Evaluation of the Geologic CO₂ Sequestration Potential of the Morrow B
Sandstone in the Farnsworth, Texas Hydrocarbon Field using Reactive
Transport Modeling

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Abstract

The objectives of this research were to examine the long term fate of CO₂ injected into the Morrow B Sandstone, a hydrocarbon reservoir in the Farnsworth Unit in northern Texas. A suite of numerical multi-phase reactive transport models was constructed simulating continuous and water-alternating-gas (WAG) CO₂ injection through nine wells into an initially water-saturated reservoir. The simulations predicted little change in the pressure or temperature of the reservoir as a result of fluid injection. However, the injected CO₂ temporarily reduced the pH of the formation water from near neutral to as low as 4.7, which induced further changes in the formation water composition and reservoir mineral matrix. Much of the injected CO₂ also initially existed as a separate immiscible gas phase, but this CO₂ appears to have leaked vertically through the overlying Morrow Shale cap rock and disappeared from the Morrow B Sandstone within 30-50 years. However, some of the injected CO₂ dissolved into the Morrow B formation water and migrated westward. This acidified CO₂-enriched formation water initially dissolved native calcite and ankerite in the reservoir but later in the simulations calcite, dolomite, and siderite began to precipitate, serving as minor sinks for CO₂. Among non-carbonate minerals, albite and illite, both initial constituents of the Morrow B Sandstone matrix, were predicted to dissolve, whereas quartz, kaolinite, and smectite were predicted consistently to precipitate. However, these changes in mineral precipitation and dissolution caused negligible changes in porosity on the order of only 10⁻³%, causing correspondingly negligible changes in the patterns of fluid flow and CO₂ storage capacity of the Morrow B Sandstone. Based on the results of the simulations, because of significant leakage of CO₂ through the overlying Morrow Shale, the Morrow B Sandstone is judged to be a minor reservoir for CO₂ sequestration for at least decadal to century time-scales, where the CO₂ is sequestered primarily in aqueous solution in the Morrow B formation water. However, petroleum, a likely major sink for injected CO₂, was not considered

in the models and likely would significantly improve the CO₂ sequestration capacity of the Morrow B Sandstone.

Evaluation of the Geologic CO₂ Sequestration Potential of the Morrow B Sandstone in the Farnsworth, Texas Hydrocarbon Field using Reactive Transport Modeling

Introduction

Injection of CO₂ into oil reservoirs is an attractive approach for simultaneous enhanced oil recovery (EOR) and long-term sequestration of CO₂ (Hepple and Benson, 2005; Jia et al., 2016; Pan et al., 2016). The Morrow B Sandstone member in the Farnsworth Unit (FWU), northern Texas, USA, is currently under investigation by the Southwest Partnership for CO₂ Sequestration (SWP) as a test case for this purpose. The Morrow B Sandstone is the principal hydrocarbon reservoir in the Farnsworth Unit, which has yielded nearly 40 million barrels of oil and over 29 million MCF (thousand cubic feet) of natural gas since commercial production began in 1956.

The deposition, mineralogy, diagenesis, structure, reservoir properties, and production history of the Morrow B Sandstone in the FWU have been described by Parker (1956), Munson (1988, 1989), McKay and Noah (1996), Czoski (2014), Gallagher (2014), Ampomah et al. (2015a, 2016b), Hutton (2015), and Rose-Coss et al. (2016). Several recent studies have also attempted to model the behavior of fluids in the FWU. Ampomah et al. (2015a-b, 2016a-e) constructed a variety of models for the western FWU and achieved several important results, including:

- quantification of error produced from upscaling of numerical grids and hydraulic properties
- ranking of relative importance of CO₂ sequestration mechanisms: (1) CO₂ dissolution in oil, (2) CO₂ dissolution in water, (3) residual trapping of immiscible CO₂
- identification of injection strategies optimizing CO₂ sequestration and oil production
- estimates of oil initially in place in the Morrow B reservoir and of current oil reserves

White et al. (2014) extended the STOMP numerical simulator to include the treatment of oil with the composition found in the Farnsworth Unit, and demonstrated the simulator's applicability in modeling water, CO₂, and hydrocarbon transport for a test case "five spot" pattern of injection and production wells in the Morrow B Sandstone. Ahmmed et al. (2016) studied the effects of CO₂ injection on the pore water and mineral matrix composition of the Morrow B Sandstone using equilibrium speciation and reaction path modeling. They found the present pore water to be supersaturated with respect to an assemblage of zeolite, clay, carbonate, mica, and aluminum hydroxide minerals, and undersaturated with respect to feldspars, ankerite, and chlorite. They also found injection of CO₂ to cause a sharp initial drop in pH from about 7 to as low as 4.1 that caused further dissolution of the Morrow B matrix. However, as water-rock reactions progressed, pH gradually rose to about 4.6 to 5.2, leading to the precipitation of dolomite and calcite which ultimately sequestered up to about 2% of the injected CO₂. Predicted porosity changes ranged from about 3.5 to 3.6% for high (100:1) water:rock ratios that probably represent short-term conditions, to 0.14 to 0.15% for low (10:1) water:rock ratios that probably represent long-term conditions.

Pan et al. (2016) used the TOUGHREACT software (Xu et al., 2006) to conduct reactive transport simulations over a 712×712×10 m³ volume of the Morrow B Sandstone for a five-spot pattern consisting of four CO₂ injection wells at the corners of the model domain and a production well at the center of the model domain. Their simulations were carried out to 1000 years in which production and water-alternating-gas (WAG) CO₂ injection occurred during the first 25 years. Their simulations predicted a stable, long-term lowering of the pH to about 4.6 throughout the model domain, the progressive precipitation of quartz, kaolinite, smectite, ankerite, and magnesite, and the progressive dissolution of albite, chlorite, and calcite. Carbon sequestration by carbonate mineral precipitation was predicted to increase over time, accounting for about 8% of the injected CO₂ after 1000 years. By that time, porosity was predicted to have

increased by about 2.5% near the injection wells (~50 m), but to have decreased by about 0.8% far from the injection wells (~450 m).

Despite these advances, significant questions about the reactive transport of CO₂, and thus, the potential for long-term CO₂ sequestration in the Morrow B Sandstone remain. In particular, questions remain about the coupled chemical and physical behavior of injected CO₂ over a larger volume of the Morrow B Sandstone reservoir in the FWU compared to the study of Pan et al. (2016), including the effects of permeability and reservoir thickness heterogeneity, and initial and boundary conditions obtained from history matching for the reservoir (Ampomah et al., 2016e).

The purpose of the present study, therefore, was to extend the study of Pan et al. (2016) by performing numerical reactive transport simulations of CO₂ injection into the Morrow B Sandstone for a larger three-dimensional model of the western FWU. More specifically, the study sought to answer (1) how CO₂ injection may change the Morrow B formation water composition and mineralogy, (2) how CO₂ would be distributed spatially throughout the reservoir and partitioned between formation water, carbonate minerals, and an immiscible gas phase, (3) how the hydraulic properties of the Morrow B Sandstone may change as a result of CO₂ injection.

Geologic Background

The FWU covers an approximately 73 km² area in the western Anadarko basin in northern Texas (Fig. 1).

Figure 1. Major geological features around the Farnsworth unit, USA (Source: Ahmmed et al., 2016, modified from Johnson et al., 1989).

The Morrow B Sandstone, the principal hydrocarbon reservoir and target for CO₂ sequestration in the FWU, is part of a broader Morrowan-age (Lower Pennsylvanian) sequence of predominantly clastic transgressive sedimentary rocks. The Morrowan Series is unconformably underlain by Chesterian (Upper Mississippian) rocks consisting mainly of marine limestones with thinly interbedded shale and sandstone, and conformably overlain by the Atokan-age (Lower Pennsylvanian) Thirteen Finger Limestone, an aquitard consisting of finely crystalline dolomitic limestones and shales (Fig. 2).

Figure 2. Lithostratigraphy of the Upper Morrowan and Lower Atokan age formations in the Farnsworth Unit including wireline logs (spontaneous potential log on the left and resistivity log on the right) (Source: Gallagher, 2014).

The Morrowan Series consists of an upper and a lower portion. The Morrow B Sandstone is one of the sandstone units in this upper portion, which were deposited as fluvial channels during brief intervals of probably glacially-induced marine regression surrounded by broader intervals of marine transgression that deposited fine-grained clastics (Gallagher, 2014). The enclosure of the Morrow B sandstone channels within lower permeability, fine-grained clastics thus make stratigraphic trapping the main trap type for hydrocarbons and CO₂ in the FWU.

The Morrow B Sandstone has an average thickness of 9 m, lies at an average depth of about 2400 m below the land surface, and dips to the southeast at an angle of less than one degree (Munson et al., 1989; Ampomah et al., 2016a,c). The mineralogy of the Morrow B Sandstone is shown in Table 1.

Table 1. Mineral composition of the Morrow B Sandstone.

Mineral	Volume (%)
Quartz	84.26
Albite	9.0
Calcite	0.75
Ankerite	0.25
Siderite	0.25
Smectite	0.1
Illite	0.88
Chlorite	1.79
Kaolinite	2.72

* Data source: Munson (1989), Gallagher (2014)

The current composition of Morrow B formation water based on samples taken from well batteries, AWT3 and AWT4, is shown in Table 2.

Table 2. Present composition of Morrow B Sandstone formation water.

Basis species	Concentration (mg/kg)	
	Well battery AWT3	Well battery AWT4
Al ³⁺	1.05	0.00791
B(OH) ₃ (aq)	21.5	27.8
Ba ²⁺	0.592	1.37
Br ⁻	17.8	20.3
Ca ²⁺	38.5	32.9
Cl ⁻	1.47×10 ³	1.84×10 ³
F ⁻	0.654	0.911
Fe ²⁺	7.29×10 ⁻⁵	2.10×10 ⁻⁸
HCO ₃ ⁻	5.79×10 ⁴	795
K ⁺	7.87	7.11
Li ⁺	0.283	0.461
Mg ²⁺	6.27	12.3
Na ⁺	1.08×10 ³	1.41×10 ³
SO ₄ ²⁻	21.4	12.9
SeO ₃ ²⁻	0.0687	0.0827
SiO ₂ (aq)	24.5	42.1
Sr ²⁺	2.68	1.85
Zn ²⁺	1.51×10 ⁻⁵	0.108
pH	7	7
ORP (mV)	140	140

* Data source: Ahmmmed et al. (2016).

The formation water has a relatively low total dissolved solids (TDS) content ranging from about 3500 to 4000 mg/L, dominated by chlorine, sodium, bicarbonate, and calcium, a near neutral pH of about 7, an Eh of about 140 mV, a reservoir temperature of about 75° C, and an average pore fluid pressure of about 35 MPa. The porosity of the Morrow B Sandstone ranges from about 10% to 18% with an average value of 14.5%. Permeability ranges from about 1 to 250 millidarcies (mD) with an average value of 48 mD (Munson, 1989; Ampomah et al., 2015a). Rose-Coss et al. (2016) found permeability to correlate with porosity according to eight distinct hydraulic flow units distinguished from one another according to pore throat radius. The initial water:oil ratio in the Morrow B Sandstone when the FWU was put into production in 1955 was

about 31:69% (Ampomah et al., 2015). Water-flooding began in 1964, and by its conclusion in December, 2010, the water:oil ratio had increased to 73:27% (Ampomah et al., 2016a).

Methodology

Reactive transport simulations were conducted using the TOUGHREACT software with the ECO2N equation of state for NaCl brine and CO₂ (Spycher and Pruess, 2005; Xu et al., 2005) and the EQ3/EQ6 thermodynamic database (Xu et al., 2004) over a structured, three dimensional (3D) model grid representing the Morrow B Sandstone reservoir in the FWU. The grid consisted of 110 cell columns, 80 cell rows, and 7 cell layers for a total of 61,600 cells. The cells that lay outside the FWU lease boundaries were disabled, leaving 38,290 active cells in the model domain. A total of 15,357 cells in the western portion of Farnsworth grid were considered for model simulation. The porosity and permeability distributions were obtained from the geologic model of Ampomah et al. (2016b), which synthesized a variety of well log and geophysical data from the FWU.

The spectrum of porosity-permeability covariance in the Morrow B was reduced to 36 discrete porosity-permeability combinations, designated as “rock types” in the model (Table 3).

Table 3. Porosity (%) - permeability (m²) covariance in the Morrow B Sandstone modeled rock types.

Porosity (%) \ Permeability (mD)	0	>0 – 0.1	>0.1 – 0.125	>0.125 – 0.15	>0.15 – 0.2	>0.2
0.01- 0.08	Rock 1	Rock 36				
>0.01 – 24.93		Rock 2	Rock 3	Rock 4	Rock 5	Rock 6
>24.93 – 49.95		Rock 7	Rock 8	Rock 9	Rock 10	Rock 11
>49.95 – 74.98		Rock 12	Rock 13	Rock 14	Rock 15	Rock 16
>74.98 – 100		Rock 17	Rock 18	Rock 19	Rock 20	Rock 21
>100 – 124.63		Rock 22	Rock 23	Rock 24	Rock 25	Rock 26
>124.63 – 149.96		Rock 27	Rock 28	Rock 29	Rock 30	Rock 31
>149.96 – 174.28		Rock 32	Rock 33	Rock 34	Rock 35	

* Table sources: Ahmmed (2015); Ampomah personal communication (2016).

In order to simulate the effects of the cap rock, the topmost cell layer in the model was assigned a uniform low porosity of 0.087 and permeability of 0.081 mD (rock 36). Figure 3a shows the distribution of model rock types (i.e. porosity and permeability defined in Table 3) in the second cell layer from the top of the grid, which represents the top of the Morrow B Sandstone in the model and is much more heterogeneous.

Several initial conditions were prescribed in the model. Initial formation water temperature, salt mass fraction, and CO₂ mass fraction were set to 75° C, 0.004, and 10⁻⁴, respectively throughout the model domain. The assigned initial background CO₂ concentration was needed to achieve convergence of the reactive transport simulation by smoothing the CO₂ concentration gradient between the injection wells and the surrounding formation water in the reservoir. The initial fluid pressure in the model varied between 32.2 and 36.5 MPa and was calculated according to the equation,

$$P = 6.68 \times 10^8 + 218.4x - 179y - 8758z \quad (1)$$

which was regressed from the reservoir history matching study of (Ampomah personal communication, 2016) immediately before injection of CO₂ (Fig. 3b). In equation (1), P represents pressure (Pa) and x , y , and z represent the spatial coordinates (m). The initial Morrow B mineral and formation water compositions are provided in Tables 1 and 2.

Figure 3: (a) Depiction of porosity-permeability heterogeneity in the top of the Morrow B Sandstone. Each color corresponds to a discrete rock type shown in Table 3. (b) Initial pressure distribution (in Pa) in the Farnsworth model grid.

Several boundary conditions were prescribed in the model. The topmost and two lowermost cell layers in the grid were prescribed as “fixed state”, in which pressure, temperature, and solute concentrations were held constant over time at values equal to the initial values. Thus, pressure, temperature, and solute concentrations were free to evolve over time during the simulations in only four of the seven cell layers, a limitation that was found to be necessary in order to achieve numerical convergence. The lateral boundaries were open to fluid flow, heat transport, and solute transport.

Relative permeability was computed according to the van Genuchten-Mualem model (Pruess et al., 1999; van Genuchten, 1980). Relative permeability is represented by the van Genuchten-Mualem model by equations (2), (3), and (4) below:

Liquid relative permeability:

$$k_{rl} = \sqrt{S^* \{1 - (1 - [S^{*1/\lambda}]^\lambda)^2\}} \quad \text{if } S_l < S_{ls} \quad (2)$$

Gas relative permeability:

$$k_{rg} = (1 - Se)^2 (1 - Se^2) \quad \text{if } S_{igr} > 0 \quad (3)$$

In equations (2) and (3),

$$S^* = (S_l - S_{lr}) / (S_{ls} - S_{lr}) \text{ and } Se = (S_l - S_{lr}) / (1 - S_{lr} - S_{gr}) \quad (4)$$

where λ = the van Genuchten-Mualem model parameter, S_l = pore water content, S_{ls} = saturated pore water content, S_{lr} = irreducible water saturation, S_{gr} = irreducible gas saturation.

The λ parameter in the model was found by fitting the model to relative permeability versus water-CO₂ saturation data generated by Feldman et al. (2016) for core samples of the Morrow B Sandstone in the FWU, leading to λ values between 0.51 and 0.80 for a residual water saturation (S_{lr}) of 0 and a residual CO₂ gas saturation (S_{gr}) of 0.125 (Fig. 4). In order to improve model convergence, S_{lr} was raised slightly from 0 to 0.05 in the relative permeability calculations (Pruess et al., 1999). Capillary pressure was computed according to the van Genuchten model (Pruess et al., 1999; Van Genuchten, 1980). Capillary pressure is represented in the van Genuchten model by equation (5) and (6) below:

$$P_{cap} = -Po([S^*]^{-\frac{1}{\lambda}} - 1)^{1-\lambda} \quad (5)$$

subject to the restriction $-P_{max} \leq P_{cap} \leq 0$

In equation (5),

$$S^* = (S_l - S_{lr}) / (S_{ls} - S_{lr}) \quad (6)$$

where $P_{\max}$ = the maximum pressure in the reservoir, P_0 = a strength coefficient for the reservoir.

The strength coefficient (P_0) of 9,560 Pa in this model was computed by fitting the model to capillary pressure versus water- CO_2 saturation data of Feldman et al. (2016) for an average λ value of 0.64 and a maximum pressure of 3.49×10^7 Pa (Fig. 5). The fit of the computed curve with the measured data is reasonable (least root mean square error equals 2033) for water saturations above 60%, which based on subsequent simulations presented below, are likely to be maintained through the FWU except very near the CO_2 injection wells.

Figure 4. Best fit curves and their associated λ values found in the present study for relative permeability versus water saturation data acquired by Feldman et al. (2016) for (a) core plug 14, (b) core plug 20, (c) core plug 18, and (d) core plug 2 from the Morrow B Sandstone in the FWU.

Figure 5: Comparison of measured capillary pressure versus water saturation data from Feldman et al. (2016) with van Genuchten model curves calculated in the present study for variable values of P_0 at an average λ value of 0.64.

Kinetic chemical reaction parameters for the precipitation and dissolution of minerals considered in the model are shown in Table 4. Initial radii for mineral grains in the Morrow B Sandstone were obtained from Gallagher (2014). Mineral reactive surface areas were calculated using the following equation (Xu et al., 2004),

$$A_{\text{geo}} = (ar^{D-3})/\rho \quad (7)$$

where a = geometric parameter, r = grain radius, ρ = density of solid, D = coefficient, 2 for Euclidean solid properties with no fractal properties. Cation exchange and decay mechanisms were not considered in the models.

Table 4. Kinetic chemical reaction parameters used in the simulations.

Minerals	Reactive Surface area (cm ² /g of mineral)	Kinetic parameters							
		Acid Mechanism			Neutral Mechanism		Base Mechanism		
		H ⁺ ≥	E _a	K ₂₅	E _a	K ₂₅	H ⁺ ≤	E _a	K ₂₅
Quartz	9.8				87.7	1.023 x 10 ⁻¹⁴			
Albite	11.45	0.457	65.0	1.35 x 10 ⁻¹⁰	69.8	9.12 x 10 ⁻¹³	-0.572	71.0	1.04 x 10 ⁻¹⁷
Clinochlore	11.41	0.5	88.0	7.8 x 10 ⁻¹²	88.0	3.0 x 10 ⁻¹³			
Illite	43.63	0.34	23.6	1.0 x 10 ⁻¹¹	35.0	1.7 x 10 ⁻¹³	-0.4	58.9	3.0 x 10 ⁻¹⁷
Kaolinite	46.15	0.777	65.9	4.9 x 10 ⁻¹²	62.76	1.01 x 10 ⁻¹³	-0.472	17.9	8.9 x 10 ⁻¹⁸
Smectite	9.8	0.34	23.6	1.05 x 10 ⁻¹¹	35.0	1.65 x 10 ⁻¹³	-0.4	58.9	3.0 x 10 ⁻¹⁷
Calcite	11.07				23.5	1.55 x 10 ⁻⁷			
Dolomite	10.49	0.5	36.1	6.46 x 10 ⁻⁴	52.2	2.95 x 10 ⁻⁸			
Ankerite	9.84	0.5	36.1	6.46 x 10 ⁻⁴	62.76	1.26 x 10 ⁻⁹			
Siderite	9.8	0.5	36.1	6.46 x 10 ⁻⁴	62.76	1.26 x 10 ⁻⁹			
Magnesite	9.8	1.0	14.4	4.2 x 10 ⁻⁷	23.5	4.6 x 10 ⁻¹⁰			

Activation Energy (E_a) in Kj/mol; Rate Constant (K₂₅) in mol/m²/s

(Data sources: Palandri and Kharaka, 2004; Xu et al., 2004; Gallagher, 2014)

Following Ahmmed (2015), changes in permeability as a function of changes in porosity caused by mineral precipitation and dissolution were calculated according to a “tube-in-series” model (Pruess, 2005) fit to observed porosity-permeability data for the Morrow B (Dai et al., 2013)”. Ahmmed (2015) found that the best fit for this model occurred for $\Gamma = 2$ and $\phi_r = 0.75$, where Γ represents the fractional length of the pore bodies and ϕ_r represents the fraction of original porosity at which permeability is reduced to zero. Further, the “tube-in-series” model was found to represent the field porosity-permeability correlation of Dai et al. (2013) well for porosity changes of less than 5%.

Following Ahmmed (2015), the mutual solubility of water and CO₂ in one another were computed according to Spycher and Pruess (2005). The dependence of water density on CO₂ concentration was calculated according to García (2001). The enthalpies of brine and CO₂ were calculated according to Lorenz and Müller (2003) and Altunin (1975), respectively. Aqueous species and gaseous species diffusion coefficients were set to $1.0 \times 10^{-9} \text{ m}^2\text{s}^{-1}$ and $1.1 \times 10^{-5} \text{ m}^2\text{s}^{-1}$, respectively. Matrix compressibility was set to $1.0 \times 10^{-10} \text{ Pa}^{-1}$, an average value for sandstone (Ingebritsen and Appold, 2012), and the tortuosity factor was calculated to be 0.525 based on the 14.5% average porosity of the Morrow B. All of the numerical simulations employed a preconditioned bi-conjugate gradient solver for which the tolerances of relative transport concentration, relative geochemical concentration, and dissolution-precipitation rate change were set to 1×10^{-4} , 0.001 and 5×10^{-4} , respectively. Aqueous activity coefficients were calculated using the extended Debye-Hückel model (Xu et al., 2005).

In order to improve the stability of the reactive transport simulations with CO₂ injection, a preliminary physical flow and heat transport simulation without reactive transport and CO₂ injection was first executed until steady-state was reached. This resulted in minimal changes to the pressure field predicted by equation (1). The results of this simulation were then imported as initial conditions into a preliminary reactive transport simulation without CO₂ injection, which

was executed for five years. This reduced the degree of super-saturation of some minerals predicted to precipitate from the initial formation water composition shown in Table 2. The results of this simulation were then imported as initial conditions into the final reactive transport simulations with CO₂ injection.

The CO₂ injection schedule used in these simulations is shown in Figure 6. Geographic coordinates of the injection wells and screen depth intervals are shown in Table 5. The CO₂ was injected at a constant enthalpy of 3.01×10^5 J/kg, corresponding to a temperature of 60° C, for a period of ten years through nine injection wells at rates varying between 0.3 kg/s and 1.51 kg/s. Historical injection rates from the field (Ampomah personal communication, 2016) were employed for the first five years of the simulation, after which the average injection rate over the first five years was employed. A total of 2.67 million tonnes of CO₂ were injected into the reservoir over the course of the simulations.

Figure 6. CO₂ injection schedules employed in the simulations for nine wells in the Morrow B Sandstone.

Figure 7. WAG injection schedules of nine wells in Morrow B formation.

Table 5. Geographic UTM coordinates (NAD 83; Zone 13) and screen depth intervals of injection wells.

Well No	Easting (m)	Northing (m)	Screen top and bottom completion depths (-m)	Fluid enthalpy (J/Kg)
8-3	316,978	4,005,050	1399 - 1404.5	301,000
8-4	317,753.5	4,014,483	1423 - 1427	301,000
8-5	317,856.9	4,015,004	1391 - 1400	301,000
9-10	317,783.6	4,013,821	1438 - 1443	301,000
11-1	318,612.7	4,016,074	1401 - 1406.5	301,000
13-1	318,607.7	4,015,651	1399.5 - 1402	301,000
13-3	318,604	4,014,450	1403.5 - 1408	301,000
13-9	318,608.5	4,015,053	1410 - 1415	301,000
15-5	318,578.9	4,013,679	1422 - 1430	301,000

Model Scenarios

Four model scenarios were tested in the present study. Model 1 consisted of continuous injection of CO₂ according to the schedule shown in Figure 6 and the capillary pressure and relative permeability relationships derived from the Feldman et al. (2016) data shown in Figures 4 and 5. Model 2 consisted of WAG injection according to the schedule shown in Figure 7, retaining the capillary pressure and relative permeability relationships of Model 1. Model 3 consisted of continuous CO₂ injection as in Model 1 but using the capillary pressure and relative permeability relationships (Fig. 8) in Pan et al.'s (2016) study of a five-spot injection-withdrawal pattern in the Morrow B Sandstone in the FWU. Model 4 consisted of WAG injection as in Model 2 but using Pan et al.'s (2016) capillary pressure and relative permeability relationships (Fig. 8) in Model 3.

A smaller λ value (0.4438) and a much larger P_0 in Pan et al.'s (2016) model compared to Feldman et al.'s (2016) model caused a significantly higher capillary pressure (P_a) with respect to pore fluid saturation. The reason for the higher aqueous and CO₂ gas relative permeability in Pan et al.'s (2016) model versus the respective pore fluid saturation (water and CO₂) was because of a larger S_{ir} value (0.3) and a smaller S_{gr} value (0.05) used in that model. It is noteworthy to mention that aqueous relative permeability was lower in the Feldman et al. (2016) model at higher pore

water saturation. However, gas relative permeability in Pan et al.'s (2016) model was higher at all CO₂ pore saturations.

Figure 8. A comparison of the (a) relative permeability and (b) capillary pressures relationships used in Model 1 and Model 2 versus Model 3 and Model 4.

Results and Discussion

Pressure and Temperature

Only negligible changes in fluid pressure were predicted to occur in the Morrow B Sandstone as a result of fluid injection. This is illustrated in Figures 9a,b, which show fluid pressure as function of time at well 13-9. In all four model scenarios, fluid pressure was predicted to rise by no more than 10^4 to 3×10^5 Pa over the background fluid pressure of about 3.3×10^7 Pa, and returned to these background values within about 20 years after injection ceased. This minor pressure increase is likely a result of the Morrow Shale, which comprises the uppermost cell layer in the model grid, being permeable enough to allow most (i.e. about 96-97%) of the injected CO₂ to leave the model domain as an immiscible phase.

Figure 9. Temporal variations of pressure for (a) Models 1 and 2, and (b) Models 3 and 4; of temperature for (c) Models 1 and 2, and (d) Models 3 and 4 at well 13-9.

Predicted temperature changes were significant in magnitude but highly localized around the wells (Figs.9c,d; Fig. 10). Temperature was predicted to drop to a minimum of around 50° C at the wells but returned to the background reservoir temperature of about 75° C within about fifteen years after fluid injection ceased. This minimum temperature is lower than the injection temperature of about 60° C, and may result from the lower reservoir pressure relative to the injection pressure.

Figure 10. East-west slice planes through the western FWU showing temperature distribution after 10 years of CO₂ injection for model 1.

pH

In all four model scenarios, pH was predicted to drop to a minimum of about 4.78 near the wells, which reflects the solubility of CO₂ at the reservoir pressure and temperature. Once injection ceased, pH rose quickly (Fig. 11). For models 3 and 4, after about 40 years, pH rose to and stabilized at a value of about 8.8, which reflects buffering by the mineral matrix of the Morrow B Sandstone. Models 1 and 2 ran successfully for only about 57 and 69 years, respectively, by which times the pH had only risen to about 6.2 and 6.95, respectively. The pattern of pH evolution was not sensitive to whether CO₂ was injected continuously or as part of a WAG cycle. However, the pattern of pH evolution was sensitive to the relative permeability and capillary pressure models. In model scenarios 3 and 4, which employed the Pan et al. (2016) data, pH rose more quickly after the cessation of injection than in models 1 and 2, which employed the Feldman et al. (2016) data. This difference may reflect the comparatively higher aqueous relative permeability as a function of water saturation for the Pan et al. (2016) data.

Figure 11. Variations in pH as a function of time at distances of (a) 0 m, (b) 100 m, and (c) 200 m from well 13-9 for all four model scenarios.

Immiscible CO₂ gas phase

In all four model scenarios, the amount of CO₂ injected into the Morrow B Sandstone exceeded the amount that could be dissolved in the formation water, leaving an immiscible CO₂ gas phase. However, this immiscible gas phase was relatively short-lived and restricted to the immediate vicinity of the injection wells (Figs. 12 and 13).

Figure 12. CO₂ pore saturation (fraction) as a function of time at (a) 0 m and (b) 100 m from well 13-9 in all four model scenarios. Mass of carbon (tonnes) present as immiscible CO₂ in the entire model domain as a function of time comparing (c) model scenarios 1 and 2 (which show the effects of continuous versus WAG injection schemes), and (d) model scenarios 2 and 4 (which show the effects of the Feldman et al. (2016) versus Pan et al. (2016) capillary pressure-relative permeability relationships).

In all four models, the immiscible CO₂ had vanished between about 15 to 30 years. Much of the immiscible CO₂ (>90%) probably leaked through the top of the model domain via the Morrow Shale. Most of the remaining immiscible CO₂ was probably diminished by formation water advection. That is, as the formation water transported dissolved CO₂ westward from the wells, more and more of the immiscible CO₂ remaining near the wells could dissolve into the formation water. The abundance of immiscible CO₂ in the models was not found to be very sensitive to whether CO₂ was injected continuously or as part of a WAG cycle. However, the abundance of immiscible CO₂ was sensitive to the capillary pressure and relative permeability models employed, with the Feldman et al. (2016) models leading to greater abundances of immiscible CO₂. This probably reflects lower CO₂ relative permeabilities as a function of CO₂ pore saturation for the Feldman et al. (2016) model compared to the Pan et al. (2016) model (Figs. 12 and 13).

Figure 13. Iso-surfaces of immiscible CO₂ pore saturation (fraction) after 10 years for model scenarios (a) 1, (b) 2, (c) 3, and (d) 4 and after 25 years for model scenarios (e) 1, (f) 2, (g) 3, and (h) 4. The 10× lower immiscible CO₂ pore saturation (fraction) was chosen in order to illustrate the spatial extent of immiscible CO₂.

Aqueous CO₂

All of the models predicted a significant amount of the injected CO₂ to be dissolved into the Morrow B Sandstone formation water and to migrate westward in the prevailing formation water flow regime (Figs. 14-15).

Figure 14. Concentration of CO₂ dissolved in Morrow B Sandstone formation water as a function of time at distances of (a) 0 m, and (c) 200 m west of well 13-9 for all four model scenarios. (Mass of carbon occurring as CO₂ dissolved in Morrow B formation water summed over the entire model domain for model scenarios (c) 1 and 2 (which show the effects of continuous versus WAG injection schemes), and (d) 2 and 4 (which show the effects of the Feldman et al. (2016) versus Pan et al. (2016) capillary pressure-relative permeability relationships).

The amount of CO₂ that was dissolved in water was not sensitive to whether CO₂ was injected continuously or as part of a WAG cycle. However, higher aqueous CO₂ concentrations were reached using the Pan et al. (2016) relative permeability and capillary pressure model than the Feldman et al. (2016) models, likely due to a higher sensitivity of relative permeability with respect to water saturation of the Feldman et al. (2016) models, which would increase CO₂ dispersion. Also, advective CO₂ transport was faster and the total mass of CO₂ in aqueous solution throughout the model domain was greater using the Feldman et al. (2016) capillary pressure and relative permeability models than the Pan et al. (2016) models. The total mass of

CO₂ in aqueous solution peaked between 10 and 30 years as all of the initially immiscible CO₂ finally dissolved into the formation water. Thereafter, without further dissolution of CO₂, carbonate mineral precipitation began to lower the mass of CO₂ in aqueous solution throughout the model domain. In addition, by as early as 59 years in model 1, CO₂ began to be transported across the western boundary of the FWU (Fig. 15).

Figure 15. Isosurfaces of aqueous CO_2 concentration after 10 years for models (a) 1, (b) 2, (c) 3, and (d) 4, and after 57 years for models (e) 1, (f) 2, (g) 3, and (h) 4 (The 10 $\times$ lower immiscible CO_2 pore saturation (fraction) was chosen in order to illustrate the spatial extent of aqueous CO_2).

Carbonate mineral precipitation

An important concern in the study was how much of the injected CO₂ could be expected to be sequestered as carbonate minerals through reaction of the CO₂ with aqueous species in the formation water and with the host rock. This is represented in the simulations through the “SMCO₂” parameter, which expresses the mass of CO₂ sequestered as minerals in kg/m³ of porous medium.

Figure 16 shows SMCO₂ and the volume of carbonate minerals precipitated at discrete distances from a well and over the entire model domain, respectively, as a function of time. In all four model scenarios, carbonate mineral abundance was predicted to decline during the period of CO₂ injection, which reflects the dissolution of native carbonate mineral cements caused by the acidification of Morrow B formation water by the injected CO₂. This carbonate mineral dissolution was greatest near the wells for WAG injection. Little difference in carbonate mineral dissolution was predicted for the Feldman et al. (2016) and Pan et al. (2016) relative permeability and capillary pressure models. Once CO₂ injection ceased, the pH of the acidified formation water rose due to reaction with the host rock matrix and mixing with ambient formation water, allowing net precipitation of carbonate minerals until at least around 50 years of simulation time. The spatial distribution of carbonate mineral precipitation coincided closely with that of aqueous CO₂ (Figs. 15 and 18). Thereafter, based on models 3 and 4, which were carried out to 200 years, newly precipitated carbonate minerals began to dissolve as the formation water returned to its pre-injection composition due to progressive mixing with formation water from the surroundings. This may mean that mineral trapping is not an effective means for long-term CO₂ sequestration in the FWU.

Figure 17 provides further insights into the nature of the predicted carbonate mineral precipitation and dissolution. Calcite was predicted to be the most abundantly precipitated carbonate mineral, followed by siderite and dolomite. Ankerite, which like calcite and siderite

was initially present in the matrix of the Morrow B Sandstone (Table 2), was predicted to dissolve.

Figure 16. SMCO₂ (i.e. kg CO₂ precipitated as carbonate minerals per m³ of porous medium) versus time for all four models at distances of (a) 0 m and (b) 200 m west of well 13-9. Total volume of carbonate minerals precipitated or, dissolved over the entire model domain as a function of time for (c) models 1 and 2, and (d) models 2 and 4.

Figure 17. Predicted total volumetric abundances of carbonate minerals precipitated or dissolved over the entire model grid domain after (a) 55 years, (b) 70 years, and (c) 200 years.

Figure 18. Isosurfaces in the western FWU of the maximum SMCO2 and a value 10× lower than the maximum value after 10 years for models (a) 1, (b) 2, (c) 3, and (d) 4, and after 57 years for models (e) 1, (f) 2, (g) 3, and (h) 4 (The 10× lower value was chosen in order to illustrate the spatial extent of carbonate minerals precipitated).

Calcite

Prior to CO₂ injection, calcite accounted for about 0.75% of the Morrow B Sandstone matrix (Table 1) and was slightly supersaturated in the Morrow B formation water (Ahmmed et al., 2016). In all four of the model scenarios considered in the present study, calcite was predicted to dissolve near the injection wells as a result of the pH decrease of the formation water caused by CO₂ injection (Fig. 19). The magnitude of calcite dissolution was greater for the WAG models (2 and 4) than for the continuous CO₂ injection models (1 and 3), probably because the fresh water introduced during WAG injection was strongly undersaturated with respect to calcite, whereas in the continuous CO₂ injection models a continuous supply of aqueous carbonate species would have been produced that would have moved the formation water closer to saturation with respect to calcite. Nonetheless, the volume reduction of calcite was predicted to be very small, with a maximum value of only 0.0022. In the continuous CO₂ injection models, a brief period of net calcite gain was predicted to occur at the wells between about 10 and 20 years of simulation time, and then after about 200 years.

Further from the wells at a distance of 200 m, for the Pan et al. (2016) capillary pressure and relative permeability models, despite calcite dissolution from about 5 to 50 years, net calcite gain was predicted over the entire 200 year course of the simulations. For the Feldman et al. (2016) models, calcite dissolution also began after about 5 years and continued to the end of the simulations at about 59 years, by which time net calcite loss occurred.

Figure 19. Changes in volume fraction of calcite, dolomite, ankerite, and siderite at distances of 0 m (a-d, respectively) and 200 m (e-g, respectively) from well 13-9.

Dolomite

Similar patterns of dolomite precipitation were predicted in the four model scenarios (Figs. 19 and 20). In all four model scenarios, net dolomite precipitation was predicted over the entire course of the simulations near the injection wells. In fact, dolomite precipitated in greater amounts than any other carbonate minerals within about 200 m of the injection wells (Fig. 19), though for the model domain as a whole, calcite was the most abundantly precipitated carbonate mineral (Fig. 17). In model scenarios 1 and 2 using the Feldman et al. (2016) relative permeability and capillary pressure data, dolomite precipitated continuously for the entire respective 57 and 69 years of the simulations. In model scenarios 3 and 4 using the Pan et al. (2016) relative permeability and capillary pressure data, dolomite precipitated quickly for the first 40-45 years, after which it slowly started to dissolve, though dolomite persisted until the end of

the simulations at 200 years. At the wells, slightly more dolomite was predicted to precipitate in the continuous CO₂ injection scenarios compared to the WAG injection scenarios. However, farther from the wells, the amount of dolomite precipitated in the continuous CO₂ and WAG injection scenarios was nearly identical.

Figure 20. Isosurface plots showing the maximum change and an illustrative lower change in volume fraction of dolomite after 10 years for models (a) 1, (b) 2, (c) 3, and (d) 4 and after 57 years for models (e) 1, (f) 2, (g) 3, and (h) 4.

Ankerite and siderite

All four model scenarios predicted net dissolution of ankerite over the whole of the model domain. Moreover, ankerite was predicted to dissolve in the greatest amounts of any of the carbonate minerals. Ankerite dissolution occurred quickly (within the first few years of the simulations) and was never followed by precipitation as native formation water returned to the regions invaded by injected CO₂ plume. At injection wells, ankerite dissolution occurred slightly faster under WAG rather than continuous CO₂ injection conditions, and also slightly faster using the Feldman et al. (2016) rather than the Pan et al. (2016) relative permeability and capillary pressure models. By a distance of 200 m from the injection wells, ankerite dissolution patterns were essentially identical for all four model scenarios (Fig. 19).

The dissolution of ankerite released Fe into the Morrow B formation water, promoting the precipitation of siderite from the formation water, which had initially been very poor in Fe (Table 2). This is evident from the converse relationship between ankerite and siderite abundances in Figure 19c,d,h,i. At injection wells, at early times of less than about 15 years, siderite precipitated slightly more quickly under WAG rather than continuous CO₂ injection conditions, whereas at later times this pattern was reversed. In addition, at injection wells and at early times of less than about 15 years, siderite precipitated slightly more quickly for the Pan et al. (2016) than for the Feldman et al. (2016) relative permeability and capillary pressure models, whereas at later times these two models did not produce any significant difference in siderite behavior. Further from the wells at a distance of 200 m, siderite precipitation patterns were essentially identical for all four model scenarios. After about 5 to 15 years of simulation time, siderite abundance remained relatively constant (Fig. 19).

Non-carbonate minerals

Figure 21. Changes in volume fractions of quartz, albite, clinocllore, illite, kaolinite, and smectite at distances of 0 m (a-f, respectively) and 200 m (g-l, respectively) from well 13-9 as a function of time.

The model simulations also predicted changes in the abundances of non-carbonate minerals (Fig. 21). Quartz, the main mineral constituent of the Morrow B Sandstone, was

predicted to increase steadily in abundance over time for all four model scenarios. This is in part because quartz is slightly supersaturated with respect to the initial Morrow B formation water composition (Ahmmed et al., 2016) and subsequent changes in formation water composition caused by CO₂ injection had little direct effect on quartz solubility. However, the dissolution of other silicate minerals (albite, clinocllore, illite) as a result of CO₂ injection increased aqueous silica concentrations in the formation water, promoting greater quartz precipitation near the injection wells compared to far from them.

Albite, the second most abundant mineral constituent of the Morrow B Sandstone, was predicted to decrease steadily in abundance over time for all four model scenarios. Albite is slightly undersaturated with respect to the initial Morrow B formation water composition (Ahmmed et al., 2016) and is likely naturally undergoing alteration to kaolinite. The acidification of the formation water due to CO₂ injection likely accelerates that alteration process, as can be seen by the sharp decrease in albite abundance and the sharp increase in kaolinite abundance in the early years of the simulations before the changes in their abundances become more gradual over time (Fig. 21b,e,h,k). The formation of smectite in the Morrow B Sandstone, is probably also an albite alteration product caused by the acidification of the formation water from CO₂ injection, as smectite contains Na that would have been provided in part by the dissolution of albite.

Two other minerals initially present in the Morrow B Sandstone, chlorite (clinocllore) and illite, were predicted to dissolve in the simulations apparently because of CO₂ injection, though clinocllore is undersaturated with respect to the initial Morrow B formation water composition and should naturally dissolve in the formation water (Ahmmed et al., 2016). Near the injection wells, clinocllore was predicted to decrease sharply in abundance in the first decades of the simulations, but in the longer simulations (Models 3 and 4), clinocllore began to precipitate and thus increase in abundance again after about 50 years. In contrast, illite decreased steadily in abundance in all four model scenarios.

Changes in porosity

The changes in mineral abundances described in the preceding discussion led to very small predicted changes in porosity. The porosity changes were greatest at injection wells, where porosity increased on the order of only $10^{-3}\%$, most of which occurred within the first decade of the simulations while CO₂ was being injected (Fig. 22a). Slightly greater porosity increases were predicted for WAG than continuous CO₂ injection, and little difference was predicted for the Pan et al. (2016) and Feldman et al. (2016) relative permeability and capillary pressure models. Further from the injection wells, a greater porosity change was predicted for WAG versus continuous CO₂ injection for the Feldman et al. (2016) model, but for the Pan et al. (2016) model no difference in porosity change for WAG versus continuous CO₂ injection was predicted (Fig. 22b).

For the model domain as a whole, porosity also changed very little (a reservoir void space volume change on the order of 10^3 m^3), rising during the first decade of the simulation during CO₂ injection and declining thereafter (Fig. 22c-e). This initial porosity increase was caused by decreases in the volumes of both carbonate and non-carbonate minerals initially present in the Morrow B Sandstone. Consistent with the preceding discussion, slightly greater porosity increases were predicted for WAG versus continuous CO₂ injection. For the Feldman et al. (2016) relative permeability and capillary pressure model (Models 1 and 2), non-carbonate minerals dissolved continuously throughout the simulations whereas carbonate minerals began to precipitate after 10 years once CO₂ injection ceased. Thus, the greatest increases in porosity coincided with the changes in formation water composition caused by CO₂ injection, and once CO₂ injection ceased and the CO₂-enriched formation water progressively mixed with ambient CO₂-poor formation water, porosity declined. For the Pan et al. (2016) relative permeability and capillary pressure model (Models 3 [not shown] and 4), non-carbonate mineral volume declined continuously but only until about 60 years, after which it began increasing, and carbonate mineral volume increased after 10 years, but only until about 50 years, after which it began decreasing.

Figure 22. Porosity (%) as a function of time (years) at distances of (a) 0 m and (b) 200 m from well 13-9. Changes in the total volume (m^3) of void space in the model domain for model scenarios (c) 1, (d) 2, and (e) 4.

However overall, the predicted net changes in porosity over the model domain were too low to have a significant impact on permeability, and thus fluid migrations, or in the CO_2 storage capacity of the reservoir.

Fluid composition

The precipitation and dissolution of minerals caused by CO_2 injection results in significant changes in the Morrow B formation water composition near the injection wells (Fig. 23). The strong dissolution of albite early in the simulations caused a corresponding spike in aqueous Na concentration, which gradually became depleted by the precipitation of smectite, dilution by ambient formation water, and a reduction in the amount of albite dissolution. Aqueous concentrations of K also increased early in the simulations as illite dissolved. After about 30-40 years, aqueous K concentrations began gradually to decline due to the effect of smectite precipitation. Aqueous HCO_3 concentrations increased immediately at the start of the simulations

directly as a result of the injection of CO₂, and remained high for the first few decades of the simulations. As noted previously, the great increase in dissolved CO₂ concentration in the formation water significantly lowered its pH, which led to the dissolution of calcite, ankerite, and clinochlore initially present in the Morrow B Sandstone, and correspondingly increased the concentrations of Ca, Mg, and Fe in the formation water. With increasing precipitation of dolomite, siderite, and eventually calcite, as well as dilution by ambient formation water, the concentrations of Ca, Mg, HCO₃, and Fe declined.

Figure 23. Total aqueous concentrations of Na, K, Ca, Mg, HCO_3 and Fe at distances of 0 m (a-f, respectively) and 200 m (g-l, respectively) from well 13-9 as a function of time.

Limitations of the present numerical simulations:

Although the models were able to simulate much of the complexity in the response of the Morrow B reservoir in the FWU to CO₂ injection, the models had important limitations that introduced uncertainties into the results:

- 1) Models 1 and 2, which employed the relative permeability and capillary pressure models derived from Feldman et al.'s (2016) data for the FWU and thus are likely more representative of actual field conditions than the relative permeability and capillary pressure models derived from Pan et al.'s (2016) data, could not simulate beyond 70 years. This is a relatively short time over which to track the behavior of the CO₂, given the goal of permanent sequestration of the CO₂ in the subsurface.
- 2) The proximity of the western boundary of the model domain to the injection wells, which was necessitated by the available field data, created two limitations in the models. One is that it prevented tracking the progress of the leading edge of the aqueous CO₂ plume and the chemical reactions it caused beyond about 70-100 years after the plume crossed western boundary of the model domain. A second is that simulations were more sensitive to the choice of boundary conditions on the model domain's western boundary than they would have been had the distance between that boundary and the injection wells been greater.
- 3) Uncertainty in the grain size distribution of the Morrow B Sandstone and corresponding uncertainty in reactive surface areas, which appear in the kinetic rate equations for mineral precipitation and dissolution reactions, led to significant uncertainty in reaction rates.
- 4) To facilitate numerical convergence, the Morrow B formation water composition in all four model scenarios was first allowed to equilibrate with the Morrow B mineral matrix for five years before CO₂ injection began. This altered the formation water saturation index of the field values due to water-rock reactions shown in Table 2.
- 5) Heterogeneity in the permeability of the Morrow Shale, which functioned as a cap rock in the models, was not considered. Instead, a uniform average porosity and permeability were assigned

to the Morrow Shale in the models, which were 0.087% and 0.081 milliDarcy (mD) respectively. The Thirteen Finger Limestone, a thicker cap rock that overlies the Morrowan sequence in the FWU (Fig. 2) (mean permeability 0.1 mD) than the Morrow Shale, was not considered in the models.

6) Although several fractures and faults are known to exist in the FWU, these were not directly taken into account as discrete features, though they did affect the bulk permeability and porosity of individual cells in the numerical grid.

7) Due to unavailability of the necessary data in the existing literature, the pH dependence of the kinetic parameters for calcite and quartz were not considered in the models, which may significantly affect the rates at which these minerals precipitated or dissolved as the CO₂ plume evolved.

8) No measured capillary pressure and relative permeability data were available for the Morrow Shale, so the data for the Morrow B Sandstone were used, possibly introducing some error into the flow and transport predictions in the Morrow Shale. In addition, error was introduced in fitting the relative permeability and capillary pressure models to the Feldman et al. (2016) and Pan et al. (2016) data.

9) A separate immiscible petroleum phase was not considered in the models. Petroleum is an effective solvent for CO₂, and the presence of petroleum would also alter the relative permeability and capillary pressure relationships in the models, affecting the migration of CO₂ both as an immiscible gas phase and in aqueous solution, as well as any CO₂-dependent chemical reactions.

Summary and conclusions

The injection of fluids into the Morrow B Sandstone did not significantly perturb the initial pressure distribution in the model domain, in part because of sufficient leakage of immiscible CO₂ from the Morrow B Sandstone through the Morrow Shale but also because of rapid diffusion of pressure laterally through the permeable Morrow B Sandstone. Most of the injected CO₂ leaked through the overlying Morrow Shale as an immiscible phase. Most of the remaining CO₂ dissolved into the Morrow B formation water. The immiscible CO₂ disappeared completely within the first 30-50 years of the simulations. Injection of CO₂ caused a significant temporary drop in the pH of the Morrow B formation water to as low as 4.7, which initiated a number of responses, mostly within about 400 m west of the injection wells. One response included dissolution of carbonate minerals mainly near the injection wells and during the first decades of the simulations, though in Model 4, carbonate dissolution continued until the end of the simulation at 200 years. For the other models, net carbonate precipitation began over the model domain as a whole within a few years after CO₂ injection ceased. Calcite was predicted to be the most abundantly precipitated carbonate mineral over the entire model domain, though in the immediate vicinity of the injection wells, dolomite was the abundantly precipitated carbonate mineral. Net ankerite dissolution was predicted throughout the simulations. Non-carbonate minerals were also affected by the CO₂ injection. Albite, clinocllore, and illite, all minerals that were initially present in the Morrow B Sandstone matrix, were predicted to dissolve, whereas quartz, kaolinite, and smectite were predicted to precipitate. These changes in mineral precipitation and dissolution produced concomitant changes in the composition of the Morrow B Sandstone formation water. Overall, however, the dissolution and precipitation of minerals in the Morrow B Sandstone induce negligible changes in its porosity on the order of 10⁻³%. These changes are too small to cause significant changes in the migration and storage of CO₂ in the Morrow B Sandstone. Based on the numerical modeling results of this study, the Morrow B

Sandstone is judged to be a suitable site for large-scale CO₂ sequestration, where much of the injected CO₂ would be sequestered in aqueous solution for at least decadal to century time-scales. Although more of the injected CO₂ was predicted to leak through the overlying Morrow Shale, this CO₂ should not travel far before becoming trapped by capillary effects.

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