is Residual gas saturation of imbibition process, Sgh is Historical-maximum-attained gas saturation. Sgic Critical reversal saturation for trapping and Sgcrit is the critical gas saturation.



Figure 2. Imbibition and drainage curves used in hysteresis modelling effect (Ampomah et al,2016)

The Residual Trapping efficiency can be calculated using the following formula in equation 12,

$$Residual Trapping index = \frac{Total Trapped mass of injected CO2}{Total injected CO2 mass}$$
(12)

Reservoir Simulation Model setup

A three-dimensional reservoir model was constructed using CMG GEM to explore two main objectives: (1) assessing the performance of CO2 flooding for enhanced oil recovery (EOR), and (2) determining the amount of CO2 sequestered in the reservoir through Residual and solubility trapping. The reservoir model consists of 36 grids in the x-direction, 36 grids in the y-direction, and 10 grids in the z-direction, with horizontal grid sizes of 120 ft and 122 ft in the i and j directions. A five-spot pattern, depicted in Figure 3, is employed for evaluating CO2 injection for both EOR and carbon capture, utilization, and storage (CCUS). The initial oil saturation is assumed to be at a residual saturation of 0.4. Relative permeability curves, as shown in Figure 4, are referenced from the Goldsmith-Landreth San Andres Unit. Injectors and producers are assumed to be completed over the entire reservoir interval. CO2 injection occurs for a period of 10 years, concurrent with simultaneous production from producers over the same duration. The simulation is conducted for 100 years, encompassing a 90-year post-injection period. A maximum bottomhole pressure (BHP) constraint, set at the rock fracturing pressure of 4000 psi, is imposed on injectors. Reservoir rock properties, including porosity, permeability, thickness, Sor (residual oil

saturation), Sorg (initial oil saturation), formation water salinity, producer BHP, and CO2 injection rate, are considered as variables for sensitivity analysis, as outlined in Table 1.





Figure 4. Relative Permeability Curves (Oil-water (right), Gas-liquid(left))

Table 1. Summary of sensitivity variable for generation of the reservoir simulation dataset

Parameter	Lower Bound	Upper Bound
Porosity	0.05	0.3
Permeability,md	0.01	250
Kv/Kh	0.01	1
Salinity,ppm	50,000	250,000
Residual Oil saturation to water	0.2	0.4
Residual Oil saturation to gas	0.1	0.25
CO2 injection Rate, MMSCF/D	5	20
Producer BHP, Psia	250	1500
Net Pay Thickness, ft	50	350

Reservoir fluid composition is referenced to the ROZ composition in Residual Oil Zone, Seminole Field, Permian Basin in (Honarpour et al, 2010) study as shown in table 2.

Component	Composition (Mole %)
N2	0.04
CO2	0.02
H2S	0
C1	20.10
C2	9.07
C3	6.95
iC4	0.04
nC4	3.90
iC5	0.04
nC5	2.49
C6	2.69
C7+	54.66
MWC7+	261

Table 2. Reservoir Fluid composition

Minimum miscible pressure (MMP) Determination and Reservoir Fluid Characterization

The minimum miscible pressure (MMP) was calculated using UH_MMP Calculator (Sinha et al,2021) yielded MMP about 1500 psia which is lower than reservoir pressure of 2000 psia. The components of reservoir oil were lumped into 10 pseudo-components, and the parameters of the Peng-Robinson equation of state were fitted based on the experiment data from the constant composition expansion (CCE) test, the differential liberation (DL) test.

Workflow for generating the Dataset for Machine learning Model

After building the physics-based compositional reservoir simulation model, a large dataset needs to be generated to train the predictive model using machine learning. In this study, a numerical model was employed to generate an appropriate dataset covering all uncertainties in geological and reservoir properties. Nine parameters were investigated in this study. The sampling method for sensitivity analysis was established using the Latin Hypercube sampling method. This method involves dividing the cumulative density function (CDF) into equal segments and then choosing a random data point in each segment. By employing this sampling method, the optimum number of reservoir simulation runs is determined. After generating all possible cases, the reservoir simulation is run to produce results in terms of cumulative oil production, cumulative CO2 trapped in each phase due to residual trapping and solubility trapping. The outcomes of the reservoir simulation model are evaluated to ensure the quality of the results before passing them to the machine learning model. The machine learning model divides the dataset into training and testing/validation portions. The performance of the machine learning model is then evaluated using the root mean square error (RMSE) and the coefficient of determination (R^2).

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (actual \ y_i - predicted \ y_i)^2}$$
(13)

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (Actual \, yi - predicted \, yi)^{2}}{\sum_{i=1}^{n} (Actual \, yi - y \, mean)^{2}}$$
(14)



Figure 5. Workflow for Dataset generation

Results and Discussion

Base Case Reservoir Simulation Results

The Base Case Reservoir simulation model was run with geological and operational parameters summarized in table 3. CO2 is injected for 10 years with cumulative oil production about 32 MMSTB were recovered as shown in Figure 6. The Storage profile for residual, solubility trapping, and structural trapping is shown in Figure 7. The most of CO2 volume stored due to structural trapping and residual trapping due to hysteresis effect mentioned earlier. However, lower amount of CO2 dissolved in water due to high salinity of 200,000 ppm. Additionally, it is noticeable that the total CO2 in the supercritical phase decreases when CO2 breakthrough occurs in the producer well. This is evident in the cumulative CO2 production profile at the producer well.

|--|

Parameter	Value
Thickness, ft	200
Permeability, md	200
Porosity	0.25
Producer BHP, Psia	500
KV/KH	0.1
Salinity, ppm	200,000
Residual Oil saturation to water	0.4
Residual Oil saturation to gas	0.2
CO2 injection Rate, MMSCF/D	20



Cumulative Oil Production Vs Time

Figure 6. Cumulative Oil Production vs time for the base case

CO2 Stored vs Time



Figure 7. Cumulative CO2 Stored vs time for the base case

Machine Learning Model

Dataset Description

Reservoir Simulation Realization used as input for the Machine Learning Model in our study Artificial Neural Network (ANN). The Reservoir rock and fluid, and operational parameter range summarized in table 1 was used to generate several cases. The input for the ANN model were Net pay thickness, Horizontal Permeability, Ratio of Vertical to Horizontal Permeability, Porosity, Residual oil Saturation to water flood, Residual gas Saturation to gas flood, formation water salinity, Producer Bottom Hole Pressure, CO2 injection rate. These input parameters were used to generate different ANN models to predict the Cumulative Oil Produced, CO2 Dissolved in water, CO2 trapped due to residual hysteresis and CO2 trapped structurally.

Summary of Correlation coefficient of the dataset per input parameter

To assess the impact of each input on the output values, a correlation coefficient analysis was conducted, and the results are summarized in Figure 8. The analysis revealed that an increase in the vertical permeability/horizontal permeability ratio led to an increase in cumulative oil production while decreasing the amount of CO2 stored in the reservoir. This effect can be attributed to the enhanced sweep efficiency, facilitating the injected CO2 to reach and mobilize more oil, thereby increasing cumulative oil production. Conversely, an increase in kv/kh resulted in a rise in CO2 levels due to gravity, leading to a faster migration of CO2 toward the top of the reservoir. This, in turn, reduced the amount of CO2 trapped and stored in the reservoir.

Residual saturation for both water and gas flooding exhibited a small correlation with both cumulative oil production and CO2 storage. Increased horizontal permeability showed a positive correlation with cumulative oil production, while decreasing structural trapping. Porosity increases demonstrated a positive correlation with both cumulative oil production and CO2 storage. The producer bottom hole pressure showed a negative correlation with cumulative oil production and a positive correlation with CO2 storage.

Furthermore, the CO2 injection rate exhibited a positive correlation with both CO2 injection and cumulative oil production. Salinity displayed a negative correlation with CO2 dissolved in water, as expected. As salinity increases, it decreases the storage capacity of CO2 solubility in water



Figure 8. Correlation Coefficient Analysis between input parameters vs the Cumulative oil production and CO2 Storage

ANN Models Configuration

In this study, an Artificial Neural Network (ANN) model was constructed to predict the Cumulative Oil Production in a reservoir based on a set of selected input parameters. The model architecture consists of multiple dense layers with rectified linear unit (ReLU) activation functions, allowing the network to capture complex relationships within the data. The input features were initially standardized using Min-Max scaling to ensure consistent input ranges for improved model convergence. To further enhance the model's ability to capture essential patterns within the data, Principal Component Analysis (PCA) was applied to reduce the dimensionality of the input space. The resulting principal components were then utilized as input features for the ANN.

This dimensionality reduction not only streamlined the computational complexity but also facilitated the identification of key features influencing the output of Cumulative Oil Production and CO2 Storage. The model was trained using the Mean Squared Error (MSE) loss function and the Adam optimizer with a learning rate of 0.1. The training process was monitored by early stopping criteria, preventing overfitting, and ensuring the model's generalization performance. The training history showed the convergence of the training and validation losses over the epochs. The early stopping mechanism prevented the model from continuing training once the validation loss reached a plateau, ensuring optimal model performance. The summary of the model's configuration is shown in Table 4.

Model	Number of Hidden Layers	Number of Neurons
Cumulative Oil Production	5	128
CO2 Dissolved in Water	5	64
CO2 Trapped (Structural)	3	15
CO2 Residual Trapping	3	10

Table 4. Summary of Developed ANN Models

Developed Models Performance Evaluation

The performance of the developed ANN models was assessed using coefficient of determination (R2) and Mean absolute Percentage Relative error (MAPRE) as well as the Mean squared error during the training and testing process. The Cumulative Oil Production model achieved an outstanding R2 value of 0.98, demonstrating its ability to accurately predict oil production trends. Similarly, the CO2 Dissolved in Water model achieved an R2 of 0.93, indicating its effectiveness in capturing dissolved CO2 dynamics. The CO2 Trapped (Structural) and CO2 Residual Trapping models demonstrated high predictive power with R2 values of 0.9 and 0.96, respectively. All the Models showed MAPRE less than 10%. Cross plots of the testing capability of the developed Models are shown in Figure 9.





Figure 9. Cross Plots of the Performance of Developed ANN Models (a: Cumulative oil Production, b: CO2 dissolved in Water, c: CO2 trapped Structurally, d: CO2 residual Trapping)

Summary and Conclusions

In summary, this study focused on constructing a three-dimensional reservoir model using CMG GEM to assess the performance of CO2 flooding for enhanced oil recovery (EOR) and determine the amount of CO2 sequestered through residual, solubility, and Structural trapping in ROZs. A comprehensive sensitivity analysis was conducted using a physics-based compositional reservoir simulation model, considering various reservoir rock properties and operational parameters. The dataset generated from the reservoir simulation was used to train an Artificial Neural Network (ANN) model, aiming to predict cumulative oil production, CO2 dissolved in water, and CO2 trapped structurally and due to residual hysteresis.

The sensitivity analysis revealed key correlations between input parameters and output variables. For instance, an increase in the vertical permeability/horizontal permeability ratio enhanced cumulative oil production but decreased CO2 storage. Horizontal permeability, porosity, and CO2 injection rate displayed positive correlations with both cumulative oil production and CO2 storage, while producer bottom hole pressure exhibited a negative correlation with oil production but a positive correlation with CO2 storage. The developed ANN models demonstrated high predictive accuracy, with R2 values ranging from 0.9 to 0.98, indicating their effectiveness in capturing complex relationships within the data. Additionally, the Mean Absolute Percentage Relative Error (MAPRE) for all models was less than 10%, confirming their reliability. Cross plots illustrated the models' ability to predict testing data accurately. In conclusion, the integrated approach of combining reservoir simulation and machine learning, particularly the ANN model, proved successful in predicting reservoir behavior under CO2 flooding scenarios. The established correlations between input parameters and output variables provide valuable insights for optimizing EOR and carbon capture, utilization, and storage (CCUS) strategies. This study contributes to advancing the understanding of CO2 flooding dynamics and offers a robust methodology for reservoir management and decision-making in the context of CO2 EOR and CCUS.

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