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COMPARISON OF A 2D TOUGHREACT MODEL OF CO_2 INJECTION INTO A CARBONATE RESERVOIR WITH CHEMICAL DATA FROM A CO_2 ENHANCED OIL RECOVERY PROJECT

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ABSTRACT

This paper presents a numerical modeling study of CO_2 injection in an Enhanced Oil Recovery Projects (EOR) in central Alberta. Chemical and isotopic monitoring of a small EOR project in Alberta has been under way since March 2008. One objective of this project is to compare measured geochemical parameters obtained from a producing well located ~800 m from the CO_2 injection well, with modeling results obtained by using the geochemical reactive-transport model TOUGHREACT.

A two-dimensional radial symmetrical model was used for the model and was assumed to be a uniform carbonate formation. The model consisted of three carbonate layers, the Lower Ireton Cap rock, the Leduc Fore Reef storage aquifer, and the Leduc Back Reef bottom rock. CO_2 is injected into the bottom 1 m of the Leduc Fore Reef at a rate of 78 kT/y (2.6 kg/s). The integrity of the cap rock is compromised due to injected CO_2 migrated into it, owing to its permeability, 0.1 MD, resulting in carbonate dissolution.

The primary CO_2 sequestration method is solubility trapping. This is evident in the plume region where low pH and high HCO_3 concentrations were observed. The secondary trapping mechanism is ionic trapping, evident by high Mg and Ca concentrations.

A comparison of modeled values with a producing well in the Leduc Fore reef found that the arrival time of injected CO_2 was similar, ~700 days. Further, the concentrations of HCO_3, both modeled and measured were very similar in values, but after the arrival of injected CO_2, the modeled value was three times larger. The pH and Mg concentrations for the modeled and measured values both followed similar trends. With CO_2 arrival, the pH decreased and Mg concentrations increased at similar times. The modeled pH was 0.5 to 1.5 pH units higher than the calculated downhole pH. The Mg modeled concentration was three times higher than the measured concentrations from the wells.

The results show that the modeled and measured values for different species follow the same trend. The difference is probably due to the kinetic parameters, which are measured on ideal samples—and the minerals present in an oil field are not ideal. Also, the inclusion of 16 months of data which has been collected post-injection, is currently under way.

BACKGROUND

CO_2 injection into saline aquifers is considered a promising option for sequestering large amounts of CO_2 captured from point source emitters such as coal-burning power plants. Although Enhanced Oil Recovery Projects (EOR) are not true Carbon Capture and Storage projects, it is nevertheless feasible to assess the fate of injected CO_2 used in the EOR process by modeling and monitoring.

The CO_2 injection area was into the Leduc Fore Reef; the Reef Complex is subdivided into the Lower, Middle, and Upper Leduc members. The pilot area is confined to the upper northeast perimeter of the Upper Leduc member. The Leduc Formation is overlain by the tight calcitic Ireton Formation; the underlying formation is the Leduc Back Reef. Detailed mineralogical studies were conducted on all members of the formation to determine their composition. CO_2 was injected into an up-sloping pinnacle reef.

Pre-injection brine and gas samples were collected on three separate occasions. Syn-injection brine and gas samples are collected on a semi-regular basis for 30 months; post-injection samples have been collected for the past 16 months and is still ongoing. The brine and gas are analyzed for major anions, cations, and gas composition, as well as nine isotopic parameters.

NUMERICAL METHOD

All of the simulations were performed using TOUGHREACT v. 1.2 (Xu et al, 2006). The code was developed by using the existing multiphase fluid and heat flow code, TOUGH2 v.2 (Pruess, 1991) and adding in the geochemical reactive transport code. The integral finite difference method for space discretization (Narasimham and Witherspoon, 1976) is the basis of the numerical method for simulation of fluid flow. Coupling between the geochemical reactions and fluid transport involves a sequential iterative approach (Yeh and Tripathi, 1991). The fluid property module ECO2N was used in the modeling.

SETUP OF THE MODEL

Geometry

A three-layer uniform model is used: the Lower Ireton calcitic cap rock is 3 m in thickness; the Leduc Fore Reef, a mixed calcite/dolomite, is 11 m in thickness; and the Leduc Back Reef, a calcitic bottom rock, is 3 m in thickness. The formations are assumed to be uniform throughout, extend 3 km in the horizontal direction, and have a radial symmetrical with non-uniform spacing. The cap rock and bottom rock have a layer thickness of 0.5 m, with the Leduc having 0.25 m thickness. CO_2 injection occurs in the bottom 2 m of the Leduc.

The simplifications in the model geometry result in a number of shortcomings, and hence we were not able to consider non-uniform sweeps, buoyancy forces, convective mixing, etc. One justification for these simplifications are that the slow reaction rates and the long time scales for geological changes will, in the long run, make the CO_2 distribution more or less uniform over time (Xu et al., 2007).

Initial and boundary conditions

Hydrogeological parameters used in the simulations are shown in Table 1. The Leduc Fore reef is the most porous and permeable zone, with a porosity of 17.5% and a permeability of 750 md. The overlying Ireton is relatively impermeable, with a permeability value of 0.1 md and porosity of 5.0%, suggesting that it is a very good cap rock. The Van Genunchten (1980) model was used to calculate the capillary pressure and relative permeability curves for each layer in the model.

Table 1. Hydrogeological parameters for the Lower Ireton, Leduc Fore Reef and Leduc Backreef formations

	Lower Ireton	Leduc Fore Reef	Leduc Back Reef
Porosity (%)	5.0	17.5	5.0
Perm. (m^2)	0.1	750	2.0
Temperature (°C)		40	
Pressure (MPa)		8.0	
Pore Comp. (Pa^{-1})		$1\ 10^{-8}$	
Diffusivity(m2/s)		$1\ 10^{-9}$	
Torousity		0.3	

Table 2 summarizes the measured water composition of brine obtained during the pre-injection portion of the study. The water composition given in Table 2 is representative for brines measured at surface conditions, i.e., after the sample degassed while moving from depth to surface. The water used in the simulation was re-equilibrated with degassing H_2S, CH_4, and CO_2 using SOLMINEQ88 (Kharaka et al., 1988) as shown in Table 2. The waters were then equilibrated with the three-layered reservoir for 10 years using the static mode of TOUGHREACT. Two species shown in Table 1 were not measured: AlO_2^- and $O_{2(aq)}$. A small amount of each was added, since the first would probably be present due to the presence of silicate minerals, and the $O_{2(aq)}$ was necessary for redox reactions to occur.

The initial mineral compositions of the Lower Ireton, Leduc Fore Reef, and Leduc Back Reef formations used in the modeling are shown in Table 3. The Lower Ireton is composed of mainly calcite (95.51%), dolomite (3.20%), and minor amounts of quartz, k-feldspar, and pyrite.

The Leduc Fore Reef consists of mostly calcite (47.67%) and dolomite (52.01%) with a trace of quartz. The Leduc Back Reef consists primarily of calcite (98.94%) and minor amounts of dolomite.

Table 2. Initial chemical species concentrations of the brine used in the TOUGHREACT simulations

Species	Measured Concentration (mol/kg)	Equilibrium Concentration (mol/kg)
pH	6.82	7.72
Ca^{2+}	0.118	2.170×10^{-2}
Mg^{2+}	.006	0.1745
Na^{+}	1.325	1.267
K^{+}	.0073	6.970×10^{-3}
Sr^{2+}	.0017	1.637×10^{-3}
Fe^{2+}	2.15×10^{-5}	1.940×10^{-5}
$SiO_{2(aq)}$	3.79×10^{-4}	3.623×10^{-4}
HCO_3^{-}	7.97×10^{-3}	8.320×10^{-3}
SO_4^{2-}	.0175	0.0168
Cl^{-}	1.672	1.670
AlO_2^{-}	-	1.36×10^{-7}
$O_{2(aq)}$	-	4.88×10^{-70}
$H_2S_{(aq)}$	3.93×10^{-3}	3.97×10^{-2}

Table 3: Initial mineral volume fractions and secondary minerals used in TOUGHREACT simulations

Primary Minerals	Lower Ireton (%)	Leduc Fore Reef (%)	Leduc Back Reef (%)
Calcite	95.51	47.67	98.94
Dolomite	3.20	52.01	0.86
Quartz	0.74	0.32	0.21
K-feldspar	0.22	0.00	0.00
Pyrite	0.33	0.00	0.00
Secondary Minerals			
Albite-low	Anhydrite	Ankerite	Aragonite
Chlorite	Dawsonite	Illite	Kaolinite
Magnesite	Siderite	Ca-Smectite	Na-Smectite

Table 4 provides parameters for the kinetics of dissolution and precipitation by the minerals, primary and secondary, used in the models (Palandri and Kharaka, 2004). Calcite was used as an equilibrium mineral in the simulations due to its relatively fast kinetics. The secondary minerals considered in the 2-D model are given in Table 3. Specific details about the kinetics used in the simulations can be found in Xu et al. (2007).

Table 4. Parameters for calculating kinetic rate constants of minerals used (Palandri and Kharaka, 2004).

Mineral	A (cm^2/g)	Parameters for kinetic rate law							
		Neutral Mechanism		Acid Mechanism			Base Mechanism		
		k^{25} ($mol/m^2/s$)	E (kJ/mol)	k^{25}	E	$n(H^+)$	k^{25}	E	$n(H^+)$
Dolomite	9.1	$2.9512\ 10^{-8}$	52.2	$6.4565\ 10^{-04}$	36.1	0.500			
Illite	108.7	$1.6596\ 10^{-13}$	35.0	$1.0471\ 10^{-11}$	23.6	0.340	$3.02\ 10^{-17}$	58.9	-0.400
K-feldspar	9.1	$3.8905\ 10^{-13}$	38.0	$8.7096\ 10^{-11}$	51.7	0.500	$6.3096\ 10^{-22}$	94.1	-0.823
Low-Albite	9.1	$2.7542\ 10^{-13}$	69.8	$6.9183\ 10^{-11}$	65.0	0.457	$2.5119\ 10^{-16}$	71.0	-0.572
Kaolinite	108.7	$6.9183\ 10^{-14}$	22.2	$4.8978\ 10^{-12}$	65.9	0.777	$8.9125\ 10^{-18}$	17.9	-0.472
Na-smectite	108.7	$1.6596\ 10^{-13}$	35.0	$1.0471\ 10^{-11}$	23.6	0.340	$3.0200\ 10^{-17}$	58.9	-0.400
Ca-smectite	108.7	$1.6596\ 10^{-13}$	35.0	$1.0471\ 10^{-11}$	23.6	0.340	$3.0200\ 10^{-17}$	58.9	-0.400
Dawsonite	9.1	$1.2598\ 10^{-09}$	62.76	$6.4565\ 10^{-04}$	36.1	0.500			
Aragonite	9.1	$4.5709\ 10^{-10}$	23.5	$4.1687\ 10^{-07}$	14.4	1.000			
Siderite	9.1	$1.2598\ 10^{-09}$	62.76	$6.4565\ 10^{-04}$	36.1	0.500			
Ankerite	9.1	$1.2598\ 10^{-09}$	62.76	$6.4565\ 10^{-04}$	36.1	0.500			
Magnesite	9.1	$4.5709\ 10^{-10}$	23.5	$4.1687\ 10^{-07}$	14.4	1.000			
Chlorite	9.8	$3.02\ 10^{-13}$	88.0	$7.762\ 10^{-12}$	88.0				
Anhydrite	9.1	$6.457\ 10^{-04}$	14.3						
Pyrite	12.87	$2.8184\ 10^{-05}$	56.9 $n(O_{2(aq)})=0.5$	$3.2022\ 10^{-08}$	56.9 $n(H^+) = -0.5$, $n(Fe^{3+})=0.5$				

Notes: (1) all rate constants are for dissolution
(2) A is specific area, k^{25} is kinetic rate constant at 25 ºC, E is activation energy, n is power term (Eq. (3), Xu et al., 2007)
(3) power terms n for both acid and base mechanism are with respect to H^+
(4) for pyrite, the neutral mechanism has n with respect to $O_{2(aq)}$, the acid mechanism has two species involved: one n with respect to H^+ and another n with respect to Fe^{3+} (Eq. (3), Xu et al., 2007)

GEOCHEMICAL REACTIONS

The dissolution of CO_2 in water forms carbonic acid via Reaction 1, also known as solubility trapping, resulting in a decrease in the pH. If there are any reactant minerals present, such as calcite, then mineral dissolution occurs (Reaction 2) resulting in a free cation and a bicarbonate ion, causing both the pH and the cation concentration to increase.

$$CO_2 + H_2O \rightleftharpoons H_2CO_3$$
$$H_2CO_3 \rightleftharpoons H^+ + HCO_3^- \quad \text{Solubility Trapping (1)}$$

$$CaCO_3 + H^+ \rightharpoonup Ca^{2+} + HCO_3^- \quad \text{Mineral Dissolution (2)}$$

Thus, the net reaction between injected CO_2 and calcite is as follows, also known as ionic trapping:

$$CO_2 + H_2O + CaCO_3 \rightharpoonup Ca^{2+} + 2HCO_3^- \quad \text{Ionic Trapping (3)}$$

SIMULATION RESULTS

The simulations conducted for this study considered the fate of injected CO_2 in the reservoir—through geochemical interactions with the brine and comparing the simulation results with data collected from a well ~800 m from the injector. The simulation results are presented in 2-D graphical plots as a function of depth and radial distance at discrete time intervals of 0.33 and 2.5 years for the CO_2 injection. While the simulation covered a radial distance of 3 km, only the first 1 km is shown, since that is where the main reactions are occurring. Specific data are also presented in graphical form as a function of depth at discrete time intervals, 0.09, 0.33, 0.59, 1.0, 1.5, 2.0, and 2.5 years, at a distance of 817 m from the injector. The modeled injection rate of CO_2 into the Leduc Fore Reef was 78 kT/y or 2.6 kg/s.

Spatial Distibution

Supercritical CO_2 is injected into the formation and, having a density less than that of the brine (~ 10 kg/m^3), migrates from the injection region upwards to the Lower Ireton cap rock. Even at the low injection rate, 2.6 kg/s, there is enough injected CO_2 in 0.33 years to see an injection plume (Figure 1). The plume had radially dispersed ~300 m under the cap rock and appears to have migrated slightly into the lower Ireton cap rock. After 2.5 years of injection, the plume had expanded radially to ~700 m. The migration of CO_2 into the Lower Ireton cap rock is evident with a maximum Sg ~0.3 at the Ireton-Leduc interfacial region nearest the injector region. This would indicate that the Lower Ireton is not an impervious cap rock. Also, CO_2 migration has occurred in the bottom rock, the Leduc Back Reef, the bottom rock. It extends out to ~250 m in the bottom rock with a maximum S_g of~0.6 in the region nearest to the injector.

The spatial distribution of HCO_3 within the study region is shown in Figure 2. The HCO_3 has a similar plume shape and size as that of the free-phase CO_2. The concentration in the Leduc Fore reef region is quite high, >1.8 mol/kg after only 0.33 years injection. The susceptibility of the cap rock and bottom rock to CO_2 is evident in both time slices for HCO_3. In the cap rock region, the concentration is ~1.6 mol/kg at the Ireton-Leduc interfacial region. After 2.5 years, both the bottom rock and cap rock region show significant HCO_3 concentration >1.8 mol/kg, indicating poor cap rock and bottom rock integrity.

pH spatial distribution in the Leduc Fore Reef aquifer is shown in Figure 3. The initial pH of the brine is 7.5; after 0.33 years of injection, this decreases to ~5.5. The pH in the cap rock and bottom rock regions also drops to ~5.0 within 0.33 years. The low pH of ~5.5 extends out to ~775 m after 2.5 years. In the bottom and cap rock, the pH ~5.0 region extends out to ~675 and ~775 m respectively.

Figure 4 shows the spatial distribution of Mg. The background concentration of Mg is ~0.18 mol/kg. After 0.3 years of CO_2 injection, the Mg concentration has increased to ~0.52 in the plume region. The significant increase in the concentration of Mg, Ca (not shown), and HCO_3 indicates that ionic trapping, Reaction 3, is an important reaction occurring with the reservoir.

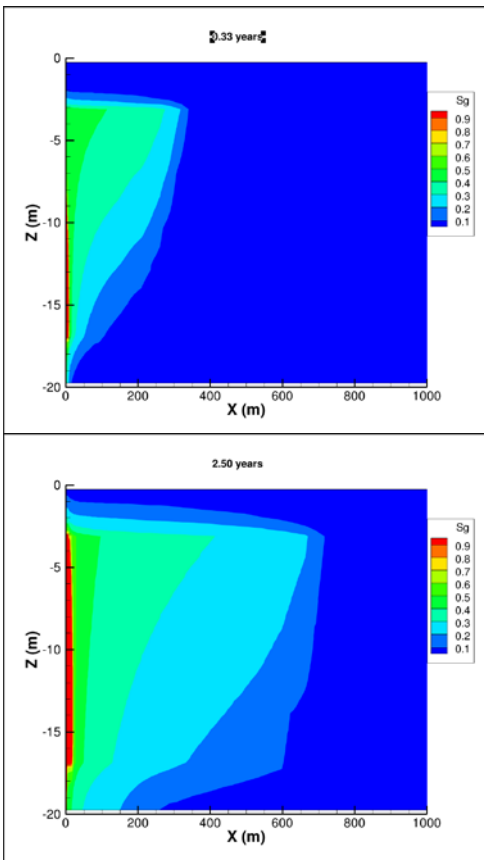

Figure 1. Spatial distribution of CO_2 gas saturation after 0.33 and 2.5 years of injection.

However, that there is no increase in the pH of the system in regions with high Mg concentration indicates that solubility trapping, Reaction 1, is the dominant reaction. This is to be expected, since the Leduc Fore Reef is calcite and dolomite (Table 3). The high Mg also occurs both within the cap rock and bottom rock region. Since there is dolomite present, albeit in smaller amounts, there are sufficient enough amounts to cause a significant increase in Mg concentration. By 2.5 years, the increased Mg occurs throughout the storage reservoir. However, the regions of highest concentration, >0.6 mol/kg, occur in the bottom rock and to a lesser extent in the cap rock. This, along with the high HCO_3 concentration, indicates that a significant amount of ionic trapping is occurring in the bottom rock. The highest concentrations in the bottom rock can be explained by the permeability. At 2.0 mD, it allows CO_2 to easily enter the region, but the formation is tight enough to impede its transport, allowing for significant dolomite dissolution to occur. The reservoir storage region has a lesser amount of dissolution due to its high permeability, 750 mD, more readily allowing the transport of CO_2, resulting in smaller amounts of dissolution but over a wider area.

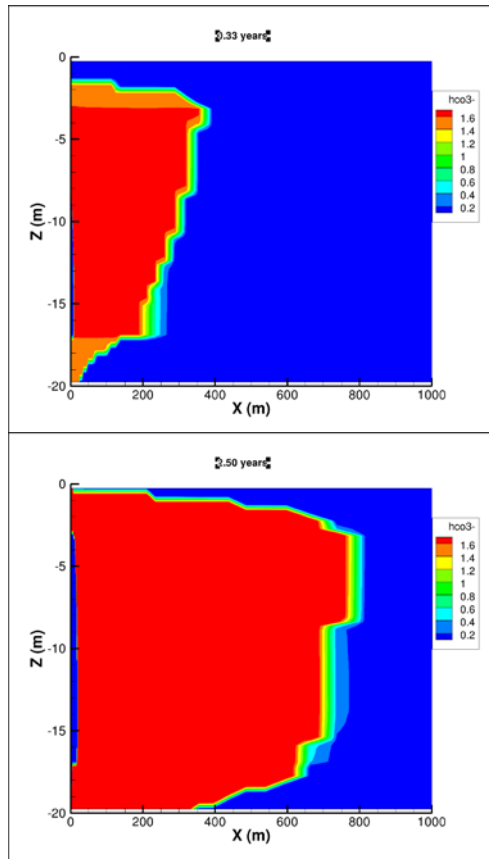

Figure 2. Spatial distribution of HCO_3 after 0.33 and 2.5 years of injection. The units of concentration are mol/kg.

Concentration vs Depth Profile at 817 m

Concentration profiles were isolated from the 2D surface plots at a distance of 817 m from the injector well. This was done to compare the species from the model with results from a producing well located ~800 m from the injector. (This comparison between model and producing well is done in the next section.) Figure 5 shows a depth profile for the concentration of HCO_3 as a function of time. There is no significant change in HCO_3 until after 2 years. The change in concentration varied radially with decreasing depth: as the depth decreased, the concentration of HCO_3 increased, reaching the maximum, twice the initial

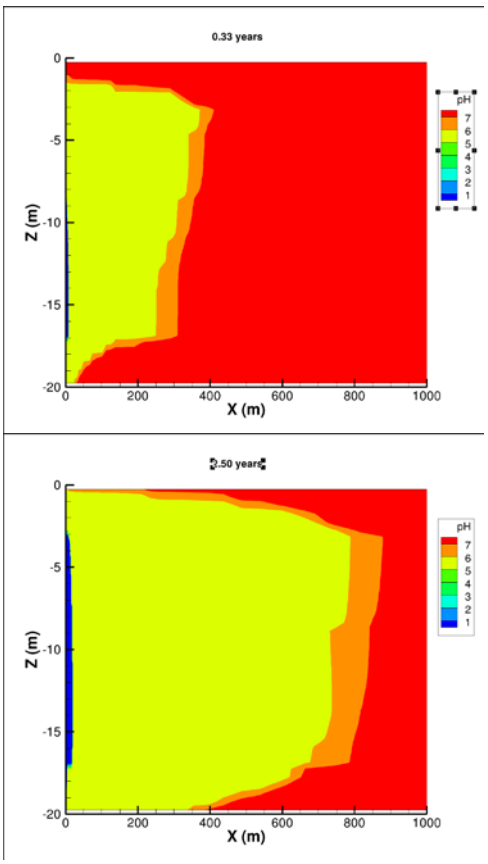

Figure 3. Spatial distribution of pH after 0.33 and 2.5 years of injection.

concentration, at the interface between the Ireton caprock and Leduc storage aquifer. After 2.5 years, the plume dispersion is evident by the concentration profile. The concentration is largest at the Ireton-Leduc interface and has a profile similar to that for plume dispersion. The time/depth profile for the pH is identical to the HCO_3 profile, except that the pH is decreasing over time. There was no change in the pH until after 2 years of CO_2 injection. At 2 years, the pH decreases slightly, from ~7.5 to 7.2, at the Ireton-Leduc interface. As depth increases, the pH increases to its background value at the bottom rock interface. The pH trend after 2.5 years is very similar to the HCO_3 trend but with decreasing pH. The Mg concentration follows that of the HCO_3; after 2 years, there is a very slight increase in Mg at the Ireton-Leduc interfacial region. After 2.5 years, the change in concentration varied radially with decreasing depth; as the depth decreased, the concentration of Mg increased, reaching the maximum at the storage-cap rock interface.

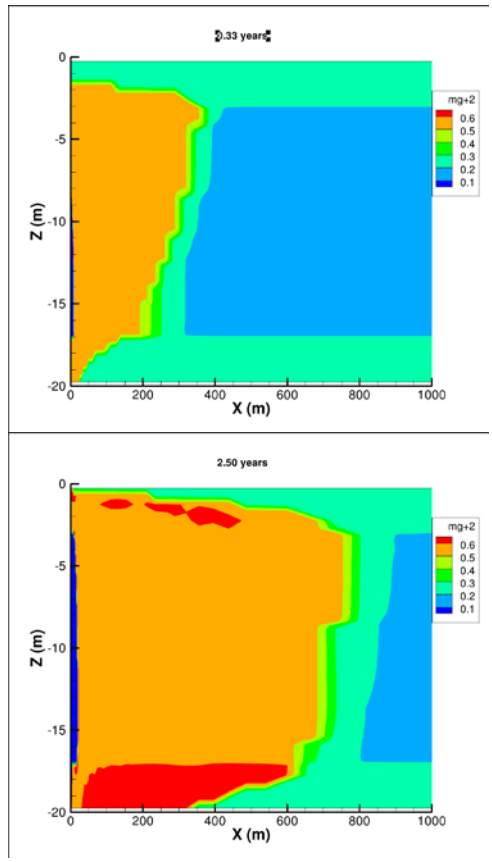

Figure 4. Spatial distribution of Mg after 0.33 and 2.5 years of injection. The units of concentration are mol/kg.

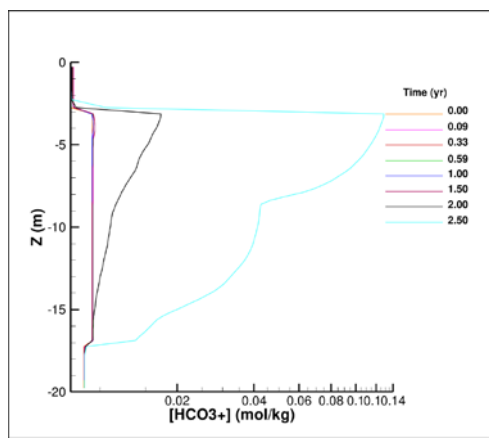

Figure 5. HCO_3 concentration profile as a function of depth.

The lack of significant increase in Mg after 2 years, while pH decreased and HCO_3 increased, indicates that solubility trapping is the primary sequestration method. After that, the continuing decrease in pH but increase in Mg and HCO_3

indicated that both ionic and solubility trapping are occurring, with solubility trapping being more dominant.

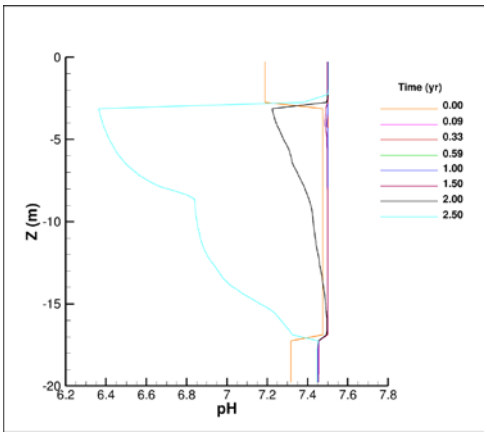

Figure 6. pH profile as a function of depth.

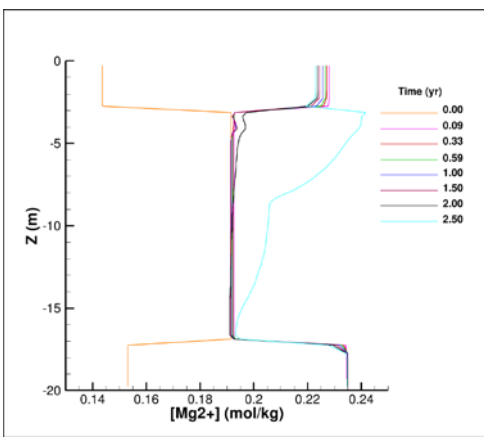

Figure 7. Mg concentration profile as a function of depth.

COMPARISON OF MODEL RESULTS AND MEASURED PARAMETERS

The exact depth of fluid production for a well producing in the Leduc Fore reef is not known. Thus, it is difficult to compare the production concentrations and the modeled concentrations. To accomplish this, the average value for the species of interest in the Leduc Fore Reef was compared with the measured value from the production well.

Figure 8 shows the HCO_3 concentrations modeled using TOUGHREACT compared to measurements from fluid samples from the production well. The observed trends are initially very similar, showing little change in concentration up to ~700 days. After ~700 days after the commencement of CO_2 injection, both modeled and measured bicarbonate concentrations increased, though at different rates.

Figure 9 shows a comparison between the downhole pH modeled with TOUGHREACT and the downhole pH based on measured results and adjusted using SOLMINEQ88 (Kharaka et al. 1988) for the producing well. SOLMINEQ88 allows for a reversal of degassing, which occurred when the sample was brought from depth to the surface, affecting the chemistry of the fluid. While the two pH values deviate by up to 1.5 pH units, the observed and modeled trends are very similar, remaining initially rather constant followed by a marked pH decrease. Also shown in Figure 9 are two linear fits of the measured and corrected downhole pH. The first linear fit is for the sampling times where the pH slowly decreased; the second fit is for the period of rapid pH decrease. The onset of the rapid decrease in the pH of the brine occurs in both the model and the measured data for samples from the well at approximately the same time, ~700 days, as shown by the blue dotted line in Figure 9. This indicates that solubility trapping of injected CO_2 has started to occur, as indicated in Reaction (1).

Figure 10 shows the changes in the calcium and magnesium concentrations obtained through measurements on fluids recovered from the production well. The modeled Mg concentration is constant at ~5000 mg/L for ~700 days, then shows a slight increase in concentration after this to 5520 mg/L. The measured concentrations have a relatively constant value of ~1650 mg/L, but it cannot be determined if there is an increase. The reason for the modeled Mg concentrations being 3 times the measured values has yet to be determined—it may be due to the kinetic parameters for dolomite requiring adjusting. The model kinetic parameters are based on measurements of kinetics for pure mineral phases. The minerals present are far from ideal in terms of surface areas, etc. These kinetic values have to be re-examined to account for real world events, e.g., water flooding corroding the ideal mineral surface areas.

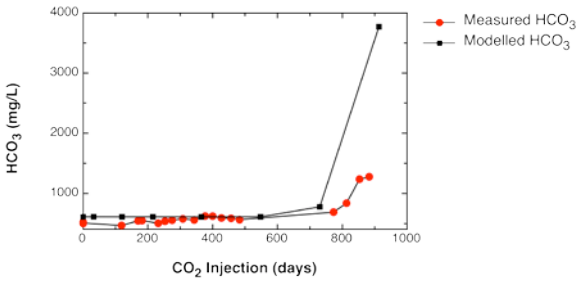

Figure 8. Measured and modeled HCO_3 versus CO_2 injection time.

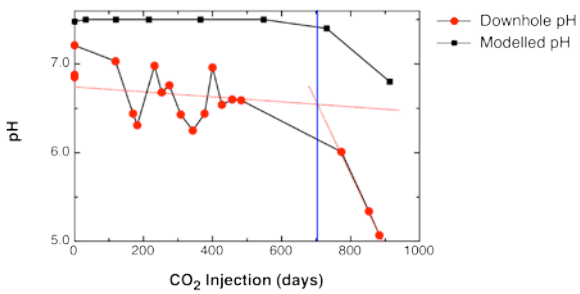

Figure 9. Measured and modeled pH versus CO_2 injection time.

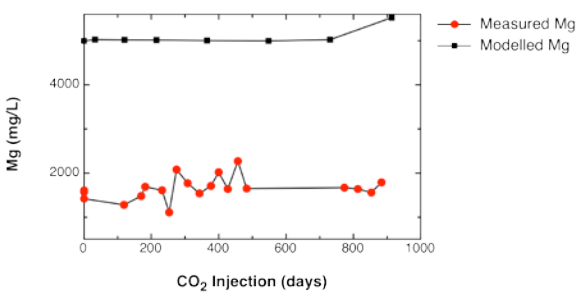

Figure 10. Measured and Modeled Mg versus CO_2 injection time.

CONCLUSIONS

For the TOUGHREACT model, the following has been determined:

1. Solubility trapping, Reaction 1, appears to be the significant method of sequestration.
2. Ionic trapping, Reaction 2, occurs very early on in the injection phase, as early as 30 days after the start of injection.
3. The Lower Ireton and Leduc Back reef are very poor seals. CO_2 infiltration occurred very early on and, in the case of the Leduc Back Reef, significant dolomite dissolution also occurred, shown by the large increase in Mg and HCO_3 concentrations and high CO_2 gas saturation values.
4. Plume dispersion occurred very quickly, evident as early as 30 days, due to the high permeability of the storage aquifer, the Leduc Fore Reef.

For the modeled well at 817 m from the injector, when compared to a well producing in the Leduc Fore Reef ~800 m from the injection well, the following was observed:

5. The arrival time of injected CO_2 was very similar, ~700 days after the onset of injection.
6. The modeled and measured concentrations of HCO_3 are nearly identical until the arrival of CO_2. Then, the modeled concentration increased significantly when compared to the measured value, three times larger.
7. The trends in the pH values are similar, but the modeled pH is 0.5–1.5 higher than the calculated downhole pH.
8. The modeled and measured trends for Mg concentration are similar, but the modeled values are 3 times the measured values.

Future work on this will include examining the kinetic parameters to see the effects on pH and cation concentrations, and adding 16 months of data that has been collected post-injection.

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