Predicting CO₂ Trapping Efficiency In Saline Aquifers By Machine Learning System: Implication To Carbon Sequestration

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**Predicting CO₂ trapping efficiency in saline aquifers by machine learning system:
Implication to Carbon Sequestration**

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Abstract

Carbon dioxide (CO₂) storage in saline formations has been identified as a practical approach to reducing CO₂ levels in the atmosphere. The residual and solubility of CO₂ in deep saline aquifers are essential mechanisms to enhance security in storing CO₂. In this research, CO₂ residual and solubility in saline formations have been predicted by adapting three Machine Learning models called Random Forest (RF), extreme gradient boosting (XGboost), and Support Vector Regression (SVR). Consequently, a diversity of the field-scale simulation database including 1509 data samples retrieved from reliable studies, was considered to train and test the proposed models to achieve this task. Graphical and statistical indicators were evaluated and compared the predictive ML model performance. The predicted results denoted that the proposed ML models are ranked from high to low as follows: XGboost>RF>SVR. Additionally, the performance analyses revealed that the XGboost model demonstrates higher accuracy in predicting CO₂ trapping efficiency in saline formation than previous ML models. The XGboost model yields very low root mean square error (RMSE) and R² for both residual and solubility trapping efficiency. At last, the applicable domain of XGboost model was validated, and only 24 suspected data points were recognized from the entire databank.

Keywords: CO₂ storage, CCS, Machine Learning, XGboost, Saline aquifers

Highlights

- CO₂ solubility and residual trapping is predicted with high accuracy using Machine Learning technique.
- XGboost exhibits the higher accuracy among developed models
- The application domain of XGboost is validated by Williams plot

1. Introduction

Global warming is one of the most pressing environmental concerns to alert throughout the world (Abas and Khan, 2014). The massive emission of greenhouse gases (GHG) is related to CO₂ sources, which estimates 30% of the total anthropogenic emission (Schmalensee et al., 1998). CO₂ emission in the atmosphere has resulted mainly from the burning of fossil fuels (Boot-Handford et al., 2014). Therefore, it is necessary to find a way to slow down CO₂ levels in the atmosphere, and one of the potential solutions is to capture carbon and store CO₂ in the subsurface (Dai et al., 2017). This solution is called Carbon Capture and Storage (CCS). CCS can be applied in geological formations, marine sediment, and saline aquifers (Vo Thanh et al., 2020a). Among these storage candidates, the saline aquifers demonstrated as the most potential candidate for CCS solution (Vo Thanh et al., 2019). CO₂ storage in deep saline formations could be evaluated by conventional simulation or analytical methods (Aminu et al., 2017; Bachu, 2008; Zapata et al., 2020). Also, CO₂ sequestration for field-scale simulation considered many data types such as geological background, petrophysical properties, and reservoir characterization (Song et al., 2020). To forecast storage efficiency and estimate field candidates' feasibility, the field study has been investigated in two approaches. Firstly, the evaluation of reservoir variables in an aquifer is affected by the potential of CO₂ storage capacity (Vo Thanh et al., 2020c; Xu et al., 2017). The second approach is emphasized on four trapping types, including structural, residual, solubility, and mineral trappings, to identify risk analysis of interest saline reservoir (Dai et al., 2017, 2016, 2014; Vo Thanh et al., 2020a). Furthermore, the geological parameters mainly influence CO₂ trapping performance to point out as follows: pay thickness, depth, residual gas saturation, porosity, permeability, salinity formation, heterogeneity (Date, 2014; Issautier et al., 2013; Jia et al., 2018; Kumar et al., 2005; Sarkarfarshi et al., 2014).

Recently, several scholars conducted the compositional reservoir simulation in field-scale model for predicting the effectiveness of CO₂ trapping in deep saline aquifers (Baz et al., 2016; Singh et al., 2021; Sohal et al., 2021; Soltanian et al., 2016). The residual and solubility trapping are two crucial factors for security and safety in geological CO₂ storage. Thus, to manage the storage of CO₂ in saline formation, it is mandatory to have reliable prediction residual and solubility trapping efficiency (Dejam and Hassanzadeh, 2018; Long Nghiem et al., 2009; Szulczewski et al., 2012). However, predicting these two trapping efficiency by the field-scale simulation requires a lot of subsurface data. Also, this data is too expensive to acquire all of the necessary information for the simulation model. To address this issue, a new approach needs to be explored for improving the accuracy of predicting trapping efficiency in brine aquifers. In the most recent years, machine learning (ML) techniques are well-known as powerful for solving the complex in the petroleum industry and environmental science (Ahmadi et al., 2016, 2015; Mahdaviara et al., 2021; Vo Thanh et al., 2020d). Also, ML algorithms have successfully developed several high accuracy predictive models in CCS. Amer et al. proposed the intelligence method for predicting CO₂ solubility in brine with a high agreement between anticipated results and experimental data (Amar et al., 2019).

In the problems of CO₂ sequestration in the subsurface, the extreme gradient boost (XGBoost) is developed for estimating the optimal sequestration depth in saline formation (Zhang et al., 2020). Similarity, Support Vector Regression (SVR) was coupled with optimization techniques to assess the permeability changing during CO₂ injection in coal seams. Another application of ML approaches in CO₂ enhanced oil recovery and storage by (Chen and Pawar, 2019), these researchers were used Random Forest (RF) and SVR to construct the high accuracy model for estimating oil production and storage performance in residual oil zones of Permian Basin. Nevertheless, these scholars were used the synthetic homogeneous model for the generation of

91 large amount of databases for training ML models. Then, the optimal ANN predicted models were
92 used to apply for real field application. Although, the predicted results were achieved between real
93 field and ML models. But the research question needs be to be solved here. Should we use the real
94 field-scale simulation results to generate the more reliable ML models for predicting CO₂ trapping
95 efficiency in saline aquifers? This question is the research gap for our study. Thus, the objective
96 of this paper is to collect the field-scale simulation results around the world available in literature
97 review for developing the robust and accuracy ML models. In this study, several popular ML
98 methods have been developed to assess the residual and solubility of brine aquifers in quick and
99 precise fashion. These methods are so-called SVR, RF, and XGboost that are used for predicting
100 CO₂ trapping index in term of geological and operation factors. Additionally, statistical analysis
101 and graphical visualization are used to rank the best ML model for future employment perspective.
102 In order to explore the stability of employed paradigm, the comparison of best ML model and
103 previous study was proceeded by analyzing the statistical indicators and fitting curves. Lastly, the
104 Williams plot was used for determining the applicable domain of the best ML model. The problem
105 of this research illustrates in **Figure 1**. This figure illustrate the sketch for the proposing research.
106 The robustness of developing ML models would be compared with the existing study that
107 considered only single reservoir for their research. In real application, the diversity of reservoirs is
108 main challenge for predicting CO₂ trapping performance. Thus, this drawback will be solved in
109 this research by considering dffirent reservoir models into one ML models for demonstration the
110 robustness as well as the applicable of our ML models.

111 To the best of our knowdege, this study is first attempt to consider muttiple simulation field data
112 around the world for developing the ML based CO₂ storage capacity. This work provide the useful
113 for reservoir engineer to monitor and evaluation CO₂ storage in the early phase of CCS project.

Ultimately, the proposing method in this paper could be adapted for related studies because it is easy to conduct and reproduce in ML applications.

Figure 1. This schematic shows the illustration of the research question

2. Methodology

This section starts with data collection and description, followed by the theory of the ML algorithms applied in this paper, and finishes with a workflow to develop the ML model.

2.1. Data preparation

The first step of developing any machine learning model is gathering the datasets. Here we collected 1509 simulation samples from reliable published literature (Ajayi et al., 2019; Al-khdheewi et al., 2018; Al-Khdheewi et al., 2018b, 2018a, 2018c; Anchliya et al., 2012; Foroozesh et al., 2018; Hsieh et al., 2013; Jin et al., 2012; Jun et al., 2019; Khudaida and Das, 2020; Kim et al., 2019; Kumar et al., 2005; Lee et al., 2010; Li et al., 2020; Liner et al., 2011; Liu et al., 2020; Mohajeri and Shariatipour, 2019; L Nghiem et al., 2009; Noushabadi et al., 2018; Pham et al., 2013; Sifuentes et al., 2009; Song et al., 2020; Sung et al., 2014; Vo Thanh et al., 2020b; Xiao et al., 2019; Zapata et al., 2020). The study area of collected data was conducted around the world, including Sleipner (Norway), Shenhua (China), Taiwan, Cuu Long Basin (Vietnam), Gorge V (Korea), Kansas (USA), Ketzin (Germany), Abu Dhabi, Israel, and UK. Also, the reservoir simulation results were produced from CMG-GEM, ECLIPSE, TOUGH2, STAR, and STOM-CO2. **Figure 2** displays the location study of simulation results to gather for ML study.

Figure 2. The study area in literature review was collected for database to develop the machine learning models

The diversity of characteristics of storage formations and simulation packages was expected to construct the powerful ML models for predicting CO₂ trapping efficiency in saline formations accurately. The calculation of trapping efficiency is determined by the following equation (Long Nghiem et al., 2009):

$$\text{Residual Trapping Index (RTI)} = \frac{\text{Total mass of CO}_2 \text{ trapped as residual (kg)}}{\text{Total mass of CO}_2 \text{ injected (kg)}} \quad (1)$$

$$\text{Solubility Trapping Index (STI)} = \frac{\text{Total mass of CO}_2 \text{ dissolved in brine (kg)}}{\text{Total mass of CO}_2 \text{ injected (kg)}} \quad (2)$$

The geological factors and injection parameters were considered as input variables for construction machine learning (ML) models, while the residual trapping index (RTI) and solubility trapping index (STI) were defined as output. **Table 1** summarizes the statistical parameters and the detailed description of input and output for employed databases. The injection time, post-injection period, porosity, permeability, thickness, Salinity, depth, residual gas saturation, pressure, temperature, and injection rate are determined as the input features for developing ML model, and the outputs consider the RTI and STI. These output was extracted from published literature using grabit tool matlab (<https://www.mathworks.com/matlabcentral/fileexchange/7173-grabit>).

Table 1. The description of inputs and outputs for ML models

		Min	Mean	Max	Standard Deviation
Outputs	RTI	0.0163	0.36805	0.98332	0.2323
	STI	0.00036	0.27481	0.89298	0.167286
Inputs	Injection period (years)	3.8	33.6952	100	24.39096
	Post injection period (years)	7.65549	917.237	7988.31	1530.578103
	Min_Porosity	0	0.08848	0.3	0.102693
	Max_Porosity	0.093	0.26138	0.47	0.095946
	Min_Permability (mD)	0.0001	26.4085	1743	199.099069
	Max_Permability(mD)	5.615	437.368	2029	455.445925
	Thickness (m)	5	244.48	1500	170.53674
	Salinity (ppm)	10000	97226.4	320000	79871.2278
	Min_Depth (m)	560.83	1464.49	3650	903.183053
	Max_Depth (m)	704.69	1725.75	3853	914.910919
	Residual gas saturation	0	0.19911	0.5	0.156826
	Temperature (°C)	30	53.9876	103	21.257944
	Pressure (MPa)	7.5	18.3503	50	11.075672
	Injection rate (ton/day)	3.47	2582.95	65753	7483.057286

2.2. Machine Learning algorithms

In this study, we develop the predictive model for prediction residual and solubility trapping in saline formations. Three powerful machine learning including Support Vector Regression (SVR), Random Forest (RF), and Extremely Gradient Boosting (XGBoost) was used to construct the intelligent prediction model. The following subsections describe the theory of these machine learning methods.

2.2.1. Support Vector Regression (SVR)

The Support Vector Regression (SVR) is the regression method that has been employed in many research themes (Chen and Pawar, 2019). The basic function of support vector regression can be described as following (Vapnik, 2013):

$$g(x) = \omega^T \phi(x) + a \quad (3)$$

where, ϕ illustrate for mapping function, w is a weight factor, x and a represent for input vector and bias. The popular regression version of SVM, ε -SVR, was adapted in this study. By using the N_s training samples, the standard formula for ε -SVR is written by (Vapnik, 2013):

$$\min_{\omega, b, \xi, \xi^*} \frac{1}{2} \omega^T \omega + C \sum_{i=1}^{N_s} (\xi_i + \xi_i^*) \quad (4)$$

$$\text{Subject to } \omega^T \phi(x_i) + b - y_i \leq \varepsilon + \xi_i,$$

$$y_i - \omega^T \phi(x_i) - b \leq \varepsilon + \xi_i^*,$$

$$\xi_i, \xi_i^* \geq 0, i = 1, 2, \dots, N_s,$$

where, C stands for the penalty parameter, and ξ_i and ξ_i^* are the slack parameters that state the minimum and maximum range training errors pointing to an error tolerance ε (Chen and Pawar, 2019). In this study, the radial basis function (rbf) kernel is used for training the SVR model. The equation of rbf can be described as (Chen and Pawar, 2019; Schölkopf and Smola, 2002):

$$(x_i, x_j) = \exp \left(-\gamma \|x_i - x_j\|_2^2 \right), \gamma > 0. \quad (5)$$

By adapting the Lagrange multipliers, α_i and α_i^* , are determined, the predictive model can be describe as below (Chen and Pawar, 2019):

$$g(x) = \sum_{i=1}^{N_s} (-\alpha_i + \alpha_i^*) K(x_i, x) + b. \quad (6)$$

The vector for the non-zero component of $(-\alpha_i + \alpha_i^*)$, $i = 1, 2, \dots, N_s$, is called the support vectors. Given an input x , the SVR model can output all the support vectors. In this research, C , γ , and ε are three tuning parameters for developing machine learning model.

2.2.2. Random Forest (RF)

The Random Forest (RF) is adapted the capacity of decision tree and ensemble techniques to generate reliable regression models. These models deliver intensive understanding into the data tree by controlling the level of nonlinearity in the training databank (Breiman, 2001). The RF is an extensive bagging and a solid opposer for boosting (Breiman, 2001). Also, the advantage of the RF model enables each regression tree to include different combinations of the predictor variables and prevents overfitting to the training dataset. This task is accomplished by switching Out-of-Bag (OOB) samples from a specific predictor to evaluate the increase in estimation error while the remaining factors are kept the same (Breiman, 2001). The mean square error (MSE_{OOB}) is defined as follows (Breiman, 2001; Chen and Pawar, 2019)

$$MSE_{OOB} = \frac{1}{N_T} \sum_{i=1}^{N_{DT}} (y_i - \hat{y}_i)^2 \quad (7)$$

where, N_{DT} presents for the number of OOB samples, and $\hat{y}_i$ knows as the OOB prediction for training samples. In RF regression modelling, the following tuning parameters need to be specified [33]: (i) the number of decision trees to grow in the random forest ($N_{estimators}$), (ii) the number of randomly defined predictor variables at each node when searching for the best split ($Max_features$), and (iii) the minimum number of observations is used for splitting an internal node ($min_samples_split$). In this study, python's Scikit-Learn package, namely "*sklearn.ensemble.RandomForestRegressor*" was used to develop RF predictive model (Pedregosa et al., 2011).

2.2.3. Extreme Gradient Boosting (XGboost)

XGBoost is an ensemble of classification and regression trees (CARTs) method developed by (Chen and Guestrin, 2016). XGBoost-based regression is adapted a decision tree (DT) based on the previous tree, adjusting DT proportion for creating step by step functionality (Gholami et al., 2020; Shin et al., n.d.; Zhang et al., 2018). Also, out of 29 winning prizes in the machine learning contest Kaggle in 2015, XGBoost was the most popular technique that 17 awards applied XGBoost (Zhang et al., 2018). The higher-ranking performance of XGBoost in supervised machine learning is the main reason it is selected to build the prediction model for CO₂ trapping performance in this study. The illustration of extreme gradient boosting depicts in Figure 3.

Figure 3. The illustration of XGboost technique

Firstly, the Xgboost has generated the difference between the prediction and data measurements to calculate the residual and misclassification. Then, the multiple regression tree models can

appropriately evaluate the misclassification achieved in the first phase. Finally, the residuals after the first two phases are adjusted to the other trees in the third phase, and this process is repeated many times (Sutton, 2005). This process leads to the final goal of XGboost that is simplified for optimization of the training loss (m) and regulations (β). The f_p stands for the function of the P-tree. The objective function (K) in round g is given by the following formula [62-64]:

$$K^{(g)} = \sum_{i=0}^n m(y_i + \tilde{y}_i) + \sum_{n=1}^P \beta(f_p) \quad (8)$$

In this work, y_i represents for the simulation CO₂ trapping efficiency from databank, and $\tilde{y}_i$ stands for the prediction values from XGboost model. The XGBRegressor library of Scikit-learn's python package is adapted for training ML model. The tuning hyperparameter was used for XGboost, including number of a tree (N_estimator), minimum loss reduction for doing a split (gamma), maximum depth of a tree (max_depth), step of each weight (learning_rate), L1 regularization of leaf weight (reg_lambda), and L2 regularization of leaf weight (reg_alpha) (Pedregosa et al., 2011).

2.3. Workflow of developing machine learning models

The framework of the machine learning (ML) model for predicting CO₂ trapping performance in deep saline aquifers consists of several steps, as depicted in **Figure 4**.

Figure 4. The schematic of machine learning modelling process

242

243 The procedure of developing ML models starts with data collection and then pre-processing
 244 input/output data. The next phase starts with a data portion that randomly divided the whole
 245 databank into two sets (training and testing). The following process is the employment of proposed
 246 ML techniques for target data. Then, the performances of each developed model are analyzed to
 247 define the best model from three ML algorithms for deployment in predicting CO₂ trapping
 248 efficiency in saline formations. In the developing ML model, the data partition is the necessary
 249 process. This step has separated the database into two groups, including train and test groups. The
 250 training group is a subset to develop the training model, while the testing group utilizes for
 251 evaluating the performance of predictive models. Unfortunately, there is no specific principle for
 252 dividing the ratio of partitioning data into training and testing. The previous work has found that
 253 the percentage of training data influences the accuracy of ML model (Ali, 2021). To improve the
 254 accuracy of the outputs for ML model, several options of data proportions need to consider for the
 255 training model. To address this issue, the entire databank is divided into four partitions as follows:
 256 60%-40%, 70%-30%, 80%-20%, 90%-10%, while the first partition is the training group and the

second part stands for the test group. However, the critical issue is how we can select the best ML model among the three techniques. To solve this problem, two popular statistical indicators are chosen; namely, coefficient of determination (R-square) and root mean squared error (RMSE). These indicators determined using the following formula:

$$R - squared = 1 - \frac{\sum_{i=1}^n (T_{i,sim} - T_{i,pred})^2}{\sum_{i=1}^n (T_{i,sim} - \bar{T}_{i,sim})^2} \quad (9)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (T_{i,sim} - T_{i,pred})^2} \quad (10)$$

T denotes the residual and solubility trapping efficiency in saline aquifers; subscripts sim and pred represent the simulation and predicted results, respectively; $\bar{Y}$ stands for average residual and solubility trapping, and n is the number of the training data point.

3. Result and Discussion

Before analyzing the prediction performance for developing ML models in this study, a brief description of the tuning hyperparameters applied in each method is presented first.

3.1. Hyperparameter tuning ML models

In addition, the ML methods need a lot of number hyperparameters for training models. However, there are only several essential parameters to be used for achieving the best model performance. The grid search technique adapts for selecting the best tuning hyperparameter for each ML method in this work. **Table 2** highlights the information of tuning parameters applied for developing the

three predictive machine learning models. All of the training and testing scenarios were conducted using open-source Scikit-learn's python package.

Table 2. The parameter for tuning ML models in this study

Model	Parameter	Specific search range	Optimal values
SVR	γ	10-200	100
	C	5-1000	100
XGboost	N_estimator	100-10000	9000
	Reg_lamda	0.01-100	4
	Max_depth	10-1000	600
	Learning_rate	0.001-1	0.01
	Reg_alpha	0.001-1	0.01
RF	N_estimator	100-6000	6000
	Min_sample split	10-100	40
	Min_sample leaf	0.5-1.0	0.95

3.2. Performance of each ML model

The four scenarios of databank portions were considered to determine the best ML method. The prediction results of three ML models are highlighted in Table X. As can be observed from this table, the developed ML models in this work can obtain an accuracy of 90% for training and testing phases on all scenarios of data proportions. These results indicated that the three ML models had predicted well in CO₂ trapping efficiency in saline aquifers using 1509 data samples.

By observation overall ML models performance on each data division, it can be found that the XGboost method has the highest prediction accuracy over XGboost and SVR. The excellent performance of XGboost could observe in **Table 3**. This table is considered as for proven the best data bank proportions. The XGboost model attains the stable prediction results of training and testing for all data portions. Among four data portions, the XGBoost model achieved the highest prediction accuracy on data portions, 80%-20%.

289

290 **Table 3. The performance of three ML models for prediction trapping index in saline aquifers.**

Databank portions	Model	RTI				STI			
		Training		Test		Training		Test	
		R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE
60%-40%	SVR	0.9412	0.0713	0.9230	0.0767	0.9049	0.0146	0.9004	0.0316
	RF	0.9971	0.0126	0.9801	0.0322	0.9980	0.0074	0.9908	0.0164
	XGBoost	0.9996	0.0046	0.9913	0.0226	0.9997	0.0028	0.9668	0.0311
70%-30%	SVR	0.9421	0.0707	0.9181	0.0769	0.9049	0.2871	0.9139	0.2756
	RF	0.9977	0.0113	0.9753	0.0354	0.9984	0.0065	0.9914	0.016
	XGBoost	0.9996	0.0043	0.9946	0.0181	0.9997	0.0027	0.9974	0.0088
80%-20%	SVR	0.9403	0.0707	0.9254	0.0759	0.9062	0.2843	0.9191	0.2847
	RF	0.9984	0.0095	0.9686	0.0410	0.9990	0.0051	0.9868	0.0208
	XGBoost	0.9997	0.0041	0.9941	0.0191	0.9998	0.0026	0.9985	0.0065
90%-10%	SVR	0.9403	0.0707	0.9133	0.0792	0.9094	0.2901	0.9107	0.2837
	RF	0.9986	0.0086	0.9451	0.0544	0.9991	0.0049	0.9780	0.02869
	XGBoost	0.9997	0.0076	0.9916	0.0241	0.9998	0.0024	0.9979	0.0080

291

292 On the other hand, SVR model has the least accuracy for prediction results on four data divisions.

293 Therefore, the overall performance ranking in terms of statistical indicators is XGboost, RF, and

294 SVR. Also, the data division of 80%-20% is used for further evaluation in this study. This data

295 division achieves excellent testing performance over three remaining data divisions. For better

296 visualization, the cross plot of testing performance using data-division 80%-20% by three ML

297 models for prediction RTI and STI is illustrated in **Figure 5**. These plots strongly demonstrate that298 the XGboost is superior to RF and SVR. As shown in **Figure 5**, the testing points of XGboost

299 distribution nearby the perfect fitting line indicate the excellent agreement between model

300 prediction and simulation data. From the view of R-squared, the Xgboost model achieves the

301 better testing effect, and its R² value of RTI and STI equal to 0.9941 and 0.9985,

302 respectively. The testing effect of SVR model is the worse, and its R-squared value of

RTI and STI is 0.9254 and 0.9191, respectively. The R-square values of the three ML models are typically above 0.92, which indicates that the ML proposed in this study have achieved the good agreement between reservoir simulation data and predictive results.

Figure 5. The fitting plots between simulated and predicted trapping efficiency for three ML models in testing phase

Moreover, for a better evaluate the performance of testing RTI and STI, bar charts of RMSE and R^2 are presented in **Figure 6**. Overall, Xgboost shows a better performance than RF and SVR in prediction CO₂ trapping efficiency. Thus, Xgboost is the most predictable ML model thanks to its highest testing R^2 and lowest RMSE. It can be remarked from **Table 3** and **Figure 6** that our nominated ML models to predict RTI and STI in saline aquifers follow the reliable ranking highlight below: Xgboost > RF > SVR

Figure 6. The comparison status of RMSE and R^2 of nominated ML models for estimation CO₂ trapping efficiency.

The better performance of XGboost in both R^2 and RMSE is demonstrated the robustness of this model for prediction CO₂ trapping efficiency. This evidence is the clear manner for demonstration the superior of XGBoost over RF and SVR. In addition, the quality of Xgboost model could be observed to deep insight by comparing the estimated CO₂ efficiency in brine formations using XGboost and the simulated testing dataset for RTI (**Figure 7a**) and STI (**Figure 7b**). The excellent fitting between simulated trapping efficiency and XGboost prediction results in the testing stage can be seen in these subfigures. Thus, all graphical analyses figure out that the XGboost is the best method in this study. Therefore, XGboost model is selected for further investigation before employing it in the actual application.

Figure 7. The relationship of simulated and predicted trapping efficiency by considering each sample testing data. (a) RTI and (b) STI

3.2. Relative important of influence predictors

CO₂ sequestration in saline aquifers has a lot of essential variables effect to trapping efficiency. Thus, the crucial variables of XGboost model need to be evaluated to understand the significance of each input feature on the CO₂ trapping efficiency in saline reservoirs. This study adopts built in function in scikit-learn library for evaluation each input variable. **Figure 8** depicts the result of ranking important features for residual trapping and solubility trapping in this study.

Figure 8. Essential features are ranking for ML models

By visualization of the bar chart, it can be found that the max_depth is an essential feature for both RTI and STI in saline reservoirs. This finding is an important notice for trapping efficiency because depth is also affected by structural trapping capacity in saline formation. In the most recent research, Iglauer et al. (Iglauer, 2018) figured out an issue in achieving an optimum storage depth where the maximum amount of CO₂ structural trapping happens in a deep saline reservoir.

Furthermore, CO₂ solubility is a function of depth in the subsurface (Duan et al., 2006). In addition, Kim et al. (Kim et al., 2017) also demonstrated that increasing depth leads to increased residual and solubility trapping efficiency in deep saline formation. Therefore, there is an agreement between the previous study and our work. In consequence, the max_depth is found as the highest-ranking feature in XGboost model.

Besides, the crucial feature is listed out from ML model. The fewer effect features are also remarked for our study. By considering the ranking charts in **Figure 8**, the minimum porosity, minimum permeability can be removed from the developed ML model. Moreover, the collection of data information with accuracy is complex in subsurface storage sites. Therefore, the developed model with fewer input features could help us to verify and easily employ the developed ML models in the actual application of the geo-sequestration project.

3.3.Comparison of the best ML model with previous models

Although the XGboost model is demonstrated as the highest accuracy over RF and SVR, it is necessary to prove the robustness of our developed models with the previous study. Therefore, the performance of XGboost is re-evaluated with previously developed ML models in the reliable published paper. **Table 4** highlights the statistical indicators for different ML methods. It is found that the XGboost model is superior to the other ML models, as confirmed by the highest R² and lowest RMSE for both training and testing phases.

Table 4. The comparison analysis for demonstration the robust of nominated ML model

			Training		Testing	
Methods	Library	Number of samples	RMSE	R ²	RMSE	R ²
XGboost (This study)	Scikit-learn	1509	0.0041	0.9998	0.0065	0.9985
ANN (Song et al., 2020)	Tensorflow	145500	0.0080	0.9842	0.0082	0.9847

For the training phases, the RMSE and R^2 from XGBoost evaluations are 0.0041 and 0.9998, respectively, whereas the RMSE and R^2 of ANN models are 0.9842, respectively.

Regarding the testing phase, the RMSE and R^2 for XGBoost evaluations are 0.0065 and 0.9985, respectively, while the RMSE and R^2 of the ANN model are 0.0082 and 0.9847, respectively.

Moreover, for better visualization of our comparison, **Figure 9** presents the bar plots of RMSE and R^2 for two ML models. The significant difference of statistical indicators in our study and previous work demonstrated that the XGboost model has better accuracy than other models by observing the bar plots.

To verify the predictability of XGboost in prediction RTI and STI in saline aquifers compared to the ANN model of Song et al. by using the same range of input features. Also, Song et al. [10] were used CMG-GEM simulation to conduct the reservoir simulation results for 300 years, including 10 years injection and 290 years post-injection, then compare the simulated results and ANN prediction. Our study updated the field simulation data from Song et al. [10] for predictive purposes to capture their idea. For better observation, the prediction results of two ML models and simulation results exhibit in **Figure 10**. As can be observed in this figure, the CO₂ trapping efficiency of XGboost achieves higher accuracy than the outputs from the multilayer ANN model. Furthermore, the advantage of our developed model utilizes less sample training data than the previous study. In this work, Xgboost has used 1509 samples while the existing research used 145500 data samples. The ML mechanism plays an essential role in determining the suitable number of training samples. Thus, the predictive-based ML should consider different methods in the same training databank to select the suitable one for a specific study.

Figure 9. Comparison study of our model and existing study for predicting CO₂ trapping

Figure 10. The comparison performance of XGboost and previous model with simulation. The XGboost exhibit the excellent fitting with simulation data by visualization the time series of RTI (a) and STI (b)

3.4.Xgboost model application perspective

The XGboost model of this study employed the supervised ML technique for predicting the CO₂ trapping efficiency in saline aquifers considering geological and operation factors available from the published paper. Specified a marked set of input-output pairs $XGboost = \{(p_i, t_i)\}_{i=1}^n$, the initial objective of each ML model is to create a map for the predictor p and the targets t (Ali, 2021) . This data part is defined as the training set. The ultimate objective of ML models build a sketch that will derive well in a database that the ML models have never learned. The blind data is adapted for estimating how well the ML models derive for specific studies. Also, these bling testing data are considered for uncertainty analysis in the prediction ML model. For instance, to employ the XGboost method as the best predictive method predicted the residual and solubility trapping in an interest saline formation. The predictors of this saline formation that are not included in the training set are collected first and processed in an excel format or text file. Then, the trained XGboost model is loaded by *joblib* function in Scikit-learn python toolkit. Finally, they load the input predictors to predict CO₂ trapping efficiency for interest saline formation whose features are stored in the input excel file.

The predictive results of ML models would help reservoir engineers deeply understand the CO₂ trapping efficiency that is useful for short-term and long-term monitoring CO₂ storage projects.

In addition, the ML help to know the impact of each predictor/feature on the CO₂ trapping efficiency in saline aquifers that will provide a valuable tool for searching the suitable values of input variables for reducing the uncertainty in the CO₂ storage project.

3.5. Applicability domain of the XGboost model

The simulation results collected in the published papers related to several uncertainty factors. Therefore, determining the legality of these data and analyzing the Xgboost of the application domain is necessary. To address this issue, the Williams plot was considered for our study. The Williams plot highlights the applicability domain of the ML model. This plot is drawn by considering the standardized residual (SR) and leverage values (Godall et al., 1993). The statistical step for the Leverage parameter can be found in (Sarapardeh et al., 2016). **Figure 11** shows the Williams plot for the XGBoost model.

Figure 11. The Williams plot demonstrates the applicaton domain of XGboost models

It can be analyzed from this plot, a massive part of the training and testing results are in the range of $-3 \leq SR \leq 3$. So, in a nutshell, the Xgboost model has a high level of reliability and statistics trueness.

Moreover, it is underlined that just 24 points from the XGboost model's feasibility realm were identified as outliers. It's worth noting that this number of suspicious data points only accounts for 1.59 % of entire datasets.

Ultimately, it is necessary to point out that the constructed Xgboost model should be employed to predict the residual and solubility CO₂ trapping in saline aquifers when input features inside the proposed applicable ranges. Nevertheless, the developed ML model can be adapted for scenarios outside the offered study range with caution because the accuracy model is not guaranteed. It can produce accurate forecasts for some values of the parameters used but erroneous predictions for others. Indeed, because the Xgboost model was built with general predictors characteristics, it may be used for a wide variety of instances with features that fall in the range of the abovementioned inputs.

4. Conclusions

In this study, three machine learning techniques, namely XGboost, RF, and SVR, were developed reliable ML models to estimate the solubility trapping index and residual trapping index for deep saline reservoirs. Based on the results, the following vital conclusions could be underlined:

- The employment ML models obtained excellent performance in predicting CO₂ trapping index in deep saline reservoirs.
- XGboost model is found as the most predictable model in prediction CO₂ trapping index in saline aquifers. Furthermore, the Xgboost outperforms RF and SVR.
- XGboost reveals the highest R² and lowest RMSE for both training and testing phases in this work.
- The Xgboost is superior to other ML models in the published literature that demonstrated the robustness of developed models.
- The maximum depth is an essential feature for residual and solubility trapping to find out from this work.
- The minimum porosity and permeability have the most negligible impact on to Xgboost model for predicting trapping index in this work.
- The highlight of this work is used fewer training data samples than previous. It is the advantage of this work to develop reliable ML models for predicting CO₂ trapping performance. Our developed models help predict the feasibility of the CO₂ storage project in the early phase.
- Also, this research was paid attention to the diversity of reservoir characteristic saline formation, whereas previous work used a homogenous reservoir model for generating data

and training ML models. The ignoring of reservoir heterogeneity for training data limits the application perspective of ML models for predicting the CO₂ trapping efficiency because the real storage sites are not homogenous conditions as realistic conditions. Thus, the more detail of reservoir models in the database is the more efficient and accurate for proposing a machine learning approach in CO₂

- The Xgboost is helpful in this work and potential for future research about and CO₂ storage and environmental study.

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Reference

- Abas, N., Khan, N., 2014. Carbon conundrum , climate change , CO₂ capture and consumptions. *Biochem. Pharmacol.* 8, 39–48. <https://doi.org/10.1016/j.jcou.2014.06.005>
- Ahmadi, M.A., Kashiwao, T., Rozyn, J., Bahadori, A., 2016. Accurate prediction of properties of carbon dioxide for carbon capture and sequestration operations. *Pet. Sci. Technol.* 34, 97–103. <https://doi.org/10.1080/10916466.2015.1107847>
- Ahmadi, M.A., Soleimani, R., Lee, M., Kashiwao, T., Bahadori, A., 2015. Determination of oil well production performance using artificial neural network (ANN) linked to the particle swarm optimization (PSO) tool. *Petroleum* 1, 118–132. <https://doi.org/10.1016/j.petlm.2015.06.004>
- Ajayi, T., Awolayo, A., Gomes, J.S., Parra, H., Hu, J., 2019. Large scale modeling and assessment of the feasibility of CO₂ storage onshore Abu Dhabi. *Energy* 185, 653–670. <https://doi.org/10.1016/j.energy.2019.07.052>
- Al-khdheewi, E.A., Vialle, S., Barifcani, A., Sarmadivaleh, M., Iglauer, S., 2018. Impact of Injection Scenario on CO₂ Leakage and CO₂ Trapping Capacity in Homogeneous Reservoirs Model description and initialization, in: *Offshore Technology Conference Asia*. Kuala Lumpur, Malaysia.
- Al-Khdheewi, E.A., Vialle, S., Barifcani, A., Sarmadivaleh, M., Iglauer, S., 2018a. Effect of wettability heterogeneity and reservoir temperature on CO₂ storage efficiency in deep saline aquifers. *Int. J. Greenh. Gas Control* 68, 216–229. <https://doi.org/10.1016/j.ijggc.2017.11.016>
- Al-Khdheewi, E.A., Vialle, S., Barifcani, A., Sarmadivaleh, M., Iglauer, S., 2018b. Enhancement of CO₂ trapping efficiency in heterogeneous reservoirs by water-alternating

502 gas injection. *Greenh. Gases Sci. Technol.* 12, 1–12. <https://doi.org/10.1002/ghg.1805>

503 Al-Khdheewi, E.A., Vialle, S., Barifcani, A., Sarmadivaleh, M., Zhang, Y., Iglauer, S., 2018c.

504 Impact of salinity on CO₂ containment security in highly heterogeneous reservoirs. *Greenh.*

505 *Gases Sci. Technol.* 8, 93–105. <https://doi.org/10.1002/ghg.1723>

506 Ali, A., 2021. Data-driven based machine learning models for predicting the deliverability of

507 underground natural gas storage in salt caverns. *Energy* 229, 120648.

508 <https://doi.org/10.1016/j.energy.2021.120648>

509 Amar, N., Hemmati-sarapardeh, A., Varamesh, A., 2019. Predicting solubility of CO₂ in brine

510 by advanced machine learning systems : Application to carbon capture and sequestration. *J.*

511 *CO₂ Util.* 33, 83–95. <https://doi.org/10.1016/j.jcou.2019.05.009>

512 Aminu, M.D., Nabavi, S.A., Rochelle, C.A., Manovic, V., 2017. A review of developments in

513 carbon dioxide storage. *Appl. Energy* 208, 1389–1419.

514 <https://doi.org/10.1016/j.apenergy.2017.09.015>

515 Anchliya, A., Ehlig-Economides, C.A., Jafarpour, B., 2012. Aquifer Management To Accelerate

516 CO₂ Dissolution and Trapping. *SPE J.* 17, 805–816. <https://doi.org/10.2118/126688-PA>

517 Bachu, S., 2008. CO₂ storage in geological media: Role, means, status and barriers to

518 deployment. *Prog. Energy Combust. Sci.* 34, 254–273.

519 <https://doi.org/10.1016/j.pecs.2007.10.001>

520 Baz, H., Noureldin, M., Allinson, W.G., Cinar, Y., 2016. A field-scale investigation of residual

521 and dissolution trapping of CO₂ in a saline formation in Western Australia. *Int. J. Greenh.*

522 *Gas Control* 46, 86–99. <https://doi.org/10.1016/j.ijggc.2015.12.032>

523 Boot-Handford, M.E., Abanades, J.C., Anthony, E.J., Blunt, M.J., Brandani, S., Dowell, N. Mac,

524 2014. Carbon capture and storage update. *Energy Environ. Sci.* 7, 130–189.

525 <https://doi.org/10.1039/c3ee42350f>

526 Breiman, L.E.O., 2001. Random Forests. *Mach. Learn.* 45, 5–32.

527 Chen, B., Pawar, R.J., 2019. Characterization of CO₂ storage and enhanced oil recovery in
528 residual oil zones. *Energy* 183, 291–304. <https://doi.org/10.1016/j.energy.2019.06.142>

529 Chen, T., Guestrin, C., 2016. XGBoost : A Scalable Tree Boosting System, in: *ACM SIGKDD*
530 International Conference on Knowledge Discovery and Data Mining. San Francisco, CA,
531 USA, pp. 785–794.

532 Dai, Z., Stauffer, P.H., Carey, J.W., Middleton, R.S., Lu, Z., Jacobs, J.F., Hnottavange-Telleen,
533 K., Spangler, L.H., 2014. Pre-site characterization risk analysis for commercial-scale carbon
534 sequestration. *Environ. Sci. Technol.* 48, 3908–3915. <https://doi.org/10.1021/es405468p>

535 Dai, Z., Viswanathan, H., Middleton, R., Pan, F., Ampomah, W., Yang, C., Jia, W., Xiao, T.,
536 Lee, S., Mcpherson, B., Balch, R., Grigg, R., White, M., 2016. CO₂ Accounting and Risk
537 Analysis for CO₂ Sequestration at Enhanced Oil Recovery Sites.
538 <https://doi.org/10.1021/acs.est.6b01744>

539 Dai, Z., Zhang, Y., Stauffer, P., Xiao, T., Zhang, M., Ampomah, W., Yang, C., Zhou, Y., Ding,
540 M., Middleton, R., Soltanian, M.R., Bielicki, J.M., 2017. Injectivity Evaluation for Offshore
541 CO₂ Sequestration in Marine Sediments. *Energy Procedia* 114, 2921–2932.
542 <https://doi.org/10.1016/j.egypro.2017.03.1420>

543 Date, N.E., 2014. Ye Zhang 1 ; Guang Yang 2 ; and Shuiquan Li 3 23 1–14.
544 [https://doi.org/10.1061/\(ASCE\)HZ.2153-5515.0000246](https://doi.org/10.1061/(ASCE)HZ.2153-5515.0000246).

545 Dejam, M., Hassanzadeh, H., 2018. Diffusive leakage of brine from aquifers during CO₂
546 geological storage. *Adv. Water Resour.* 111, 36–57.
547 <https://doi.org/10.1016/j.advwatres.2017.10.029>

548 Duan, Z., Sun, R., Zhu, C., Chou, I., 2006. An improved model for the calculation of CO₂
549 solubility in aqueous solutions containing Na⁺,K⁺,Ca²⁺,Mg²⁺,Cl, and SO₄. *Mar. Chem.*
550 98, 131–139. <https://doi.org/10.1016/j.marchem.2005.09.001>

551 Foroozesh, J., Dier, M.A., Rezk, M.G., 2018. A simulation study on CO₂ sequestration in saline
552 aquifers : Trapping mechanisms and risk of CO₂ leakage, in: *MATEC Web of*
553 *Conferences*. p. 5.

554 Gholami, H., Mohamadifar, A., Collins, A.L., 2020. Spatial mapping of the provenance of storm
555 dust: Application of data mining and ensemble modelling. *Atmos. Res.* 233, 104716.
556 <https://doi.org/10.1016/j.atmosres.2019.104716>

557 Hsieh, B.Z., Nghiem, L., Shen, C.H., Lin, Z.S., 2013. Effects of complex sandstone-shale
558 sequences of a storage formation on the risk of CO₂ leakage: Case study from Taiwan. *Int.*
559 *J. Greenh. Gas Control* 17, 376–387. <https://doi.org/10.1016/j.ijggc.2013.05.030>

560 Iglaier, S., 2018. Optimum storage depths for structural CO₂ trapping. *Int. J. Greenh. Gas*
561 *Control* 77, 82–87. <https://doi.org/10.1016/j.ijggc.2018.07.009>

562 Issautier, B.Î., Fillacier, S., Le Gallo, Y., Audigane, P., Chiaberge, C., Viseur, S., 2013.
563 Modelling of CO₂ injection in fluvial sedimentary heterogeneous reservoirs to assess the
564 impact of geological heterogeneities on CO₂ storage capacity and performance. *Energy*
565 *Procedia* 37, 5181–5190. <https://doi.org/10.1016/j.egypro.2013.06.434>

566 Jia, W., McPherson, B., Pan, F., Dai, Z., Xiao, T., 2018. Uncertainty quantification of
567 CO₂ storage using Bayesian model averaging and polynomial chaos expansion. *Int. J.*
568 *Greenh. Gas Control* 71, 104–115. <https://doi.org/10.1016/j.ijggc.2018.02.015>

569 Jin, M., Pickup, G., Mackay, E., Todd, A., Sohrabi, M., Monaghan, A., Naylor, M., 2012. Static
570 and Dynamic Estimates of CO₂-Storage Capacity in Two Saline Formations in the UK. *SPE*

571 J. 17, 1108–1118. <https://doi.org/10.2118/131609-PA>
 572 Jun, C., Kim, M., Shin, H., 2019. Optimization of well placement and operating conditions for
 573 various well patterns in CO₂ sequestration in the Pohang Basin, Korea. *Int. J. Greenh. Gas*
 574 *Control* 90, 102810. <https://doi.org/10.1016/j.ijggc.2019.102810>
 575 Khudaida, K.J., Das, D.B., 2020. A Numerical Analysis of the Effects of Supercritical CO₂
 576 Injection on CO₂ Storage Capacities of Geological Formations. *Clean Technol.* 2, 333–364.
 577 <https://doi.org/10.3390/cleantechnol2030021>
 578 Kim, J., Song, Y., Shinn, Y., Kwon, Y., Jung, W., Sung, W., 2019. A study of CO₂ storage
 579 integrity with rate allocation in multi-layered aquifer. *Geosci. J.* 23, 823–832.
 580 Kim, Y., Jang, H., Kim, J., Lee, J., 2017. Prediction of storage efficiency on CO₂ sequestration
 581 in deep saline aquifers using artificial neural network. *Appl. Energy* 185, 916–928.
 582 <https://doi.org/10.1016/j.apenergy.2016.10.012>
 583 Kumar, A., Ozah, R., Noh, M., Pope, G.A., Bryant, S., Sepehrnoori, K., Lake, L.W., 2005.
 584 Reservoir Simulation of CO₂ Storage in Deep Saline Aquifers. *SPE J.* 10, 336–348.
 585 <https://doi.org/10.2118/89343-PA>
 586 Lee, J.H., Park, Y.C., Sung, W.M., Lee, Y.S., 2010. A simulation of a trap mechanism for the
 587 sequestration of CO₂ into goraev aquifer, Korea. *Energy Sources, Part A Recover. Util.*
 588 *Environ. Eff.* 32, 796–808. <https://doi.org/10.1080/15567030903436822>
 589 Li, Y.H., Shen, C.H., Wu, C.Y., Hsieh, B.Z., 2020. Numerical study of CO₂ geological storage
 590 in saline aquifers without the risk of leakage. *Energies* 13.
 591 <https://doi.org/10.3390/en13205259>
 592 Liner, C.L., Geng, P., Zeng, J., King, H., Li, J., 2011. A CO₂ Sequestration Simulation Case
 593 Study at the Dickman Field, Ness Co., Kansas, in: *SPE Annual Technical Conference and*

Exhibition. Denver, Colorado, USA, pp. 1–15.

Liu, D., Li, Y., Agarwal, R., 2020. Evaluation of CO₂ Storage in a Shale Gas Reservoir Compared to a Deep Saline Aquifer in the Ordos Basin of China. *Energies* 13.

Mahdaviara, M., Nait, M., Hemmati-sarapardeh, A., 2021. Toward smart schemes for modeling CO₂ solubility in crude oil : Application to carbon dioxide enhanced oil recovery. *Fuel* 285, 119147. <https://doi.org/10.1016/j.fuel.2020.119147>

Mohajeri, M., Shariatipour, S., 2019. Evaluation of enhancing CO₂ sequestration by post-brine injection under different scenarios using the E300 compositional simulator. *Pet. Res.* 4, 314–333. <https://doi.org/10.1016/j.ptlrs.2019.08.001>

Nghiem, L., Shrivastava, V., Kohse, B., Hassam, M., Yang, C., 2009. Simulation of Trapping Processes for CO₂ Storage in Saline Aquifers.

Nghiem, Long, Yang, C., Shrivatava, V., Kohse, B., Hassam, M., Chen, D., Card, C., 2009. Optimization of Residual Gas and Solubility Trapping for CO₂ Storage in Saline Aquifers. *Soc. Pet. Eng.* 1–9. <https://doi.org/10.1016/j.egypro.2009.02.079>

Noushabadi, M.J., Training, T.I.F.P., Brisset, A., Thibeau, S., 2018. Investigation of CO₂ Storage Security Increase by Brine Alternative CO₂ Injection WAG _ CCS, in: Abu Dhabi International Petroleum Exhibition & Conference. Abu Dhabi, UAE, pp. 1–13.

Pedregosa, F., Weiss, R., Brucher, M., 2011. Scikit-learn : Machine Learning in Python. *J. of Machine Learn. Res.* 12, 2825–2830.

Pham, V.T.H., Riis, F., Gjeldvik, I.T., Halland, E.K., Tappel, I.M., Aagaard, P., 2013. Assessment of CO₂ injection into the south Utsira-Skade aquifer, the North Sea, Norway. *Energy* 55, 529–540. <https://doi.org/10.1016/j.energy.2013.03.026>

Sarkarfarshi, M., Malekzadeh, F.A., Gracie, R., Dusseault, M.B., 2014. Parametric sensitivity

analysis for CO₂ geosequestration. *Int. J. Greenh. Gas Control* 23, 61–71.

<https://doi.org/10.1016/j.ijggc.2014.02.003>

Schmalensee, R., Stoker, T.M., Judson, R.A., 1998. World carbon dioxide emissions: 1950 –

2050. *Rev. Econ. Stat.* 80, 15–27. <https://doi.org/https://doi.org/10.1162/003465398557294>

Schölkopf, B., Smola, A.J., 2002. *Learning with Kernels: Support Vector Machines,*

Regularization, Optimization, and Beyond. MIT Press.

Shin, Y., Kim, Taekgeun, Hong, Seoksu, Lee, S., Lee, E., Hong, Seungwoo, Lee, C., Kim,

Taeyeon, Park, M.S., Park, J., Heo, T., n.d. Prediction of Chlorophyll- a Concentrations in

the Nakdong River Using Machine Learning Methods.

Sifuentes, W., Blunt, M.J., Giddins, M. a., 2009. Modeling CO₂ Storage in Aquifers : Assessing

the Key Contributors to Uncertainty. *SPE Offshore Eur. Oil Gas Conf. Exhib.* SPE123582.

<https://doi.org/10.2118/123582-MS>

Singh, M., Chaudhuri, A., Reza, M., Stauffer, P.H., 2021. Coupled multiphase flow and transport

simulation to model CO₂ dissolution and local capillary trapping in permeability and

capillary heterogeneous reservoir. *Int. J. Greenh. Gas Control* 108.

<https://doi.org/10.1016/j.ijggc.2021.103329>

Sohal, M.A., Le, Y., Audigane, P., Dios, J.C. De, Rigby, S.P., 2021. Effect of geological

heterogeneities on reservoir storage capacity and migration of CO₂ plume in a deep saline

fractured carbonate aquifer. *Int. J. Greenh. Gas Control* 108.

Soltanian, M.R., Amooie, M.A., Cole, D.R., Graham, D.E., Hosseini, S.A., Hovorka, S., Pfiffner,

S.M., Phelps, T.J., Moortgat, J., 2016. Simulating the Cranfield geological carbon

sequestration project with high-resolution static models and an accurate equation of state.

Int. J. Greenh. Gas Control 54, 282–296. <https://doi.org/10.1016/j.ijggc.2016.10.002>

640 Song, Y., Sung, W., Jang, Y., Jung, W., 2020. Application of an artificial neural network in
 641 predicting the effectiveness of trapping mechanisms on CO₂ sequestration in saline
 642 aquifers. *Int. J. Greenh. Gas Control* 98, 103042.
 643 <https://doi.org/10.1016/j.ijggc.2020.103042>
 644 Sung, R.T., Li, M.H., Dong, J.J., Lin, A.T.S., Hsu, S.K., Wang, C.Y., Yang, C.N., 2014.
 645 Numerical assessment of CO₂ geological sequestration in sloping and layered
 646 heterogeneous formations: A case study from Taiwan. *Int. J. Greenh. Gas Control* 20, 168–
 647 179. <https://doi.org/10.1016/j.ijggc.2013.11.003>
 648 Sutton, C.D., 2005. Classification and Regression Trees, Bagging, and Boosting. *Handb.*
 649 *of Statistics* 24, 303–329. [https://doi.org/10.1016/S0169-7161\(04\)24011-1](https://doi.org/10.1016/S0169-7161(04)24011-1)
 650 Szulczewski, M.L., Macminn, C.W., Herzog, H.J., Juanes, R., 2012. Lifetime of carbon capture
 651 and storage as a climate-change mitigation technology. *Proc. Natl. Acad. Sci.* 109, 5185–
 652 5189. <https://doi.org/10.1073/pnas.1115347109>
 653 Vapnik, V.N., 2013. *The Nature of Statistical Learning Theory*. Springer New York.
 654 Vo Thanh, H., Sugai, Y., Nguele, R., Sasaki, K., 2020a. Robust optimization of CO₂
 655 sequestration through a water alternating gas process under geological uncertainties in Cuu
 656 Long Basin, Vietnam. *J. Nat. Gas Sci. Eng.* <https://doi.org/10.1016/j.jngse.2020.103208>
 657 Vo Thanh, H., Sugai, Y., Nguele, R., Sasaki, K., 2020b. Robust optimization of CO₂
 658 sequestration through a water alternating gas process under geological uncertainties in Cuu
 659 Long Basin, Vietnam. *J. Nat. Gas Sci. Eng.* 76, 103208.
 660 <https://doi.org/10.1016/j.jngse.2020.103208>
 661 Vo Thanh, H., Sugai, Y., Nguele, R., Sasaki, K., 2019. Integrated workflow in 3D geological
 662 model construction for evaluation of CO₂ storage capacity of a fractured basement reservoir

663 in Cuu Long Basin, Vietnam. *Int. J. Greenh. Gas Control* 90, 102826.
 664 <https://doi.org/10.1016/j.ijggc.2019.102826>
 665 Vo Thanh, H., Sugai, Y., Sasaki, K., 2020c. Impact of a new geological modelling method on the
 666 enhancement of the CO₂ storage assessment of E sequence of Nam Vang field, offshore
 667 Vietnam. *Energy Sources, Part A Recover. Util. Environ. Eff.* 42, 1499–1512.
 668 <https://doi.org/10.1080/15567036.2019.1604865>
 669 Vo Thanh, H., Sugai, Y., Sasaki, K., 2020d. Application of artificial neural network for
 670 predicting the performance of CO₂ enhanced oil recovery and storage in residual oil zones.
 671 *Sci. Rep.* 10, 18204. <https://doi.org/10.1038/s41598-020-73931-2>
 672 Xiao, T., McPherson, B., Esser, R., Jia, W., Moodie, N., Chu, S., Lee, S.Y., 2019. Forecasting
 673 commercial-scale CO₂ storage capacity in deep saline reservoirs: Case study of Buzzard's
 674 bench, Central Utah. *Comput. Geosci.* 126, 41–51.
 675 <https://doi.org/10.1016/j.cageo.2018.12.006>
 676 Xu, R., Zeng, K., Zhang, C., Jiang, P., 2017. Assessing the feasibility and CO₂ storage capacity
 677 of CO₂ enhanced shale gas recovery using Triple-Porosity reservoir model. *Appl. Therm.*
 678 *Eng.* 115, 1306–1314. <https://doi.org/10.1016/j.applthermaleng.2017.01.062>
 679 Zapata, Y., Kristensen, M.R., Huerta, N., Brown, C., Kabir, C.S., Reza, Z., 2020. CO₂
 680 geological storage: Critical insights on plume dynamics and storage efficiency during long-
 681 term injection and post-injection periods. *J. Nat. Gas Sci. Eng.* 83, 103542.
 682 <https://doi.org/10.1016/j.jngse.2020.103542>
 683 Zhang, D., Qian, L., Mao, B., Huang, C.A.N., Huang, B.I.N., 2018. A Data-Driven Design for
 684 Fault Detection of Wind Turbines Using Random Forests and XGboost. *IEEE Access* 6,
 685 21020–21031. <https://doi.org/10.1109/ACCESS.2018.2818678>

686 Zhang, J., Feng, Q., Zhang, X., Shu, C., Wang, S., Wu, K., 2020. A Supervised Learning
687 Approach for Accurate Modeling of CO₂ – Brine Interfacial Tension with Application in
688 Identifying the Optimum Sequestration Depth in Saline Aquifers. *Energy & Fuels* 34, 7353–
689 7362. <https://doi.org/10.1021/acs.energyfuels.0c00846>
690 C.R. Goodall, Computation using the QR decomposition, Chapman Hall. *Handb. Mod. Stat.*
691 *Methods* 9 (1993) 467–508, [https://doi.org/10.1016/S0169-7161\(05\)80137-3](https://doi.org/10.1016/S0169-7161(05)80137-3).
692 A. Hemmati-Sarapardeh, F. Ameli, B. Dabir, M. Ahmadi, A.H. Mohammadi, On the evaluation
693 of asphaltene precipitation titration data: modeling and data assessment, *Fluid Phase*
694 *Equilib.* 415 (2016) 88–100.
695