

# The Wabamun Area Sequestration Project (WASP): Modeling CO<sub>2</sub> Injection into an H<sub>2</sub>S Containing Saline Aquifer using Toughreact

Maurice Shevalier, Michael Nightingale, Bernhard Mayer and Ian Hutcheon  
Applied Geochemistry Group, Dept. of Geoscience, University of Calgary  
2500 University Drive NW, Calgary, AB, T2N 1N4, Canada

## Introduction

CO<sub>2</sub> captured from point source emitters such as coal-burning power plants can be sequestered by injection into saline aquifers. This is considered a promising option for sequestering large amounts of CO<sub>2</sub>. If the deep saline aquifers contain even minor amounts of anhydrite or other sulfate sources, H<sub>2</sub>S may be present. If the unit in question has been buried to reach a temperature of 120°C, H<sub>2</sub>S will almost certainly form via the process of thermochemical sulfate reduction (TSR) (Krouse et al. 1988; Hutcheon, 1999; Simpson, 1999). On a volume basis, the amount of anhydrite required to produce 50% H<sub>2</sub>S in gas at 5% porosity is less than 1% of the rock. Typical anhydrite amounts e.g. in Devonian strata of the Western Canadian Sedimentary Basin, are much higher.

The Wabamun Area CO<sub>2</sub> Sequestration Project (WASP) investigates the feasibility of injecting one gigaton of CO<sub>2</sub> (20 Mt-CO<sub>2</sub> year<sup>-1</sup> for 50 years) into a saline aquifer in the Western Canadian Sedimentary Basin. In the WASP study area in central Alberta, the Devonian Nisku formation was identified as a suitable aquifer for CO<sub>2</sub> injection due to its non-association with current oil and gas production, adequate depth, adequate containment, and good reservoir quality. Computer modeling was undertaken to determine what effects H<sub>2</sub>S present in the reservoir would have on the injection of CO<sub>2</sub> into the Nisku formation.

## TOUGHREACT Modeling Details

TOUGHREACT v. 1.2 (Xu and Pruess, 2001) was used to perform all of the simulations using the fluid property module ECO2N. A single layer uniform homogeneous carbonate formation with a thickness of 70 m which extended infinitely in the horizontal direction is considered in the present model. A one dimensional radial symmetrical geometry was used with non-uniform spacing. Injection of carbon dioxide was simulated at 31.69 kg/s (1 MT/year) for 50 years. The initial pressure was 16 MPa at the top of the formation. The measured water composition from brine obtained from a well located in the Nisku formation (Shevalier and Mayer, 2009) and an initial mineral composition from a representative sample of the Nisku formation (Nightingale et al., 2009) were used in the simulation.

The simulations conducted for this study considered the fate of injected CO<sub>2</sub> in the reservoir through geochemical interactions with the brine, with minerals present in the formation and residual trapping, i.e. how much CO<sub>2</sub> remained as a gas in the reservoir. Two sets of simulations were performed, one with and one without dissolved H<sub>2</sub>S present in the brine in order to evaluate the effect of ambient dissolved H<sub>2</sub>S on the geochemistry of the reservoir when large amounts of CO<sub>2</sub> (1 MT/year for 50 years) are injected.

## Results and Discussion

Initially, the pH of the brine was 6.10 across the entire reservoir. The pH distribution along the radial distance appeared to increase from values below 4.0 to 5.11 (see Figure 1). The region of  $\text{pH} < 4.0$  is the region where there was no water present, i.e. the value of the gas saturation was  $\sim 1.0$ . This complete dehydration was probably due to the high rate of  $\text{CO}_2$  injection and the region ranges from 19.7 m after one year to 136.1 m after 50 years (see Table 1). Beyond this region, the pH was initially at a value of 5.11 and remained constant, then increased over a very short distance from 5.11 to 6.44 and remained constant over the rest of the radial distance. This represents the region where  $\text{CO}_2$  had diffused into the reservoir fluids and solubility trapping is occurring causing the pH to remain slightly acidic. This pattern was observed for both  $\text{H}_2\text{S}$  and non- $\text{H}_2\text{S}$  aquifers.

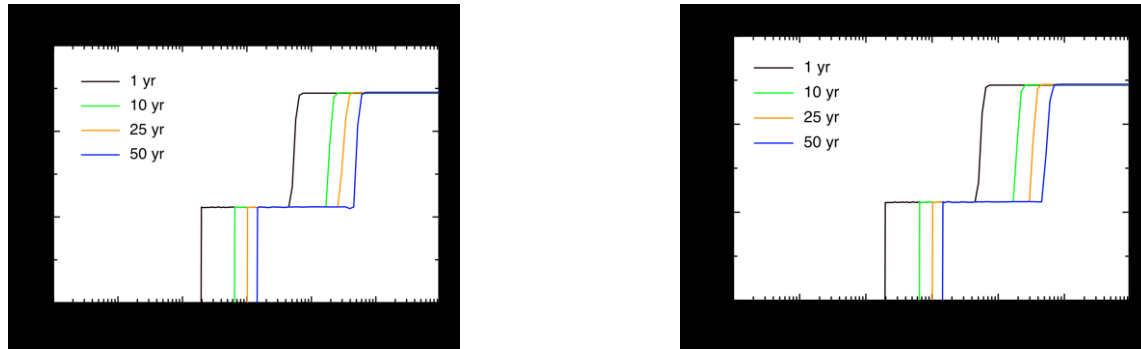


Figure 1. pH of aquifer as a function of radial distance after initiation of  $\text{CO}_2$  injection for both non- $\text{H}_2\text{S}$  and  $\text{H}_2\text{S}$  aquifers.

The initial concentration of bicarbonate in the brine was  $\sim 0.02$  moles/kg across the entire modeling area. After one year of injection the concentration of bicarbonate in the brine was  $\sim 1.25$  moles/kg at a distance of  $\sim 20$  m from the injector (see Figure 2). At a distance of  $\sim 500$  m the concentration decreased to the ambient value of  $\sim 0.02$  moles/kg. A similar increase and decrease in bicarbonate concentration was evident for all times but at increasing distances from the injector (see Figure 2). The increase in bicarbonate concentrations along with the decrease in pH indicated that solubility trapping was occurring in this region. The gradual increase in sequestration of  $\text{CO}_2$  over time was due to the larger fluid volumes available as the  $\text{CO}_2$  travels radially outward into the reservoir. Further, as time progressed the amount of injected  $\text{CO}_2$  sequestered by solubility trapping increased from 34% to 56% (see Table 1). Results for simulations with or without  $\text{H}_2\text{S}$  in the aquifer were similar.

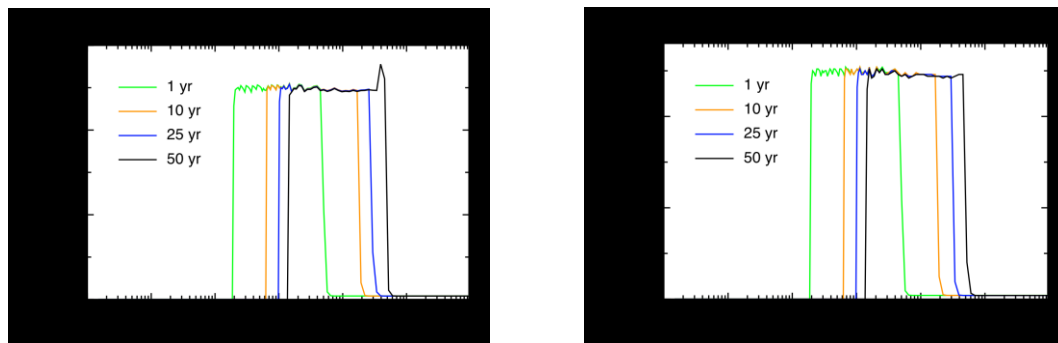


Figure 2.  $\text{HCO}_3^-$  concentration as a function of radial distance after initiation of  $\text{CO}_2$  injection for both non- $\text{H}_2\text{S}$  and  $\text{H}_2\text{S}$  aquifers.

Time (years)	Amount of CO <sub>2</sub> stored in brine as HCO <sub>3</sub> <sup>-</sup> (MT)	Percentage of injected CO <sub>2</sub> stored as HCO <sub>3</sub> <sup>-</sup>
1.0	0.28	34%
5.0	1.66	33%
10.0	3.96	39%
12.5	5.50	44%
25.0	10.8	43%
37.5	17.8	48%
50.0	27.8	56%

Table 1: Injection time of CO<sub>2</sub> and amount of CO<sub>2</sub> stored as HCO<sub>3</sub><sup>-</sup> in the reservoir waters for both H<sub>2</sub>S and non-H<sub>2</sub>S aquifers.

There was a small decrease in dolomite present to ~100 m (see Figure 3). Thereafter the amount of dolomite present remained constant as the radial distance increased followed by a small increase. The radial distance of this volume change increased with time, from ~500 m after 1 year of injection to ~5000 m after 50 years. Calcite displayed an opposite trend, i.e. the volume fraction of calcite increased at similar radial distances then remained stable and then decreased slightly at similar distances to the dolomite change (see Figure 4). Mineral precipitation represents another method of CO<sub>2</sub> sequestration, but in this case the net C sequestration via mineral trapping was negligible compared to the amount of CO<sub>2</sub> sequestered as HCO<sub>3</sub><sup>-</sup>. The presence of H<sub>2</sub>S did not significantly change the simulation results.

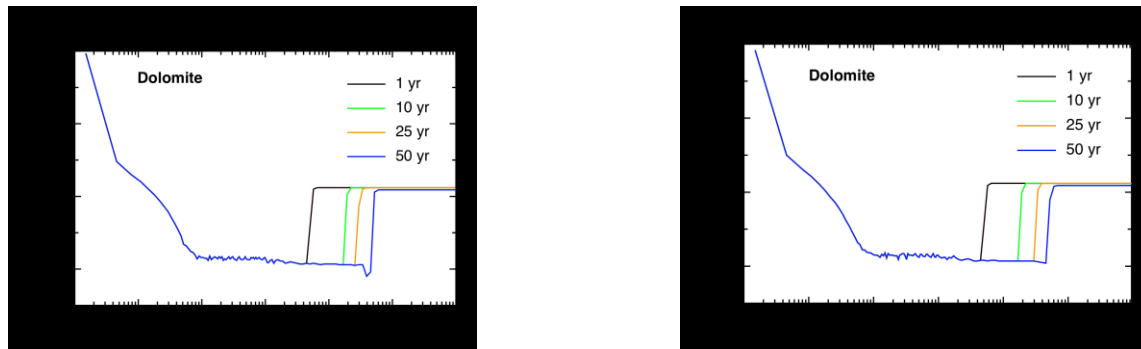


Figure 3. Dolomite mineral abundance as a function of radial distance after initiation of CO<sub>2</sub> injection for both non-H<sub>2</sub>S and H<sub>2</sub>S aquifers.

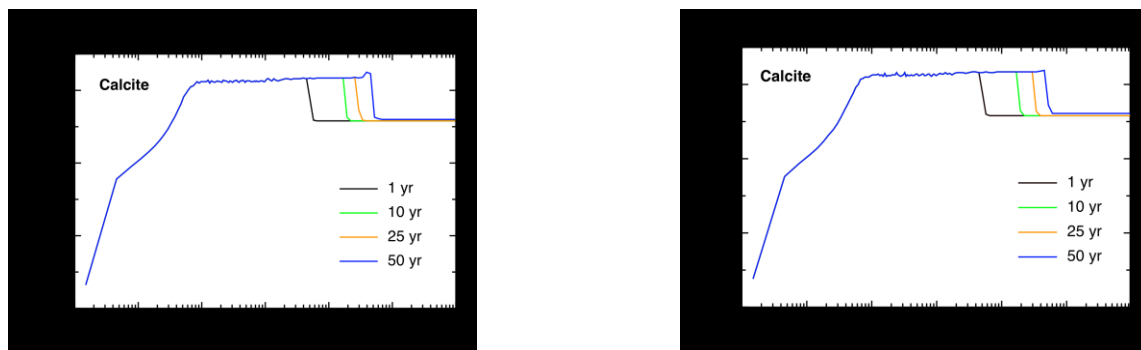


Figure 4. Calcite mineral abundance as a function of radial distance after initiation of CO<sub>2</sub> injection for both non-H<sub>2</sub>S and H<sub>2</sub>S aquifers.

## References

- Hutcheon, I., Controls on the distribution of non-hydrocarbon gases in the Alberta Basin, *Bull. Can. Pet. Geol.*, 47(4), 573-593, 1999.
- Krouse, H.R., Viau, C.A., Eliuk, L.S., Ueda, A. and Halas, S., Chemical and isotopic evidence of thermochemical sulphate reduction by light hydrocarbon gases in deep carbonate reservoirs, *Nature*, 333, 415-419, 1988.
- Nightingale, M., Shevalier, M., Mayer, B., *Wabamun Area Sequestration Project: Mineralogy Report*, Wabamun Area CO<sub>2</sub> Sequestration Project (WASP) Internal Report, University of Calgary, 2009
- Shevalier, M., Mayer, B., *Wabamun Area Sequestration Project: Baseline Geochemistry and Preliminary Geochemical Modelling*, Wabamun Area CO<sub>2</sub> Sequestration Project (WASP) Internal Report, University of Calgary, 2009
- Simpson, G., 1999, Sulfate reduction and fluid chemistry of the Devonian Leduc and Nisku formations in south-central Alberta. Ph.D. Thesis, University of Calgary (unpublished).
- Xu, T., Pruess, K., On fluid flow and mineral alteration in fractured caprock of magmatic hydrothermal systems, *J. Geophys. Res.*, 106, 2121–2138, 2001.