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CO_2 injection-based enhanced methane recovery from carbonate gas reservoirs via deep learning

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ABSTRACT

CO_2 injection is a promising technology for enhancing gas recovery (CO_2-EGR) that concomitantly reduces carbon emissions and aids the energy transition, although it has not yet been applied commercially at the field scale. We develop an innovative workflow using raw data to provide an effective approach in evaluating CH_4 recovery during CO_2-EGR. A well-calibrated three-dimensional geological model is generated and validated using actual field data—achieving a robust alignment between history and simulation. We visualize the spread of the CO_2 plume and quantitatively evaluate the dynamic productivity to the single gas well. We use three deep learning algorithms to predict the time histories of CO_2 rate and CH_4 recovery and provide feedback on production wells across various injection systems. The results indicate that CO_2 injection can enhance CH_4 recovery in water-bearing gas reservoirs—CH_4 recovery increases with injection rate escalating. Specifically, the increased injection rate diminishes CO_2 breakthrough time while concurrently expanding the swept area. The increased injection rate reduces CO_2 breakthrough time and increases the swept area. Deep learning algorithms exhibit superior predictive performance, with the gated recurrent unit model being the most reliable and fastest among the three algorithms, particularly when accommodating injection and production time series, as evidenced by its smallest values for evaluation metrics. This study provides an efficient method for predicting the dynamic productivity before and after CO_2 injection, which exhibits a speedup that is 3–4 orders of magnitudes higher than traditional numerical simulation. Such models show promise in advancing the practical application of CO_2-EGR technology in gas reservoir development.

I. INTRODUCTION

The increasing urgency to mitigate greenhouse gas emissions, particularly carbon dioxide (CO_2), from the combustion of fossil fuels, and to combat global warming underscores the critical need for innovative solutions.[20,31,35] Carbon capture, utilization, and storage (CCUS), including CO_2-enhanced gas recovery (CO_2-EGR), CO_2-enhaced oil recovery (CO_2-EOR), and CO_2-enhanced deep brine recovery (CO_2-EWR), are all promising strategies to achieve net-zero emissions by 2050.[1,21,22,42] As one of the promising CCUS options, CO_2-EGR can reduce CO_2 emission by sequestering it into gas reservoirs and simultaneously enhancing CH_4 production.[32,42] Despite its potential, the commercialization and field-scale application of CO_2-EGR technologies have not yet been widely implemented.[25,60] Advanced evaluation and prediction of well performance during CO_2 injection based on the specific characteristics of the targeted gas reservoirs are crucial in facilitating the implementation of such techniques and leveraging their full potential in carbon mitigation efforts.

Various studies have identified key parameters affecting the performance of CO_2 storage and CH_4 production for CO_2-EGR.[6,65] Critical parameters include reservoir characteristics, including permeability, porosity, thickness, depth, initial reservoir pressure, and *in situ* gas and water volume, together with operational conditions such as injection and production pressures.[44,48] A notable impediment to CH_4 recovery is the ascending gas–water interface during CH_4 production, which increases gas phase flow resistance and heterogeneity of saturation.[41] Reservoir heterogeneity plays a crucial role in CO_2-EGR efficiency as it can reduce the size of the region swept by CO_2 and leads to early breakthrough of CO_2.[45,63] This identifies a gap in optimizing the interplay between injection parameters and formation heterogeneity. The behavior of CH_4, CO_2, and water in the reservoir, particularly under CO_2 injection remains ambiguous.

Extensive research has been conducted on CO_2-EGR at the lab scale, focusing on understanding CO_2–CH_4–H_2O interactions, refining petrophysical mechanisms, and assessing the impact of reservoir heterogeneity and rock–fluid interactions.[19,30,47] Recent investigations exploring the behavior of H_2O–CH_4–CO_2 mixtures in porous media have considered more petrophysical mechanisms, such as advection, dispersion, and diffusion.[5] However, a large gap between theoretical studies and practical application still exists. Thus, there is a need for effective methodologies to evaluate gas production behavior and to define optimal operational conditions that maximize gas production and CO_2 sequestration.

A comprehensive multi-field-coupled process-based modeling approach is necessary to address the complex phenomena that control such systems. While attempts to simulate and predict the variations in key parameters influencing reservoir development, including using history matching, have been explored,[29,40,55] the inherent complexity of CO_2-EGR as a coupled multi-scale transport process characterized by nonlinear relationships presents challenges to numerical simulators in accurately modeling gas production dynamics during CO_2 injection and displacement.[7] Laboratory experiments and simulations often fall short of fully replicating the subsurface conditions of the reservoir, generally relying on idealized models.[15,16,33] However, the development of data-driven artificial intelligence (AI) technologies offers promising avenues in navigating these complexed reservoir conditions, especially in applications of CO_2-enhanced oil recovery (CO_2-EOR).[3,66,67] Machine learning (ML) and deep learning (DL) algorithms offer unique advantages for analyzing complex reservoir datasets and predicting reservoir performance.[36,37] ML algorithms, such as support vector machines (SVM), random forests, and gradient boosting machines, can analyze vast amounts of reservoir data to identify patterns and relationships that may not be apparent through traditional analysis methods.[46] By learning from historical reservoir data, ML models can make accurate predictions about future reservoir behavior and optimize gas injection strategies to maximize recovery.[46,62] DL, a subset of ML, has emerged as a powerful tool for analyzing large and complex datasets in various domains.[56,57] DL algorithms, such as convolutional neural networks (CNN) and recurrent neural networks (RNN), are capable of learning intricate features from raw data and performing sophisticated tasks.[15,18] DL algorithms can analyze seismic data, well logs, and gas well productivity to identify subtle patterns and anomalies indicative of reservoir properties and performance.[4,11,43] Thus, the capacity of deep learning (DL) algorithms to predict fluid displacement effects from the perspective of CO_2 injection into gas reservoirs, is a promising field for further investigation.

In this study, we introduce a methodology that merges numerical simulation and DL methods to predict CH_4 production behavior and evaluate CH_4 recovery potential. This is completed for CO_2-EGR in carbonate gas reservoirs of the Longwangmiao formation in the Sichuan Basin. We first construct an accurate three-dimensional geological model based on actual field parameters. This is then calibrated and validated, demonstrating a robust match between historical and simulated production data over 7 years. Then, we simulate CO_2 injection processes at the gas–water interface after depletion and analyze the production rates of CH_4, CO_2, and H_2O under diverse injection conditions. Furthermore, to forecast CH_4 and CO_2 production rates under various CO_2 injection scenarios, DL models are developed by training on multiple datasets derived from numerical simulations within this high-fidelity geological model. The prediction capability of three deep learning models, including temporal convolutional network (TCN), long short-term memory (LSTM), and gated recurrent unit (GRU) models, are evaluated in this study. The innovative approach of integrating conventional numerical simulation with DL techniques is poised to offer rapid, precise, and extensive quantitative insights in applications of CO_2-EGR in gas reservoirs. This facilitates the real-time optimization of injection–production strategies across different reservoir conditions and operational conditions, enhancing workflow efficiency and speeding up CO_2-EGR evaluation in real time and in support of field-scale operations.

II. MODELING

A. Gas reservoir characteristics

The overall recovery of CH_4 from water-bearing gas reservoirs is generally low due to the rising gas–water interface. This phenomenon leads to the formation water occluding the pore structure, thereby impeding CH_4 production as water saturations increase.[59] We use the Cambrian Longwangmiao formation gas reservoir in the Sichuan Basin, China, as a type example. This reservoir is primarily composed of carbonates, with complex geological structure, including dissolved open-pores and natural fractures.[27] The reservoir is strongly heterogeneous with permeability in the range ∼0.01–100 mD and porosity in the range ∼0.1%–10%.[58] Such conditions provide favorable conditions for formation water channeling and the blocking of the flow of CH_4. This issue is further exacerbated by the presence of bottom water—with a critical need to resolve such issues.[61]

B. Model description

We assembled an accurate geological model for this reservoir by combining the observed conditions within the area surrounding the well (Table I). The reservoir simulation model comprises $150 \times 150 \times 19$ grid blocks, with each block 100 m in the x and y directions and divided into 19 stacked horizontal layers. The reservoir fluids comprise three components: CO_2, CH_4, and H_2O. The reservoir temperature is 137 °C with a reference pressure gradient anchored at a reference depth of 4370 m with a reference pressure of 66 MPa. Reservoir thickness is 201 m, with an initial gas–water interface height of 4375 m. The original geological reserves are 1.06×10^{10} m^3, and the average gas saturation is 37.62%. We use a dual-porosity, dual-permeability model to represent fracture and matrix characteristics based on well logging data. The average porosity and permeability of the matrix are 2.1% and 2.34 mD and for the fractures are 6.8% and 25 mD. Average tortuosity is recovered from core observations as 1.52 with a diffusion coefficient of 2.0×10^{-6} m^2/s.

C. Simulation and history matching

We use CH_4 and H_2O production data from well-1 as daily histories of gas and water production, bottom hole pressure and production

TABLE I. Model parameters representing the reservoir.

Parameter	Value
Grid	150 × 150 × 19
Average pressure (MPa)	66.14
Reservoir depth range (m)	4315–4516
Average matrix porosity (%)	2.1
Average fracture porosity (%)	6.8
Average matrix permeability (mD)	2.34
Average fracture permeability (mD)	25
Rock compressibility (1/MPa)	1.62×10^{-9}
Water–gas contact elevation (m)	4375
Average gas saturation (%)	37.62
Temperature (°C)	137
Diffusion coefficient (m^2/s)	2.0×10^{-6}
Tortuosity	1.52
Fraction of CO_2/CH_4 (injected well)	1.0/0.0
Original gas in place, OGIP (m^3)	1.06×10^{10}
Original water in place, OWIP (m_3)	3.58×10^7

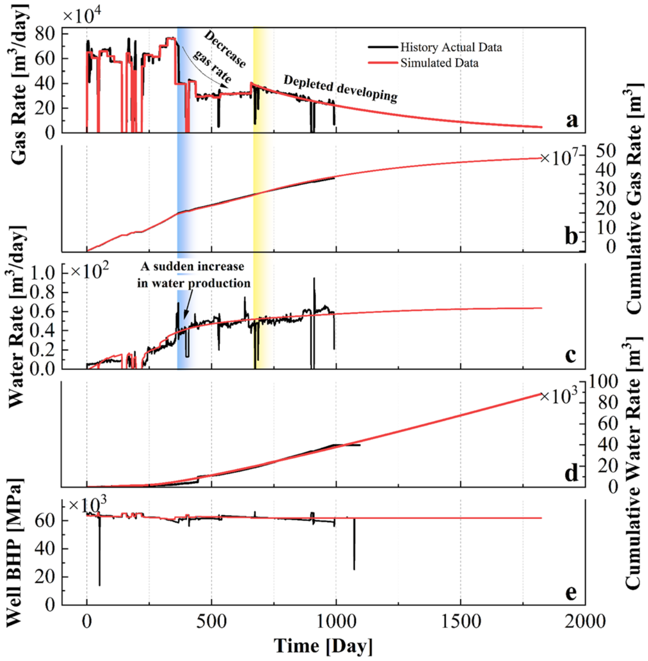

FIG. 1. Actual production data and historical fitting results of well-1 in the Longwangmiao formation gas reservoir: (a) daily gas rate, (b) cumulative gas rate, (c) daily water rate, (d) cumulative water rate, and (e) well bottomhole pressure. For a more intuitive comparison and analysis, the time-axis is consistent across all five subplots. The fitting results are excellent, indicating that well-1 initially adopts constant-rate production then switches to constant-pressure production (depleted development) after approximately 700 days due to an increase in water rate.

system to history match production by adjusting the relative permeability and capillary pressure curves. We achieve a good fit, as shown in Fig. 1. Based on the actual production from well-1, we observe that the presence of formation water significantly impacts the production of CH_4. After approximately 300 days of production, water production suddenly increases, accompanied by a decrease in gas production. According to our predictive results, if we do not implement measures to increase the recovery efficiency of the gas reservoir in time, the gas well will face abandonment under depleting development.

D. CO_2 injection

Injecting CO_2 into water-bearing gas reservoirs can improve production of CH_4 as demonstrated and supported by laboratory experiments.[24] Mechanisms contributing to CO_2-EGR include the following:

1. Replenishing reservoir energy: Injecting CO_2 increases pore fluid pressures and gradients and thereby enhances gas flow.[21,38,39]
2. Displacement and diffusion: Competitive adsorption between CO_2 and CH_4 on mineral surfaces such as clay, calcite, and quartz aid fluid displacement.[8,9,14,34] Injected CO_2 present on rock surfaces and diffusion of CO_2 in matrix pores effectively spreads out and increases the CO_2-swept area.[13,23]
3. Gravity differentiation: Under reservoir conditions, CO_2 is supercritical.[12] This state favors plug or piston flow over mixing with CH_4, thereby improving fluid displacement efficiency.[10] A barrier also forms between the water and gas phases, slowing the intrusion of formation water.[41,53]
4. Porosity and permeability enhancement: CO_2 reacts with formation water to generate carbonic and other acids, etching the pore space and increasing permeability and porosity.[54] This enhances reservoir connectivity and, thereby, gas flow.[2]
5. Reducing capillary pressure: The dissolution of CO_2 into formation water reduces the interfacial tension at the gas–water–solid interface by lowering the density of the formation water.[50,51] This process effectively alleviates the blockage of flow channels characterized by high capillary pressures, resulting in a reduction of flow resistance.[52]

Given these many interacting processes, the challenges of implementing this technique at field scale requires accurate prediction and evaluation of the effects of CO_2 injection. We use a model for CO_2 injection at a second well (well-2) that is strategically positioned 2200 m away from well-1 during the depleted production stage. CO_2 is injected into the reservoir at six different injection rates: 5.5, 6.5, 7.0, 7.5, 8.0, and 8.5×10^5 m^3/day, each with a CO_2 mole fraction of 100%.

E. Characteristics of CO_2 injection into gas reservoirs

From the simulation results, it is evident that CO_2 injection can effectively enhance CH_4 production. CH_4 production rates are shown after 100 days at injection rates of 0, 5.5, 6.5, 7.0, 7.5, 8.0, and 8.5 $\times 10^5$ m^3/day and are 1.899, 2.681, 2.821, 2.891, 2.961, 3.031, and 3.121×10^5 m^3/day, respectively, as shown in Fig. 2. More importantly, there is a significant increase in CH_4 recovery. Compared to continuing depletion of the reservoir without CO_2-EGR, CH_4 recovery rates increase by 1.61%, 1.85%, 1.97%, 2.08%, 2.19%, and 2.29% at the respective injection rates. The breakthrough time for CO_2 in well-1 also decreases (earlier) with increasing injection rates, as 594, 524, 436,

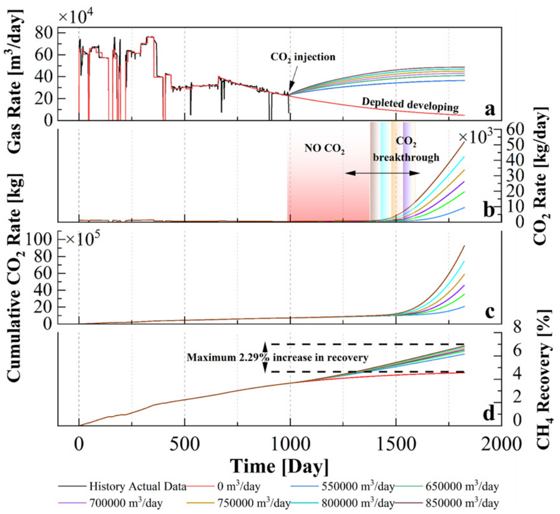

FIG. 2. Full-cycle dynamic productivity of well-1 at different CO_2 injection rates: (a) daily gas rate, (b) daily CO_2 rate, (c) cumulative CO_2 rate, and (d) CH_4 recovery rate. For more intuitive comparison and analysis, the time-axis is consistent across all four subplots. Well-2 is injected with CO_2 into the gas reservoir at rates of 5.5, 6.5, 7.0, 7.5, 8.0, and 8.5 $\times$ 10^5 m^3/day, respectively. Compared to depleted development, the productivity of Well-1 shows a significant increase in CH_4 production after CO_2 injection, with production increasing with the injection rate.

378, 311, and 292 days, respectively. Therefore, higher injection rates contribute to improved gas recovery efficiency. Figure 3 illustrates that injection velocity is directly proportional to the spread of the CO_2 plume.

III. DEEP LEARNING METHODS AND ALGORITHM

The subsurface displacement of CH_4 via CO_2 injection engenders complex physical processes, which are challenging for the current numerical simulation methods. While these methods can represent the underlying processes, they are often hampered by high computational demands. In response to these challenges, we explore the application of deep learning algorithms to replicate the complex physical processes associated with CO_2 injection into carbonate gas reservoirs.[3,64,67,68] We use three neural network models, LSTM, TCN, and GRU, to train the simulation results obtained in Sec. III to predict the CH_4 production rates in scenarios that were not directly modeled, thereby enhancing the predictive capability beyond the limitations of traditional numerical simulation.

A. LSTM

Long short-term memory (LSTM) is a type of recurrent neural network (RNN) designed to overcome the vanishing gradient problem in traditional RNNs, enabling the model to capture long-range dependencies in sequential data. It has memory cells with self-connections that allow them to maintain information over long sequences. The key

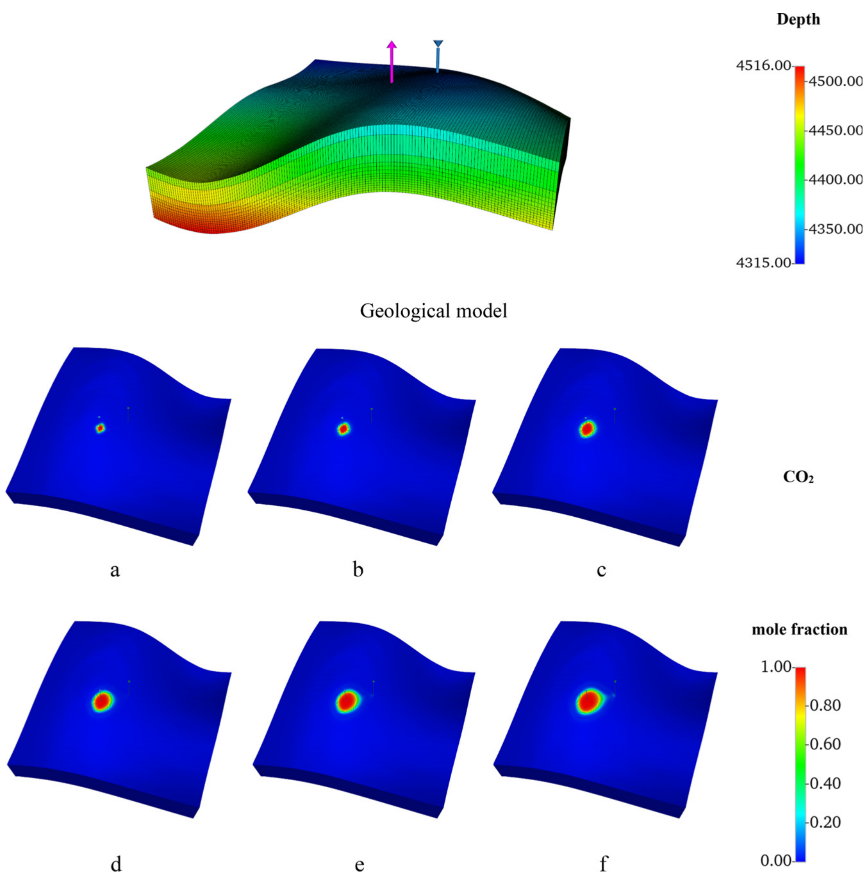

FIG. 3. Two wells in the geologic model. Production well-1 in red and injection well-2 in blue. Spread of the CO_2 plume after 200d for injection at rates of: (a) 5.5, (b) 6.5, (c) 7.0, (d) 7.5, (e) 8.0, and (f) 8.5 $\times$ 10^5 m^3/day, respectively.

components of an LSTM cell include a cell state, an input gate, a forget gate, and an output gate.[15,26]

The LSTM architecture and equations allow the model to selectively update and retrieve information from the cell state, facilitating the learning of long-term dependencies in sequential data.[49] In the provided problem of predicting gas well production over time, LSTM is suitable for capturing dependencies in sequential data. Gas production may be influenced by historical injection rates, and LSTM can learn to capture these long-term dependencies, making it effective for time series prediction.

B. GRU

Gated recurrent unit (GRU) models are another type of recurrent neural network like LSTM but with a simpler structure. They combine the memory cell and hidden state into a single state, making it computationally more efficient. GRU has reset and update gates that control information flow.[18,43]

The GRU architecture consists of specialized gating mechanisms that control the flow of information through the network. It has two gates: the reset gate and the update gate. The reset gate decides how much past information to forget, and the update gate decides how much of the new information to store.[37]

GRU models have fewer parameters compared to traditional LSTMs, making them computationally more efficient. GRUs are effective when dealing with shorter sequences where preserving long-term dependencies is less critical. GRU models have proven effective in various sequence-related tasks, including natural language processing, time series prediction, and speech recognition.[56]

For the gas well production problem, GRU can be effective in learning dependencies in the input sequence. Its simplified structure makes it computationally less expensive compared to LSTM, but it can still capture the temporal dynamics of gas production in response to varying injection rates.

C. TCN

Temporal convolutional network (TCN) models are convolutional neural networks designed for sequence modeling tasks. They use dilated convolutions to increase the receptive field exponentially without increasing the number of parameters. This allows TCN to efficiently capture long-range dependencies.[36]

TCN uses dilated causal convolutions, which operate on a sequence in a way that respects the temporal order. The dilation rate controls how far apart the elements of the convolutional kernel are. TCN often includes multiple stacked blocks, each containing dilated causal convolutions followed by activation functions like ReLU.[37]

These convolutions allow TCN to capture long-range dependencies effectively. Multiple blocks are stacked to increase the receptive field and improve the ability of the model to capture complex patterns. The outputs from different blocks are summed to produce the final output sequence. The architecture and operations of TCNs make them well-suited for sequence modeling tasks and they have demonstrated success in various applications, including time series prediction.[46]

In the context of predicting gas well production, TCNs can effectively capture the temporal patterns and dependencies in the input data. The varying injection rates and their impact on gas production can be learned by the dilated convolutions of TCNs, making them suitable for time series forecasting.

D. Hyperparameters

The hyperparameters used in the deep learning algorithms play critical roles in training the model effectively.[17,28] The model efficiently processes training data with an optimal batch size and iterations by balancing computational resources repeatedly. Employing a single dense layer with ReLU activation ensures simplicity and nonlinearity, essential for capturing complex patterns. A dropout rate of 0.01 mitigates overfitting by randomly dropping out input units during training. The Adam optimizer dynamically adjusts learning rates based on recent gradients, optimizing model performance. Meanwhile, the choice of mean squared error as the loss function accurately quantifies prediction accuracy. These hyperparameters were thoughtfully selected after repeated attempts to ensure the deep learning model effectively predicts gas reservoir performance during CO_2 injection. The hyperparameters of the model selected in this study are presented in Table II.

IV. MODEL PERFORMANCE AND PREDICTION

A. Dataset and evaluation metrics

We predict the three parameters of gas rate, CO_2 rate, and CH_4 recovery separately. Each parameter is related to time, production pressure difference, injection rate, and other production conditions. The training set consists of numerical outputs at injection rates of 5.5, 6.5, 7.0, and 8.5×10^5 m^3/day. The validation set includes data at an injection rate of 8.0×10^5 m^3/day, while the prediction set involves data at an injection rate of 7.5×10^5 m^3/day. We utilize three deep learning algorithms to learn the relationship between the feature parameters and production conditions in the training set, enabling us to predict well feedback under unknown production conditions.

LSTM is effective when there are long-term dependencies in the gas well production data and can learn to remember injection rate patterns over extended periods. TCN is suitable for capturing temporal patterns and dependencies efficiently, making it effective for modeling the complex relationships between injection rates and gas production over time. GRU, being computationally efficient, is suitable when a

TABLE II. Hyperparameter settings of each model.

Deep learning algorithm	Hyperparameters
LSTM	Batch size = 32, Iteration = 1500, Dense = 1, Activation = relu, Dropout rate = 0.01, Optimizer name = adam, Loss function name = MSE,
TCN	Batch size = 32, Iteration = 1500, Dense = 1, Activation = relu, Kernel size = 2, Optimizer name = adam, Loss function name = MSE,
GRU	Batch size = 32, Iteration = 1500, Dense = 1, Activation = relu, Dropout rate = 0.01, Optimizer name = adam, Loss function name = MSE,

balance between model complexity and computational resources is desired and it can still capture temporal dependencies in the input data.[4] Each algorithm addresses the gas well production prediction problem differently, offering various trade-offs in terms of model complexity and computational efficiency. The choice among them depends on factors such as the nature of the data, the desired model interpretability, and available computational resources. Root mean square error (*RMSE*), mean absolute error (*MAE*), and *R*-squared errors (R^2) are selected to describe the performance of the deep learning model in predicting the effect of CO_2 injection to enhance gas recovery.[17] *RMSE* measures the average magnitude of the errors between the predicted and actual values, giving greater weight to larger errors due to squaring. *MAE* computes the average absolute differences between the predicted and actual values, providing a straightforward measure of prediction accuracy.

B. Model performance

The evaluation of model efficacy relies on how well the predictive model aligns with the validation data. Consequently, the alignment of the predictive model enables the extraction of dataset patterns and relationships during training. Figure 4 depicts the predictive outcomes derived from the validation dataset of each model. As illustrated in Fig. 4, the predictive outcomes of all models correspond to the general trend of the actual values. Figure 5 demonstrates that both ends of the 100% agreement line perfectly accommodate the predictive and actual values of all models. Moreover, the quantitative assessment of model predictions is conducted (as shown in Table III). This suggests that the GRU model is adept at capturing the overall data trend and is less likely to yield extreme predictive outcomes. The predictive results of the validation set indicate that all models can effectively grasp the fundamental dataset patterns and relationships. These models exhibit a high level of adaptability to validation datasets. Furthermore, in comparison to LSTM and TCN models, the GRU model demonstrates superior predictive performance for the dataset.

C. Model prediction

Once the model undergoes training, forecasting responses for an independent test set offers a more accurate assessment of the model's performance on novel and unobserved data. Figure 6 illustrates the predicted efficacy of all models on the test set. The predicted outcomes of all models on the test sets resemble those on the training sets, with the actual and predicted values following the same trajectory (refer to Fig. 6). However, there exists a discrepancy between the projected outcomes of all models and the actual values. The disparity between the TCN model and the actual values is the most substantial.

Figure 7 displays the optimization results of three algorithms for subterranean fluid displacement via CO_2 injection. The x-axis depicts the predicted data, while the y-axis represents the simulated data. The GRU model continues to exhibit strong performance on the test set (as shown in Table IV). In addition to the alignment of the actual and predicted values at both extremities of the 100% agreement line, all evaluation metrics identify it as the most precise prediction model. Elevated R^2 values signify the GRU model's ability to elucidate a significant portion of the dataset's variability. This underscores the model's heightened accuracy and reliability in predicting the methane production rate from the gas reservoir under CO_2 injection-induced displacement—thus, rendering it the optimal model for precisely forecasting gas flow rates via CO_2 displacement.

D. Advantages of deep learning

The forecasting outcomes presented in Secs. IV B and IV C demonstrate that the three models effectively anticipate the synthetic dataset of fluid displacement driven by CO_2. Nonetheless, the precision of the predictive outcomes varies among LSTM, TCN, and GRU.

(1) The prognostications of the GRU model within the training and testing sets exhibit relative stability, yielding superior predictive efficacy. This is primarily attributed to the resilience of the model to noisy data. The GRU model adeptly filters out noise via specialized gating mechanisms, whereas the LSTM and TCN models might excessively conform to noise within the input sequence. This distinction is reflected in the heightened R^2 value of the GRU model.

(2) The GRU model demonstrates notable potential in optimizing fits. Both the training and test sets' R^2 values of the LSTM algorithm exceed 0.99, indicating commendable predictive performance. However, the GRU model achieves high and accurate

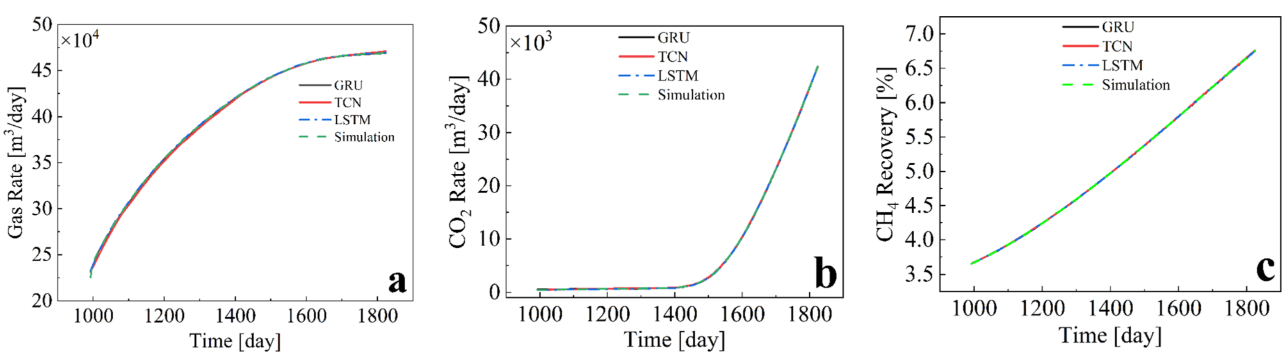

FIG. 4. Predicted results of the deep learning model on the validation set: (a) predicted daily gas rate at an injection rate of 8.0×10^5 m^3/day, (b) predicted daily CO_2 rate, and (c) predicted CH_4 recovery. Each model is trained on feedback data from well-1 at injection rates of 5.5, 6.5, 7.0, and 8.5×10^5 m^3/day. The validation set consists of feedback data from well-1 at an injection rate of 8.0×10^5 m^3/day.

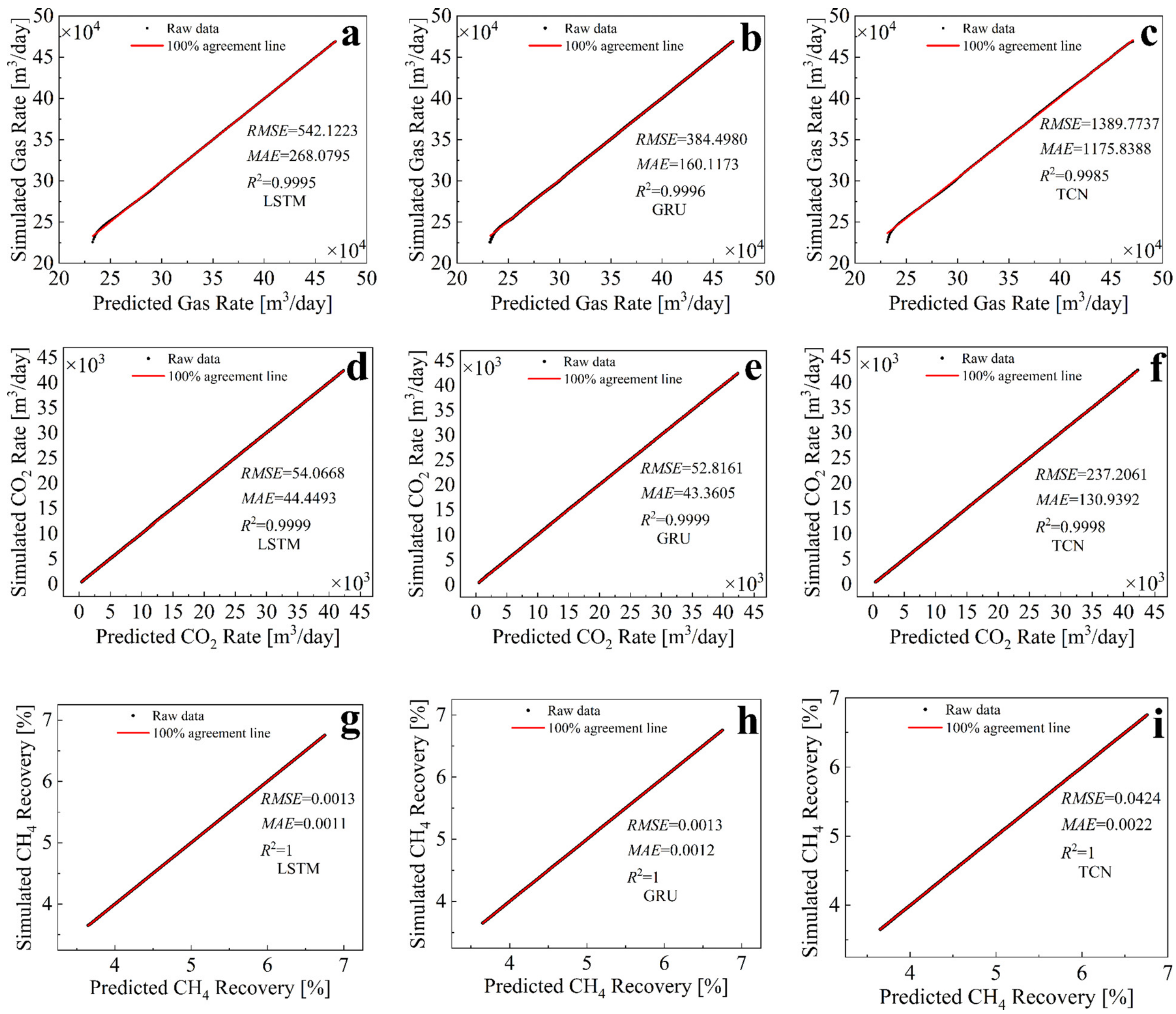

FIG. 5. Evaluation index for the validation set. We evaluated the predicted gas rate, CO_2 rate, and CH_4 recovery under the CO_2 injection rate of 8.0×10^5 m^3/day using three metrics: *RMSE*, *MAE*, and R^2. Smaller values of these metrics indicate closer proximity between the predicted and raw values, reflecting better algorithm performance (more details in Table III).

TABLE III. Evaluation results for the validation set.

Metrics	Prediction variables	LSTM	GRU	TCN
RMSE	Gas rate	542.1223	384.4980	1389.7737
	CO_2 rate	54.0668	52.8161	237.2061
	CH_4 recovery	0.0013	0.0013	0.0424
MAE	Gas rate	268.0795	160.1173	1175.8388
	CO_2 rate	44.4493	43.3606	130.9392
	CH_4 recovery	0.0011	0.0012	0.0022
R^2	Gas rate	0.9995	0.9996	0.9985
	CO_2 rate	0.9999	0.9999	0.9998
	CH_4 recovery	1	1	1

predictive outcomes in merely 100 epochs, compared to the LSTM model's requirement of 2000 epochs. This discrepancy primarily stems from the GRU model's ability to selectively retain crucial information from previous sequence steps, whereas the LSTM model operates fundamentally sequentially, constraining its scalability and computational efficiency. Consequently, the GRU model boasts superior computational efficiency.

(3) With regard to a small dataset, the GRU model more effectively assimilates sequence features from the data than the LSTM and TCN models, thereby enhancing prediction accuracy and generalizability. Precise prediction of this limited sample data holds significant implications, offering reliable forecasts of gas flow rates and furnishing valuable insights into key process

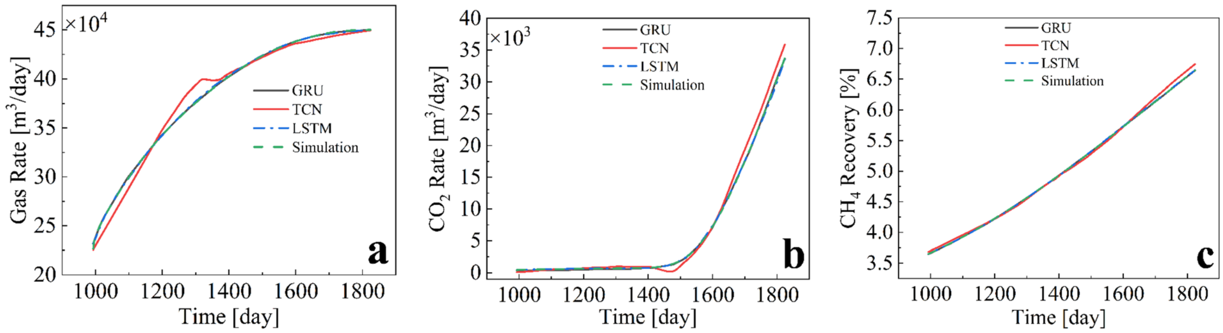

FIG. 6. Predicted results of the deep learning model on the test dataset. (a) Predicted daily gas rate at an injection rate of 7.5×10^5 m^3/day, (b) predicted daily CO_2 rate, and (c) predicted CH_4 recovery.

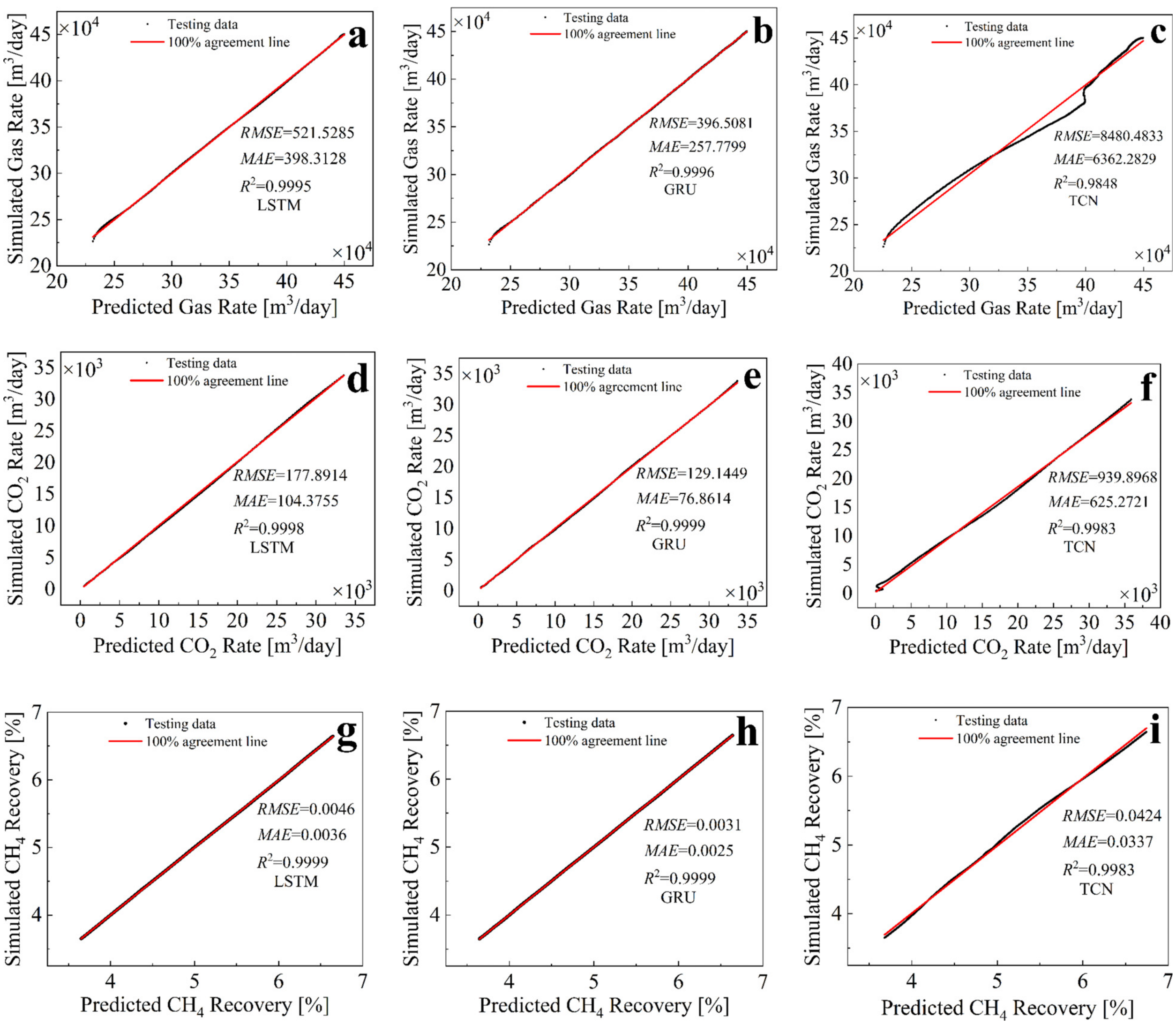

FIG. 7. Evaluation index for the testing set. We evaluated the predicted gas rate, CO_2 rate, and CH_4 recovery under the test set using three metrics: *RMSE, MAE*, and R^2. Smaller values of these metrics indicate closer proximity between the predicted and raw values (more details in Table IV).

TABLE IV. Evaluation results for the testing set.

Metrices	Prediction variables	LSTM	GRU	TCN
	Gas rate	521.5285	396.5081	8480.4833
RMSE	CO_2 rate	177.8914	129.1449	939.8968
	CH_4 recovery	0.0046	0.0031	0.0424
	Gas rate	398.3128	257.7799	6362.2829
MAE	CO_2 rate	104.3755	76.8614	625.2721
	CH_4 recovery	0.0036	0.0025	0.0377
	Gas rate	0.9995	0.9996	0.9848
R^2	CO_2 rate	0.9998	0.9999	0.9983
	CH_4 recovery	0.9999	0.9999	0.9983

interactions, as well as predictions concerning gas recovery, gas pressure, and CO_2 fraction within gas reservoirs. Such insights carry substantial practical significance.

(4) To sum up, the test results underscore GRU's prowess in handling nonlinear dynamic relationships and capturing long-term dependencies within irregular sequences more effectively. This achievement is facilitated through its information flow selection network, which proficiently discerns patterns across varied time scales.

V. DISCUSSIONS

A. Optimization of deep learning in the prediction workflow

Deep learning models are capable of handling complex nonlinear relationships, without requiring the comprehension of complex theoretical equations and ideal assumptions about field properties. They can adapt to different data and applications and help optimize CO_2 injection for CH_4 recovery process in ways that traditional mathematical models cannot—this reflects significant potential for their application. Gas that is difficult to desorb at normal pressure can be discharged using underground CO_2 injection, benefiting from its displacement. The accurate prediction of CH_4 flow rate facilitates the optimization of the CO_2 injection process and reasonable use of the "gas injection start-stop" opportunity to maximize the CH_4 recovery. This mitigates potential safety hazards and improves the safety of production and its capacity. Simultaneously, by optimizing CO_2 injection, gas fields can minimize the volume of CO_2 required to achieve ideal production, thereby increasing their carbon "efficiency." This has immense practical significance for optimizing production systems, improving gas production, and reducing gas drainage costs. The GRU model, which accurately predicts the change in CH_4 flow rate in the CO_2 injection process to enhance CH_4 recovery, was further evaluated to reduce the time cost of numerical simulation. A few improvements proved beneficial: a) Only the CO_2 injection rate, CO_2 rate, and mixture flow rate are used as input layers. The dimension of the input features could be increased. Additionally, the dynamics of the CO_2 injection process and prediction accuracy could be improved by analyzing the changes in injection rate and CO_2 range in the plume spread during CO_2 injection. b) The GRU model can be combined with other methods to enhance prediction accuracy and efficiency. For example, using machine learning techniques to preprocess data can help remove outliers and improve data quality. c) The reliability of the model can be further tested through field experiments and by implementing GRU on a hardwired device. This may facilitate the identification of differences between the model prediction and actual field data and guide further model optimization.

B. Exploring applications of deep learning in CO_2-EGR

CO_2-EGR is an integral mechanism in the implementation of CCUS. The application of deep learning algorithms in the field of gas reservoir development has emerged as a promising path, demonstrating considerable potential for revolutionizing traditional approaches to well productivity evaluation and in predicting the effectiveness of different CO_2 injection rates on CH_4 recovery.

One notable application of deep learning algorithms lies in the accurate evaluation of productivity. By leveraging neural networks and advanced data analytics, these algorithms can process vast datasets, including production histories of gas and water, bottomhole flowing pressures, and other relevant parameters. The models thus enable the prediction and optimization of well performance, offering a dynamic and data-driven approach to well productivity assessment. The models may also need to consider additional factors, such as plume shape, spread area, actual gas behavior, and real reservoir heterogeneity, providing valuable insights into the intricate interplay between CO_2 and CH_4 transport within the reservoir. While the application of deep learning in gas reservoir development shows great promise, challenges remain, including the need for extensive and diverse datasets for training robust models. Additionally, the integration of actual injection–production data into these algorithms poses a challenge that demands further research. Future directions also may involve enhancing the adaptability of deep learning models to different geological settings. The ability to assess productivity accurately and optimize CO_2 injection strategies for enhanced CH_4 recovery signifies a transformative shift in the field.

As technology advances and challenges are addressed, the application of deep learning in gas reservoir engineering holds the promise of unlocking new efficiencies and insights, ultimately contributing to sustainable and optimized gas reservoir development practices.

VI. CONCLUSIONS

We apply deep learning algorithms to predict CH_4 production from a carbonate reservoir using CO_2 injection for enhanced gas recovery (CO_2-EGR). This, first-of-its-time application captures the relationships among different features, including injection rates, gas production, CH_4 recovery, and other features. The analysis confirms that underground fluid displacement using the CO_2 injection could enhance CH_4 recovery and with good predictive results. Specific conclusions are as follows:

(1) Injecting CO_2 into depleted water-bearing gas reservoirs effectively increases CH_4 recovery and mitigates the rise of the gas–water interface. A positive gradient variance is quantitatively observed between injection rate and CH_4 recovery. The injection rate influences CO_2 breakthrough time and swept area, with higher injection rates resulting in earlier CO_2 breakthrough times and larger swept area.

(2) Deep learning algorithms predict performance of the models with greater computation efficiency. We focus on pressure gradients and time series among training sets and employed the TCN, LSTM, and GRU models to learn from CH_4 rate, CO_2 rate, and CH_4 recovery under varying CO_2 injection rates. We predict the performance and feedback of production wells over a spectrum of production systems. The GRU algorithms exhibit the most reliable and effective predictive performance. For gas well time series as features, it exhibits the smallest values for *RMSE*, *MAE*, and R^2. GRU is computationally faster than numerical simulation by 3–4 orders of magnitude.
(3) The application of deep learning models in gas reservoir engineering presents a transformative opportunity. These models, adept at handling intricate nonlinear relationships without necessitating complex theoretical equations, offer a dynamic approach to optimizing CO_2 injection for CH_4 recovery. By accurately predicting CH_4 rates and analyzing CO_2 injection dynamics, they enable the precise optimization of injection processes. However, challenges persist, including the need for diverse datasets and the integration of actual injection–production data. Future directions may involve enhancing model adaptability to diverse reservoir settings. Despite challenges, the application of deep learning promises to revolutionize traditional approaches to well productivity evaluation, offering insights into CO_2–CH_4 transport dynamics and contributing to sustainable gas reservoir development.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Yize Huang: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Methodology (equal); Software (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Xizhe Li:** Conceptualization (equal); Funding acquisition (equal); Project administration (equal); Resources (equal); Supervision (equal); Writing – review & editing (equal). **Derek Elsworth:** Conceptualization (equal); Formal analysis (equal); Resources (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – review & editing (equal). **Xiaohua Liu:** Data curation (equal); Funding acquisition (equal); Project administration (equal); Resources (equal); Supervision (equal). **Pengliang Yu:** Data curation (equal); Formal analysis (equal); Methodology (equal); Software (equal); Supervision (equal); Writing – review & editing (equal). **Chao Qian:** Data curation (equal); Software (equal); Supervision (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

NOMENCLATURE

AI	Artificial intelligence
CCUS	Carbon capture, utilization, and storage
CO2-EGR	CO2-enhanced gas recovery
CO_2-EOR	CO2-enhanced oil recovery
CO2-EWR	CO2-enhanced deep brine recovery
DL	Deep learning
GRU	Gated recurrent unit
LSTM	Long short-term memory
MAE	Mean absolute error
ML	Machine learning
R^2	R-squared error value
RMSE	Root mean square error
RNN	Recurrent neural network
TCN	Temporal convolutional network

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