Research Article
Numerical Modeling Study on Mineral Alteration and Sealing Performance for CO₂ Geological Sequestration with Enhancing Water Recovery in Hydraulic Fractured Shale Reservoirs

Maosen Yan,1,2 Chi Ai,2 Xiaofei Fu,1 Jun Zhang,2 Xu Han,2 Ziyuan Cong,3 Fahao Yu,4 Wei Li,2 and Yuwei Li1,2,3

1Key Laboratory of Continental Shale Hydrocarbon Accumulation and Efficient Development, Ministry of Education, Northeast Petroleum University, Daqing 163318, China
2Department of Petroleum Engineering, Northeast Petroleum University, Daqing 163318, China
3School of Environment, Liaoning University, Shenyang 110036, China
4Bohai Oilfield Research Institute, CNOOC Tianjin Branch Company, Tianjin 300459, China

Correspondence should be addressed to Yuwei Li; liyuweibox@126.com
Received 22 June 2021; Accepted 21 October 2021; Published 19 November 2021

Academic Editor: Hao Liu

Copyright © 2021 Maosen Yan et al. Exclusive Licensee GeoScienceWorld. Distributed under a Creative Commons Attribution License (CC BY 4.0).

Recently, CO₂ geological sequestration combined with enhancing deep saline water/brine recovery is regarded as a potential strategic choice for reduction of CO₂ emissions. This technology not only achieves the relatively secure storage of CO₂ which was captured during industrial processes but also can enhance the recovery of water for drinking, industrial, and agricultural utilization. However, the impact of CO₂-water-rock reactions on the shale reservoir in the system is unclear and the sealing performance of mudstone caprock has not been investigated. For analyzing the mechanism of mineral alteration in the shale reservoir, a three-dimensional injection-production model in the double-fractured horizontal well pattern is established according to actual parameters of shale and mudstone layers. In addition, mineral alteration was characterized and caprock sealing performance was also assessed. Numerical results showed that the presence of CO₂ can lead to the dissolution of k-feldspar, oligoclase, chlorite, and dolomite and the precipitation of clay minerals such as kaolinite, illite, and smectite (Ca-smectite and Na-smectite). Due to positive ion released by dissolved primary minerals, the precipitation of secondary carbonate occurs including ankerite and dawsonite, which induces the mineral sequestration capacity of the shale reservoir. The amount of CO₂ sequestration by mineral is 51430.96 t after 200 years, which equals 23.47% of the total injection (219145.34 t). Besides, the height of the sealing gas column is used for evaluating the sealing performance of the shale-mudstone interface. Results show that the height of the sealing gas column at the interface above the injection well is lower but the maximum value of CO₂ gas saturation is only 0.00037 after 200 years. The height of the sealing gas column at the interface is greater than 800 m, which can be classified as level II and guarantee the security of the CO₂ storage. The analysis results provide reliable guidance and reference for the site selection of CO₂ geological sequestration.

1. Introduction

Carbon dioxide (CO₂) has contributed to the major increase in the atmospheric concentration of greenhouse gas, which is mainly caused by the combustion of fossil fuels in power plants and other industrial processes. In recent years, carbon capture and storage (CCS) has been widely regarded as one of the effective methods to achieve the reduction of CO₂ emissions [1]. Instead of injection into saline aquifers, carbon capture utilization and storage (CCUS) is considered as a better option for economic benefit, such as CO₂-EGS and CO₂-EOR [2, 3] Nowadays, a novel approach of CCUS is proposed, which is called the CO₂ geological storage combined with deep saline water/brine recovery (CCS-EWR).
This technology has shown the potential of simultaneously increasing the CO₂ storage and producing the underground water from the aquifers [4].

Due to CO₂ injection into the formation, CO₂-water-rock chemical interactions will induce mineral alteration. Cui et al. [5] established a comprehensive reactive transport model. Meanwhile, they carried out a series of simulation to analyze the effect of CO₂-water-rock geochemical reactions on reservoir physical properties. Actually, initial mineral composition plays a vital role in CO₂-water-rock reactions during CO₂ geological sequestration [6]. On the basis of a dataset from the test well of Knox saline reservoir in Kentucky, Zhu et al. [7] used 2-D radial-reactive transport models to evaluate mineral dissolution and precipitation. Results from the kinetic models suggested that if dawsonite is suppressed, the mineral trapping is essentially nonexistent. Wang et al. [8] developed radial models to determine the impacts of mineralogical compositions on trapping amounts for the CO₂ geological storage. Their study indicated that dissolution of chlorite is beneficial to the formation of secondary carbonate minerals and CO₂ mineral trapping. Xu et al. [9] employed a 2-D horizontal model in a five-spot well pattern and studied on the rock-fluid interaction for a CO₂-based geothermal system.

Acting as a seal for CO₂ rising from the reservoir, the caprock must be able to withstand the changes in physical and chemical properties due to the CO₂-brine-rock mineral interactions [10]. Gherardi et al. [11] presented 1-D and 2-D numerical simulations of reactive transport in the process of CO₂ geological storage. The simulation results demonstrated that the occurrence of CO₂ leakage from the reservoir may have an influence on the geochemical evolution of the caprock. Tian et al. [12] considered clay-rich shale and mudstone as two types of caprock for modeling analyses. Their results indicate that the mudstone is more suitable to be used as a caprock. Na et al. [13] used reaction experiments under in situ reservoir pressure conditions of 35 MPa and various temperatures (from 150 to 170 °C) to analyze mineral alteration induced by mixtures of CO₂ and water. After 12 days CO₂-brine-rock reaction, XRD and SEM analysis results indicated that the existence of CO₂ induced the dissolution of primary rock minerals such as calcite and feldspar. Thus, the precipitation of secondary carbonate (calcite and ankerite) was observed. Both geochemical recovery and CO₂ geological storage could be achieved by the above geochemical processes. Khather et al. [14] carried out core-flood experiments to evaluate changes in the properties of dolostone samples. Overall, a slight increase in the porosity was observed in most samples, which might be caused by the dissolution of carbonate (dolomite and calcite). Wollenweber et al. [15] studied the effects of high-pressure CO₂ exposure on fluid transport properties and mineralogical composition of two pelitic caprocks, a limestone, and a clay-rich marl lithotype. In repetitive gas breakthrough experiments, the capillary CO₂ sealing efficiency of the initially water-saturated sample plugs was found to decrease for both caprocks. Espinoza and Santamaria [16] measured the breakthrough pressure and ensuing CO₂ permeability through homogeneous specimens made of sand, silt, kaolinite, and smectite. Their experimental results and data gathered from previous studies highlight the inverse relationship between breakthrough pressure and pore size, as anticipated by Laplace’s equation.

Compared with traditional CCUS methods, CCS-EWR has two advantages: (1) on the basis of reasonable pumping well engineering design, reservoir pressure release and water production can be controlled to achieve the safety and stability of large-scale CO₂ geological sequestration and (2) deep saline water can be collected and treated for life drinking, industrial, and/or agricultural utilizations to alleviate water shortage as well as ecological impact [17]. Shale has the potential to store a portion of the injected CO₂ into the reservoir [18]. Once shale gas is depleted from shale, CO₂ could be trapped in the reservoirs by taking advantage of the newly available pore space and existing well infrastructure [19, 20]. In this study, a simulation model was established to perform the CCS-EWR process in the shale reservoir. However, each CCUS system may behave differently due to differences in compositions of brine and rock. For this reason, it’s advisable to perform a specific case study for each type of reservoir before the CO₂ sequestration process [21]. Thus, the numerical simulation method was employed in this study to investigate the CO₂-brine-rock interaction occurring in the CCS-EWR system. Meanwhile, mineral trapping capacity and sealing performance of caprock were assessed.

2. Simulation Approach

2.1. Governing Equations. The governing equations used in this study have been discussed in detail by Xu et al. [24]. All flow and transport equations can be derived from the principle of mass conservation. In this study, heat transfer was not considered, so mass transfer can be denoted as equations (1) and (2).

\[
\frac{\partial M}{\partial t} = -\nabla F + q, \quad (1)
\]

\[
u_\beta = -\frac{\eta_\beta}{\mu_\beta} \left( \nabla P - \rho_\beta g \right) \quad (\beta = l, g), \quad (2)
\]

where \(M\) is mass accumulation, kg/m³, \(t\) is time step, \(F\) is mass flux, kg/m²/s, and \(q\) is source/sink terms, kg/m²/s. Equation (2) is the expression of Darcy’s law. Subscript \(\beta\) is the phase index which can be represented as \(l\) (liquid phase) and \(g\) (gas phase). In equation (2), \(u\) is Darcy velocity, m/s, \(\eta\) is permeability, m², \(\eta_\beta\) is relative permeability, \(\mu\) is viscosity, kg/m/s, \(P\) is pressure, Pa, \(\rho\) is density, kg/m³, and \(g\) is acceleration of gravity, 9.8 m/s². Water and CO₂ transport equations can be represented as equation (3). Where \(\phi\) is porosity, \(S\) is saturation, and \(X\) is the mass fraction.
Water and CO₂ transport equations can be represented as equation (3), where \( \phi \) is porosity, \( S \) is saturation, and \( X \) is the mass fraction. Because CO₂ is subject to local chemical interactions, \( q_j \) is a part of source/sink terms which takes part in chemical reactions.

\[
\begin{align*}
\text{Water} & \quad \left\{ \begin{array}{l}
M_w = \phi \left( S_i \rho \xi_X \omega + S_g \rho_g \xi_X \omega_g \right), \\
F_w = X_{w \omega} \rho \xi \mu + X_{w \omega} \rho_g \xi \mu_g,
\end{array} \right. \\
q_w = q_{w \omega} + q_{w \omega_g}, \\
(3)
\end{align*}
\]

Chemical components

\[
\begin{align*}
M_j & = \phi S_j C_j, \\
F_j &= \mu C_j - \left( \tau \phi S_j D_j \right) \nabla C_j, \quad (j = 1, 2, \ldots, N), \\
q_j &= q_{j \omega} + q_{j \omega_g} + q_{j \omega_g}, \\
\end{align*}
\]

2.2. Model Setup. In this study, a three-dimensional model was developed with the size of 1000 m x 700 m x 119.33 m. As shown in Figure 1, the formation consists of two parts, which are shale and mudstone. At their interface, a thin layer is divided from mudstone to monitor the evolution characteristic of the mudstone layer. Shale #2 is the injection reservoir which has already been hydrofractured. Considering the actual exploring mode of shale gas, the double-horizontal well pattern was employed for the current simulation study. The distance between the injection well and the production well is 300 m, and the spacing of the fracture is 100 m. With the injection rate of 0.3472 kg/s (30 t/day), the entire injection time is 20 years. After half-year injection, the production well is activated with the rate of 0.2 kg/s. When the injection period is ceased, we monitor the model for additional 180 years.

2.3. Initial Conditions and Parameters. Simulation was carried out for isothermal condition at 97.3°C, which corresponds to the values measured at the top of the shale gas reservoir in the X site. According to the fluid flow test results of the core, the basic data (i.e., density, porosity, and permeability) was acquired. It should be noted that the core sample of shale came from three depths (2554.36 m, 2581.59 m, and 2593.87 m) but their results of porosity and permeability are very close. Therefore, we use the average value of porosity and permeability as shown in Table 1.

The pore pressure of the shale gas reservoir (shale #2) is 26.8 MPa which has been measured, and the pore pressure equilibrium is required before simulation solution. The pressure equilibrium simulation was conducted firstly, and the results are used for the initial pore pressure condition which is shown as Figure 2.

As shown in Table 1, rock grain density, porosity, and permeability are obtained by rock sample test. Parameters of relative permeability and capillary pressure for rock matrix are from Tian et al. [22]. Due to the existence of the hydraulic fracture, the MINC method is adopted which is used for modeling the fluid flow in fractured-porous media [23]. On the basis of hydraulic fracturing design and microseismic data, fracture basic data was obtained as shown in Table 2.

2.4. Mineralogy and Aqueous Composition. According to X-ray diffraction (XRD) mineralogical analysis of core samples from mudstone and shale in the X site, mudstone consists mainly of quartz and clay minerals (i.e., kaolinite, chlorite, illite, and smectite). For shale samples from three depths, their mineral compositions are obviously different from each other. In Table 3, primary minerals mean existing at the beginning of the simulation and secondary means minerals could be formed after simulations. For revealing the process of mineral evolution, three common secondary minerals are specified which could be formed after CO₂ injection.

Initial aqueous composition used in the model (Table 4) is based on water samples taken from a nearby well completed in the X site.

2.5. Thermodynamic and Kinetic Parameters. The present simulation was performed with the TOUGHREACT code, which is a comprehensive multicomponent reactive fluid flow and geochemical transport simulator [24]. In this code, the primary source used for equilibrium constants of aqueous species and minerals is originally obtained from EQ3/6 V7.2b database [25]. Moreover, a portion of thermodynamic properties of several minerals and aqueous species has been revised on the basis of Xu et al. [26]. In the modeling of geochemical systems, a subset of aqueous species is selected as basis species and all other species (including aqueous complexes, minerals, and gaseous species) are referred to as secondary species. The kinetic rate law is used to describe the dissolution and precipitation of minerals. In TOUGHREACT, the rate expression in equation (5) given by Lasaga et al. [27] is employed for the simulation of mineral reactions.

\[
r_m = f \left( c_1, c_2, \ldots, c_{N_c} \right) = \pm k_m A_m \left[ 1 - \Omega_m \right]^{\eta}, \quad (5)
\]

The positive and negative signs of \( r_m \) in equation (5) indicate dissolution and precipitation, respectively. \( k_m \) is the rate constant which is temperature and pH dependent.
Am is the specific reactive surface area per kg H$_2$O of each mineral, and $\Omega_m$ is the kinetic mineral saturation ratio. $\theta$ and $\eta$ are two constants which depend on experimental data, and they are taken equal to 1 in this study. The rate constant $k_m$ is calculated on the basis of reaction rate constant at 25°C, $k_{25}$, and activation energy $E_a$ with equation (6) given by Palandri and Kharaka [28]. Furthermore, the rate constant includes three mechanisms including neutral, acid, and base, which are expressed by subscripts $nu$, H, and OH, respectively. $R$ is the gas constant and $T$ is the absolute temperature. The term $a$ is the activity of the species, and $n$ is the power term (constant).

\[
k = k_{25}^{nu} \exp \left[ \frac{-E_n^{nu}}{R} \left( \frac{1}{T} - \frac{1}{298.15} \right) \right]^{a_n^{nu}} + k_{25}^H \exp \left[ \frac{-E_n^{H}}{R} \left( \frac{1}{T} - \frac{1}{298.15} \right) \right]^{a_n^H} + k_{25}^{OH} \exp \left[ \frac{-E_n^{OH}}{R} \left( \frac{1}{T} - \frac{1}{298.15} \right) \right]^{a_n^{OH}}. \tag{6}
\]

The parameters for calculating kinetic rate constants of minerals are presented in Table 5. Note that (1) $A$ is the specific surface area, $k_{25}$ is kinetic constant at 25°C, $E_a$ is

---

**Table 1: Initial values for hydrogeological parameters.**

| Parameters                          | Shale     | Mudstone  |
|-------------------------------------|-----------|-----------|
| Temperature ($^\circ$C)             | 97.3      | 97.3      |
| Rock grain density (kg/m$^3$)       | 2120      | 2350      |
| Porosity                           | 0.0352    | 0.0127    |
| Permeability (m$^2$)                | 2.35 × 10$^{-17}$ | 7.30 × 10$^{-19}$ |

Liquid relative permeability, parameters for the van Genuchten-Mualem (van Genuchten, 1980) function: $k_{rl} = \sqrt{S^\ast \left(1 - \left(1 - (S^\ast)^{1/\lambda} \right)^{2} \right)}$, where, $S^\ast = (S_t - S_{lr})/(S_{ls} - S_{lr})$

$\lambda = 0.475$, $S_{lr} = 0.3$, $S_{ls} = 1.0$

Gas relative permeability, parameters for the Corey (Corey, 1954) model: $k_{rg} = (1 - S^\wedge)^2 (1 - S^\wedge^2)$, here, $S^\ast = (S_t - S_{lr})/(S_{ls} - S_{lr})$

$S_{gr} = 0.05$

Capillary pressure, parameters for the van Genuchten (1980) function: $P_{cap} = -P_0 \left(\left[S^\ast\right]^{-1/\lambda} - 1 \right)^{1-\lambda}$, here, $S^\ast = (S_t - S_{lr})/(S_{ls} - S_{lr})$

$\lambda = 0.475$, $S_{lr} = 0.2$, $S_{ls} = 0.999$

$P_{max}$ (Pa) $1.0 \times 10^7$, $1.0 \times 10^8$

$P_0$ (a) $2.4 \times 10^5$, $2.1 \times 10^6$
activation energy, and $n$ is the power term (equation (6)); (2) the power term $n$ for both acid and base mechanisms is with respect to $H^+$; and (3) for pyrite, the neutral mechanism has $n$ with respect to $O_2(aq)$ and the base mechanism has two species involved: one $n$ with respect to $H^+$ and another $n$ with respect to $Fe^{3+}$. The reaction kinetic data of minerals are listed in Table 5, which are given by Tian et al. [22], Liu et al. [29], Yang et al. [30], and Xu et al. [31].

3. Results and Discussion

3.1. Mineral Alteration in the Shale Layer. As shown in Figure 3, with the injection of $CO_2$ into the shale layer, $CO_2$ saturation close to the injection well reaches the maximum value 0.54 after 20 years. Due to dissolution of $CO_2$ into groundwater, pH decreases to 4.98 which will induce dissolution of primary minerals and precipitation of secondary minerals in the shale layer.

Figure 4 shows the dissolved primary minerals including K-feldspar, oligoclase, chlorite, and dolomite. Because of the larger kinetic constant, dolomite dissolves more severely and easier to reach the equilibrium state, which results in a smaller dissolution volume fraction in hydraulic fractures. Meanwhile, the change of $Ca^{2+}$ concentration which is caused by dolomite dissolution affects oligoclase dissolution. Due to larger permeability, sufficient reaction cannot occur in fractures which leads K-feldspar and chlorite to dissolve obviously around fractures.

Figure 5 shows changes in the volume fraction of quartz and clay minerals. Precipitation of clay minerals requires $SiO_2(aq)$ and $AlO_2^-$ provided by the dissolution of feldspar minerals and chlorite. Illite is precipitated in the period of injection. K-Feldspar provides $K^+$ which is needed for illite precipitation, so the spatial distribution of changes in volume fractions of illite precipitation and K-feldspar dissolution negatively correlates. The dissolution of Na- and Ca-bearing oligoclase supplies $Na^+$ and $Ca^{2+}$ for the precipitation of smectite-Na and smectite-Ca; thus, both are formed with a volume fraction amount of about 0.0019 near hydraulic fractures. Meanwhile, a small amount of quartz is precipitated.

Figure 6 shows changes in the volume fraction of carbonate. Calcite dissolution occurs close to the injection side, which is with a volume fraction about 0.0069 near hydraulic fractures. $Mg^{2+}$ is released by dissolution of chlorite and dolomite, and it causes magnesite precipitation. At the same time, precipitation of secondary carbonate ankerite and dawsonite is obtained. All of the precipitation of the above carbonate will eventually increase the effective mineral trapping capacity of $CO_2$ in the shale layer.

Porosity changes are induced by mineral dissolution-precipitation reactions. Therefore, porosity can be calculated by the following relationship [32]:

$$\phi = 1 - \sum_{m=1}^{nm} fr_m - fr_p,$$

where $nm$ is the number of minerals, $fr_m$ is the volume fraction of mineral $m$ in the rock ($V_{mineral}/V_{medium}$, including porosity), and $fr_p$ is the volume fraction of nonreactive rock.

As shown in Figure 7, because of mineral alteration in the period of injection, the porosity of the shale layer decreases slightly which causes small changes in permeability. But those tiny decreases will not significantly lower the connectivity of the shale layer.

3.2. $CO_2$ Mineral Trapping of the Shale Layer. Carbonate dissolution enhances the effect on the $CO_2$ trapping capacity of the shale layer, and it is of great significance to $CO_2$ storage. According to the result of $CO_2$ sequestration by mineral (SMCO$_2$, kg/m$^3$ medium) in Figure 8, the performance of $CO_2$ mineral trapping is consistent with precipitation of carbonate which includes magnesite, ankerite, and dawsonite.

The amount of $CO_2$ trapped in mineral increases significantly in the process of injection, and the rate of increase obviously reduces after injection stops. The amount of $CO_2$ sequestration by mineral is 51430.96 t after 200 years which
The results show that the current CCS-EWR system has an excellent effect on CO$_2$ mineral trapping.

3.3. Sealing Performance of the Mudstone Layer. Since the section of the caprock affected by geochemical reactions is very thin, mineral trapping of CO$_2$ in the caprock can be negligible [33]. The injected CO$_2$ plume initially migrates towards the top of the shale reservoir due to buoyancy until it reaches the mudstone layer. Hence, the mudstone layer above the shale layer is the key to prevent CO$_2$ from large leakage, whose sealing performance would ensure the security of the CCS-EWR system. In Figure 9, the simulation results show that the porosity of the shale-mudstone interface above the injection well increases from the initial value of 0.0127 to the maximum value of 0.0180 after 200 years. Those increases will induce small leakage of CO$_2$. The results of CO$_2$ gas saturation after 200 years show that maximum value is only 0.00037; hence, the large amount of CO$_2$ leakage does not occur.

When the CO$_2$ fluid pressure in the reservoir exceeds the breakthrough pressure, CO$_2$ may migrate through the water-saturated pore network of caprock. The relationship between breakthrough pressure and the pore throat with an equivalent radius $r$ can be expressed as the Washburn equation:

$$P_c = \frac{2\sigma \cos \theta}{r},$$  \hspace{1cm} (8)

where $P_c$ is the breakthrough pressure, MPa, $\sigma$ is interfacial tension between the liquid phase and the gaseous phase, N/m, $\theta$ is the wetting (contact) angle between the wetting fluid and the mineral surface, and $r$ is the equivalent radius of the pore throat, m.

The breakthrough pressure of caprock can be converted to the height of the sealing gas column (HSGC), which is used for evaluating the sealing performance of caprock. Once the gas column exceeds HSGC of the caprock-reservoir interface, CO$_2$ will displace the upper fluid of formation and escape through caprock. Ultimately, it will cause the failure of the caprock sealing system and the significant leak of CO$_2$. HSGC of the caprock-reservoir interface under CO$_2$ leakage, whose sealing performance would ensure the security of the CCS-EWR system.

| Mineral | Chemical formula | Mudstone | Shale #1 | Shale #2 | Shale #3 |
|---------|------------------|----------|----------|----------|----------|
| Calcite | CaCO$_3$         | 0.0096   | 0.0853   | 0.1672   | 0.3103   |
| Chlorite| Mg$_{52}$Fe$_{25}$Al$_2$Si$_{10}$O$_{10}$(OH)$_8$ | 0.0385   | 0.2351   | 0.1427   | 0.1361   |
| Dolomite| CaMg(CO$_3$)$_2$ | 0.0194   | 0.0558   | 0.0638   | 0.0755   |
| Illite  | $K_{0.4}Mg_{0.3}Al_{1.7}Si_{2}O_{10}$(OH)$_2$ | 0.1253   | 0.1064   | 0.0981   | 0.0778   |
| K-Feldspar| KAlSi$_3$O$_8$ | 0.0520   | 0.0382   | 0.0617   | 0.0295   |
| Kaolinite| Al$_2$SiO$_3$(OH)$_4$ | 0.0211   | 0.0616   | 0.0624   | 0.0505   |
| Oligoclase| CaNa$_2$Al$_2$Si$_4$O$_{10}$ | 0.0030   | 0.0737   | 0.0525   | 0.0388   |
| Quartz | SiO$_2$ | 0.5216   | 0.1338   | 0.1167   | 0.1223   |
| Ca-Smectite | $Ca_{0.145}Mg_{0.26}Al_{1.77}Si_{2}O_{10}$(OH)$_2$ | 0.1268   | 0.0728   | 0.0758   | 0.0739   |
| Na-Smectite | $Na_{0.29}Mg_{0.26}Al_{1.77}Si_{2}O_{10}$(OH)$_2$ | 0.0827   | 0.0840   | 0.0669   | 0.0505   |
| Hematite | FeO$_3$ | 0.0090   | 0.0247   | 0.0153   |          |
| Pyrite | FeSO$_4$ | 0.0153   | 0.0380   | 0.0827   | 0.0505   |
| Magnesite | MgCO$_3$ | 0.0038   | 0.0400   | 0.0040   | 0.0010   |
| Siderite | FeCO$_3$ | 0.0252   | 0.0255   | 0.0113   |          |

| Component | Shale | Mudstone |
|-----------|-------|----------|
| AlO$_2^-$ | $0.174 \times 10^{-8}$ | $0.890 \times 10^{-8}$ |
| Ca$^{2+}$ | $0.870 \times 10^{-3}$ | $0.230 \times 10^{-4}$ |
| Cl$^-$ | $0.929 \times 10^{-3}$ | $0.938 \times 10^{-3}$ |
| Fe$^{3+}$ | $0.773 \times 10^{-6}$ | $0.111 \times 10^{-6}$ |
| HCO$_3^-$ | $0.361 \times 10^{-4}$ | $0.364 \times 10^{-4}$ |
| K$^+$ | $0.100 \times 10^{-4}$ | $0.167 \times 10^{-4}$ |
| Mg$^{2+}$ | $0.125 \times 10^{-5}$ | $0.161 \times 10^{-5}$ |
| Na$^+$ | $0.136 \times 10^{-3}$ | $0.130 \times 10^{-3}$ |
| SiO$_2$ (aq) | $0.554 \times 10^{-3}$ | $0.213 \times 10^{-4}$ |
| SO$_4^{2-}$ | $0.505 \times 10^{-4}$ | $0.453 \times 10^{-4}$ |
| pH | 7.38 | 6.87 |
Table 5: Parameters for calculating kinetic rate constants of primary and secondary minerals.

| Mineral       | A (cm$^2$/g) | Parameters for kinetic rate law | Parameters for kinetic rate law |
|---------------|--------------|---------------------------------|---------------------------------|
|               |              | Neutral mechanism | Acid mechanism | Base mechanism |
|               |              | $k_{25}$ (mol/m$^2$/s) | $E_a$ (KJ/mol) | $n$(H$^+$) | $k_{25}$ (mol/m$^2$/s) | $E_a$ (KJ/mol) | n(H$^+$) | Ref |
| Albite        | 9.8          | 2.75 x 10$^{-13}$ | 69.8          | 6.92 x 10$^{-11}$ | 65.0 | 0.457 | 2.51 x 10$^{-16}$ | 71.0 | -0.572 | (a) |
| Calcite       | 9.8          | 1.55 x 10$^{-9}$  | 23.5          | 5.01 x 10$^{-4}$  | 14.4 | 1.0   |                     |       |       | (b) |
| Chlorite      | 9.8          | 3.02 x 10$^{-13}$ | 88.0          | 7.76 x 10$^{-12}$ | 88.0 | 0.5   |                     |       |       | (b) |
| Dawsonite     | 9.8          | 1.26 x 10$^{-9}$  | 62.76         | 6.46 x 10$^{-4}$  | 36.1 | 0.5   |                     |       |       | (b) |
| Dolomite      | 9.8          | 2.95 x 10$^{-8}$  | 52.2          | 6.46 x 10$^{-4}$  | 36.1 | 0.5   |                     |       |       | (b) |
| Hematite      | 12.87        | 2.51 x 10$^{-15}$ | 66.2          | 4.07 x 10$^{-10}$ | 66.2 | 1.0   |                     |       |       | (b) |
| Illite        | 151.63       | 1.66 x 10$^{-13}$ | 35.0          | 1.05 x 10$^{-11}$ | 23.6 | 0.34  | 3.02 x 10$^{-17}$ | 58.9 | -0.4  | (b) |
| K-Feldspar    | 9.8          | 3.89 x 10$^{-13}$ | 38.0          | 8.71 x 10$^{-11}$ | 51.7 | 0.5   | 6.31 x 10$^{-22}$ | 94.1 | -0.823| (b) |
| Kaolinite     | 151.63       | 6.92 x 10$^{-14}$ | 22.2          | 4.9 x 10$^{-12}$  | 65.9 | 0.777 | 8.91 x 10$^{-18}$ | 17.9 | -0.472| (d) |
| Magnesite     | 9.8          | 4.57 x 10$^{-10}$ | 23.5          | 4.17 x 10$^{-7}$  | 14.4 | 1.0   |                     |       |       | (b) |
| Oligoclase    | 9.8          | 1.45 x 10$^{-13}$ | 69.8          | 2.14 x 10$^{-11}$ | 65.0 | 0.457 |                     |       |       | (b) |
| Quartz        | 9.8          | 1.02 x 10$^{-14}$ | 87.7          |                     |       |       |                     |       |       | (d) |
| Siderite      | 9.8          | 1.26 x 10$^{-9}$  | 62.76         | 6.46 x 10$^{-4}$  | 36.1 | 0.5   |                     |       |       | (b) |
| Smectite-ca   | 151.63       | 1.66 x 10$^{-13}$ | 35.0          | 1.05 x 10$^{-11}$ | 23.6 | 0.34  | 3.02 x 10$^{-17}$ | 58.9 | -0.4  | (d) |
| Smectite-Na   | 151.63       | 1.66 x 10$^{-13}$ | 35.0          | 1.05 x 10$^{-11}$ | 23.6 | 0.34  | 3.02 x 10$^{-17}$ | 58.9 | -0.4  | (d) |
| Pyrite        | 12.87        | 4.0 x 10$^{-11}$  | 56.9          | 3.02 x 10$^{-8}$  | 56.9 | 2.82 x 10$^{-3}$ | 56.9 | n(H$^+$) = -0.5     | (d) |

n(O$_2$(aq)) = 0.5

n(Fe$^{3+}$) = 0.5

(a) Tian et al. [22]; (b) Liu et al. [29]; (c) Yang et al. [30]; (d) Xu et al. [31].
breakthrough pressure can be calculated as the equation given by Smith [34]:

$$T_h = \frac{P_c}{\left( \rho_w - \rho_{CO_2} \right) g}.$$  \hspace{1cm} (9)

where $\rho_w$ is the density of formation water, kg/m$^3$, $\rho_{CO_2}$ is the density of supercritical CO$_2$ fluid, $g$ is the acceleration of gravity, 9.8 N/kg, and $T_h$ is the column height of gas sealing under $P_c$, m.

The HSGC of shale-mudstone interface after 200 years is presented in Figure 10, and the result shows that HSGCs are all greater than 800 m. The pore size of the shale-mudstone interface above the injection well increases; thus, HSGCs are smaller than those of the above production well. According to the evaluation index in Table 6 [35], generally, HSGC of the mudstone layer can be classified as level II. For maintaining the high sealing performance of caprock in the period of CO$_2$ geological sequestration, it is crucial to take breakthrough pressure into consideration before site selection. Due to the existence of natural cracks, microfractures,
Figure 5: Changes in the volume fraction of quartz, kaolinite, illite, and total smectite (Ca-Smectite and Na-Smectite) (negative values indicate dissolution and positive precipitation) after 200 years. (a) Changes in the volume fraction of quartz. (b) Changes in the volume fraction of kaolinite. (c) Changes in the volume fraction of illite. (d) Changes in the volume fraction of total smectite.

Figure 6: Changes in the volume fraction of calcite, magnesite, ankerite, and dawsonite (negative values indicate dissolution and positive precipitation) after 200 years. (a) Changes in the volume fraction of calcite. (b) Changes in the volume fraction of magnesite. (c) Changes in the volume fraction of ankerite. (d) Changes in the volume fraction of dawsonite.
and fault systems in caprocks, the actual sealing performance of caprock will be worse than theoretical value. Consequently, it is reasonable to take the sealing performance index as high as possible.

4. Discussion

In this study, the conceptual model was established based on a particular depleted shale gas reservoir. The model was built on the assumption that the initial shale gas saturation was 0. In fact, there should have been residual shale gas in the reservoir. The existence of shale gas (CH$_4$) would cause CO$_2$-CH$_4$ competitive adsorption and have an effect on CO$_2$ transport [36–38]. However, this factor was not considered in this study due to the lack of shale gas saturation data.

Deformation of the formation will occur because of CO$_2$ injection. Considering the existence of shale the bedding plane, natural fractures, and faults [39–53], the deformation behavior and the effect on fluid transport will be extremely complicated. The reactivation potential of faults does exist,
which may provide a leak path for CO$_2$ to escape the storage formation [54–56]. In addition, the acid mixture of CO$_2$ and formation water will cause the influence on the strength and fracture behavior and induce the mechanical failure of the reservoir, caprock, or their interface [57, 58]. The fractures caused by mechanical damage will have an impact on the sealing performance of the CCS-EWR system. The next step is to further study the influence of rock mechanical property degradation, natural fracture properties, injection-production rates, and other factors on the sealing performance of the CCS-EWR system and further investigate effective measures for the security of CO$_2$ storage.

### 5. Conclusions

In this paper, according to actual parameters of shale and mudstone layers in the CCS-EWR system, a three-dimensional injection-production model in the double-fractured horizontal well pattern is established to investigate the mechanism of mineral alteration. With the developed model, the mineral sequestration capacity of the shale reservoir is analyzed and the sealing performance of mudstone caprock is assessed. The main conclusions obtained from this research are as follows:

1. Mineral alteration is driven by pH decrease due to the presence of CO$_2$. The dissolved primary minerals include K-feldspar, oligoclase, chlorite, and dolomite. Meanwhile, clay minerals such as kaolinite, illite, and smectite (Ca-smectite and Na-smectite) are precipitated. Because of large permeability, sufficient reaction cannot occur in fractures. Hence, significant mineral alterations are observed around fractures on the side of the injection well.

2. Due to positive ion released by dissolved primary minerals, the precipitation of secondary carbonate occurs including ankerite and dawsonite, which induces the mineral sequestration capacity of the shale reservoir. The amount of CO$_2$ sequestration by mineral is 51430.96 t after 200 years, which equals 23.47% of total injection (219145.34 t).

3. The height of the sealing gas column (HSGC) is used for evaluating the sealing performance of the shale-mudstone interface. Results show that HSGCs of the interface above the injection well are lower because of the decrease of porosity but the maximum value of CO$_2$ gas saturation is only 0.00037 after 200 years. The entire HSGCs of the interface are greater than 800 m, which can be classified as level II and guarantee the security of CO$_2$ storage.

### Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

### Conflicts of Interest

The authors declare no conflict of interest.

### Authors’ Contributions

The conceptualization was done by Yuwei Li; the methodology was done by Maosen Yan and Yuwei Li; the investigation was done by Jun Zhang, Xu Han, and Ziyuan Cong; writing and original draft preparation were done by Maosen Yan and Chi Ai; writing, review, and editing were done by Maosen Yan; visualization was done by Xiaofei Fu, Fahao Yu, and Wei Li.
Acknowledgments

This research was funded by the Opening Fund of Key Laboratory of Continental Shale Accumulation and Development (Northeast Petroleum University), Ministry of Education, Youth Backbone Training Program of Northeast Petroleum University (no. 15041260501), and the Research Start Project of Northeast Petroleum University (no. 1305021857).

References

[1] I. Gaus, "Role and impact of CO\textsubscript{2}-rock interactions during CO\textsubscript{2} storage in sedimentary rocks," *International Journal of Greenhouse Gas Control*, vol. 4, no. 1, pp. 73–89, 2010.

[2] F. Z. Zhang, P. X. Jiang, and R. N. Xu, "System thermodynamic performance comparison of CO\textsubscript{2}-EGS and water-EGS systems," *Applied Thermal Engineering*, vol. 61, no. 2, pp. 236–244, 2013.

[3] N. Kampman, M. Bickle, M. Wigley, and B. Dubacq, "Fluid flow and CO\textsubscript{2}-fluid-mineral interactions during CO\textsubscript{2}-storage in sedimentary basins," *Chemical Geology*, vol. 369, pp. 22–50, 2014.

[4] Q. Li, Y. N. Wei, G. Liu, and H. Shi, "CO\textsubscript{2}-EWR: a cleaner solution for coal chemical industry in China," *Journal of Cleaner Production*, vol. 103, pp. 330–337, 2015.

[5] G. D. Cui, Y. Wang, Z. Rui, B. Chen, S. Ren, and L. Zhang, "Assessing the combined influence of fluid-rock interactions on reservoir properties and injectivity during CO\textsubscript{2} storage in saline aquifers," *Energy*, vol. 155, pp. 281–296, 2018.

[6] D. Q. Liu, Y. Li, and R. K. Agarwal, "Numerical simulation of long-term storage of CO\textsubscript{2} in Yanchang shale reservoir of the Ordos basin in China," *Chemical Geology*, vol. 440, pp. 288–305, 2016.

[7] J. F. Zhu, T. M. Parris, J. Richard Bowersox, and D. C. Harris, "Modeling CO\textsubscript{2}-brine-rock interactions in the Knox Group: implications of a deep carbon storage field test in western Kentucky," *Applied Geochemistry*, vol. 37, pp. 29–42, 2013.

[8] K. R. Wang, T. Xu, H. Tian, and F. Wang, "Impacts of mineralogical compositions on different trapping mechanisms during long-term CO\textsubscript{2} storage in deep saline aquifers," *Acta Geotechnica*, vol. 11, no. 5, pp. 1167–1188, 2016.

[9] T. F. Xu, G. Feng, and Y. Shi, "On fluid-rock chemical interaction in CO\textsubscript{2}-based geothermal systems," *Journal of Geochemical Exploration*, vol. 144, Part A, pp. 179–193, 2014.

[10] R. Shukla, P. Ranjith, A. Haque, and X. Choi, "A review of studies on CO\textsubscript{2} sequestration and caprock integrity," *Fuel*, vol. 89, no. 10, pp. 2651–2666, 2010.

[11] F. Gherardi, T. Xu, and K. Pruess, "Numerical modeling of self-limiting and self-enhancing caprock alteration induced by CO\textsubscript{2} storage in a depleted gas reservoir," *Chemical Geology*, vol. 244, no. 1–2, pp. 103–129, 2007.

[12] H. L. Tian, T. Xu, F. Wang, V. V. Patil, Y. Sun, and G. Yue, "A numerical study of mineral alteration and self-sealing efficiency of a caprock for CO\textsubscript{2} geological storage," *Acta Geotechnica*, vol. 9, no. 1, pp. 87–100, 2014.

[13] J. Na, T. Xu, Y. Yuan, B. Feng, H. Tian, and X. Bao, "An integrated study of fluid-rock interaction in a CO\textsubscript{2}-based enhanced geothermal system: a case study of Songliao Basin, China," *Applied Geochemistry*, vol. 59, pp. 166–177, 2015.

[14] M. Khather, A. Saeedi, R. Rezaee, R. R. P. Noble, and D. Gray, "Experimental investigation of changes in petrophysical properties during CO\textsubscript{2} injection into dolomite-rich rocks," *International Journal of Greenhouse Gas Control*, vol. 59, pp. 74–90, 2017.

[15] J. Wollenweber, S. Alles, A. Busch, B. M. Krooss, H. Stanjek, and R. Littke, "Experimental investigation of the CO\textsubscript{2} sealing efficiency of caprocks," *International Journal of Greenhouse Gas Control*, vol. 4, no. 2, pp. 231–241, 2010.

[16] D. N. Espinoza and J. C. Santamarina, "CO\textsubscript{2} breakthrough–Caprock sealing efficiency and integrity for carbon geological storage," *International Journal of Greenhouse Gas Control*, vol. 66, pp. 218–229, 2017.

[17] Z. X. Sun, J. Yao, X. Huang et al., "CO\textsubscript{2} injection for heat extraction and carbon sequestration in a geothermal site: Huizhou Sag, the Pearl River Mouth Basin," *Geothermics*, vol. 64, pp. 331–343, 2016.

[18] S. Fakher and A. Imqam, "Application of carbon dioxide injection in shale oil reservoirs for increasing oil recovery and carbon dioxide storage," *Fuel*, vol. 265, article 116944, 2020.

[19] E. M. Myshakin, H. Singh, S. Sanguinito, G. Bromhal, and A. L. Goodman, "Numerical estimations of storage efficiency for the prospective CO\textsubscript{2} storage resource of shales," *International Journal of Greenhouse Gas Control*, vol. 76, pp. 24–31, 2018.

[20] J. S. Levine, I. Fukai, D. J. Soeder et al., "U.S. DOE NETL methodology for estimating the prospective CO\textsubscript{2} storage resource of shales at the national and regional scale," *International Journal of Greenhouse Gas Control*, vol. 51, pp. 81–94, 2016.

[21] M. Wigand, J. W. Carey, H. Schütz, E. Spangenberg, and J. Erzinger, "Geochimical effects of CO\textsubscript{2} sequestration in sandstones under simulated in situ conditions of deep saline aquifers," *Applied Geochemistry*, vol. 23, no. 9, pp. 2735–2745, 2008.

[22] H. L. Tian, T. Xu, Y. Li, Z. Yang, and F. Wang, "Evolution of sealing efficiency for CO\textsubscript{2} geological storage due to mineral alteration within a hydrogeologically heterogeneous caprock," *Applied Geochemistry*, vol. 63, pp. 380–397, 2015.

[23] K. Pruess and T. N. Narasimhan, "A practical method for modeling fluid and heat flow in fractured porous media," *SPE Journal*, vol. 25, no. 1, pp. 14–26, 1985.

[24] T. F. Xu, E. Sonnenthal, N. Spycher, and K. Pruess, "TOUGH-REACT user's guide: a simulation program for non-isothermal multiphase reactive geochemical transport in variable saturated geologic media, V1.2.1.1.1", in *LBNL-55460-2008*, Lawrence Berkeley National Lab., Berkeley, CA, 2008.

[25] T. J. Wolery, "EQ3/6: software package for geochemical modeling of aqueous systems: package overview and installation guide (version 7.0)," in *UCRL-MA-110662-Pt.1*, Lawrence Livermore National Lab., Livermore, CA, 1992.

[26] T. F. Xu, J. A. Apps, K. Pruess, and H. Yamamoto, "Numerical modeling of injection and mineral trapping of CO\textsubscript{2} with H\textsubscript{2}S and SO\textsubscript{2} in a sandstone formation," *Chemical Geology*, vol. 242, no. 3–4, pp. 319–346, 2007.

[27] A. C. Lasaga, J. M. Soler, J. Ganor, T. E. Burch, and K. L. Nagy, "Chemical weathering rate laws and global geochemical cycles," *Geochemica et Cosmochimica Acta*, vol. 58, no. 10, pp. 2361–2386, 1994.

[28] J. L. Palladri and Y. K. Kharaka, "A compilation of rate parameters of water-mineral interaction kinetics for application to geochemical modeling," *Open-File Report*, U.S. Geological Survey, Menlo Park, CA, 2004.
X. Liu, T. Xu, H. Tian, M. Wei, G. Jin, and N. Liu, “Numerical modeling study of mineralization induced by methane cold seep at the sea bottom,” *Marine and Petroleum Geology*, vol. 75, pp. 14–28, 2016.

L. L. Yang, T. Xu, B. Yang, H. Tian, and H. Lei, “Effects of mineral composition and heterogeneity on the reservoir quality evolution with CO2 intrusion,” *Geochemistry, Geophysics, Geosystems*, vol. 15, no. 3, pp. 605–618, 2014.

T. F. Xu, Y. K. Khara, C. Doughty, B. M. Freifeild, and T. M. Daley, “Reactive transport modeling to study changes in water chemistry induced by CO2 injection at the Frio-I brine pilot,” *Chemical Geology*, vol. 271, no. 3–4, pp. 153–164, 2010.

T. F. Xu, J. A. Apps, and K. Pruess, “Numerical simulation of CO2 disposal by mineral trapping in deep aquifers,” *Applied Geochemistry*, vol. 19, no. 6, pp. 917–936, 2004.

I. Gaus, M. Azaroual, and I. Czernichowski-Lauriol, “Reactive transport modelling of the impact of CO2 injection on the clayey cap rock at Sleipner (North Sea),” *Chemical Geology*, vol. 217, no. 3–4, pp. 319–337, 2005.

D. A. Smith, “Theoretical considerations of sealing and nonsealing faults,” *AAPG Bulletin*, vol. 50, no. 2, pp. 363–374, 1966.

X. Han, F. Feng, and Z. Cong, “Dynamic evaluation method of caprock microscopic sealing in CO2 sequestration project,” *Geofluids*, vol. 2020, Article ID 2648692, 12 pages, 2020.

R. Iddphonce, J. Wang, and L. Zhao, “Review of CO2 injection techniques for enhanced shale gas recovery: Prospect and challenges,” *Journal of Natural Gas Science and Engineering*, vol. 77, article 103240, 2020.

P. L. HUO, D. Zhang, Z. Yang, W. Li, J. Zhang, and S. Jia, “CO2 geological sequestration: displacement behavior of shale gas methane by carbon dioxide injection,” *International Journal of Greenhouse Gas Control*, vol. 66, pp. 48–59, 2017.

I. Klewia, D. S. Berawala, H. C. Alexander Walker, P. Ø. Andersen, and P. H. Nadeau, “Review of experimental sorption studies of CO2 and CH4 in shales,” *Journal of Natural Gas Science and Engineering*, vol. 73, article 103045, 2020.

Y. Li, M. Long, J. Tang, M. Chen, and X. Fu, “A hydraulic fracture height mathematical model considering the influence of plastic region at fracture tip,” *Petroleum Exploration and Development*, vol. 47, no. 1, pp. 184–195, 2020.

Z. Y. Cong, Y. Li, Y. Pan et al., “Study on CO2 foam fracturing model and fracture propagation simulation,” *Energy*, vol. 238, article 121778, Part B, 2022.

J. Zhang, Y. Li, Y. Pan et al., “Experiments and analysis on the influence of multiple closed cemented natural fractures on hydraulic fracture propagation in a tight sandstone reservoir,” *Engineering Geology*, vol. 281, article 105981, 2021.

Y. W. Li, D. Jia, Z. Rui, J. Peng, C. Fu, and J. Zhang, “Evaluation method of rock brittleness based on statistical constitutive relations for rock damage,” *Journal of Petroleum Science and Engineering*, vol. 153, pp. 123–132, 2017.

J. Xie, J. Tang, R. Yong et al., “A 3-D hydraulic fracture propagation model applied for shale gas reservoirs with multiple bedding planes,” *Engineering Fracture Mechanics*, vol. 228, article 106872, 2020.

X. Zhao, L. Zhou, X. Pu et al., “Formation conditions and enrichment model of retained petroleum in lacustrine shale: a case study of the Paleogene in Huanghua depression, Bohai Bay Basin, China,” *Petroleum Exploration and Development*, vol. 47, no. 5, pp. 916–930, 2020.

J. Z. Tang, K. Wu, L. Zuo, L. Xiao, S. Sun, and C. Ehlig–Economides, “Investigation of rupture and slip mechanisms of hydraulic fractures in multiple-layered formations,” *SPE Journal*, vol. 24, no. 5, pp. 2292–2307, 2019.

J. Z. Tang, K. Wu, Y. Li, X. Hu, Q. Liu, and C. Ehlig-Economides, “Numerical investigation of the interactions between hydraulic fracture and bedding planes with non-orthogonal approach angle,” *Engineering Fracture Mechanics*, vol. 200, pp. 1–16, 2018.

S. W. Mao, Z. Zhang, T. Chun, and K. Wu, “Field-scale numerical investigation of proppant transport among multicluster hydraulic fractures,” *SPE Journal*, vol. 26, no. 1, pp. 307–323, 2021.

S. W. Mao, P. Siddhamshetty, Z. Zhang et al., “Impact of proppant pumping schedule on well production for slickwater fracturing,” *SPE Journal*, vol. 26, no. 1, pp. 342–358, 2021.

N. Yalcin Erik and F. Ay, “Use of Petrolgical and Organic Geochemical Data in Determining Hydrocarbon Generation Potential of Coals: Miocene Coals of Malatyaa Basin (Eastern Anatolia-Turkey),” *International Journal of Coal Science & Technology*, vol. 8, no. 4, pp. 510–533, 2020.

F. S. Zhang, M. An, L. Zhang, Y. Fang, and D. Elsworth, “Effect of mineralogy on friction-dilation relationships for simulated faults: implications for permeability evolution in caprock faults,” *Geoscience Frontiers*, vol. 11, no. 2, pp. 439–450, 2020.

J. N. Dong, M. Chen, Y. Li, S. Wang, C. Zeng, and M. Zaman, “Experimental and theoretical study on dynamic hydraulic fracture,” *Energies*, vol. 12, no. 3, article 397, 2019.

M. K. An, F. Zhang, D. Elsworth, Z. Xu, Z. Chen, and L. Zhang, “Friction of Longmaxi shale gouges and implications for seismicity during hydraulic fracturing,” *Journal of Geophysical Research: Solid Earth*, vol. 125, no. 8, article e2020JB019885, 2020.

M. K. An, F. Zhang, Z. Chen, D. Elsworth, and L. Zhang, “Temperature and fluid pressurization effects on frictional stability of shale faults reactivated by hydraulic fracturing in the Changning block, Southwest China,” *Journal of Geophysical Research: Solid Earth*, vol. 125, no. 8, article e2020JB019584, 2020.

H. Lee, J. Y. Shinn, S. H. Ong et al., “Fault reactivation potential of an offshore CO2 storage site, Pohang Basin, South Korea,” *Journal of Petroleum Science and Engineering*, vol. 152, pp. 427–442, 2017.

Q. Tao, D. Alexander, and S. L. Bryant, “Modeling potential CO2 leakage rate along a fault in Mahogany Field,” *Journal of Petroleum Science and Engineering*, vol. 111, pp. 15–24, 2013.

J. Lee, K. B. Min, and J. Rutqvist, “Probabilistic analysis of fracture reactivation associated with deep underground CO2 injection,” *Rock Mechanics and Rock Engineering*, vol. 46, no. 4, pp. 801–820, 2013.

Y. H. Huang, S. Q. Yang, W. P. Li, and M. R. Hall, “Influence of super-critical CO2 on the strength and fracture behavior of brine-saturated sandstone specimens,” *Rock Mechanics and Rock Engineering*, vol. 53, no. 2, pp. 653–670, 2020.

Z. Shi, L. Sun, I. Haljasmaa et al., “Impact of brine/CO2 exposure on the transport and mechanical properties of the Mt Simon sandstone,” *Journal of Petroleum Science and Engineering*, vol. 177, pp. 295–305, 2019.