POTENTIAL CHEMICAL IMPACTS OF CO_2 LEAKAGE ON UNDERGROUND SOURCE OF DRINKING WATER (USDWs) ASSESSED BY QUANTITATIVE RISK ANALYSIS

Case Study of the SWP Phase 3 Project: Farnsworth Unit CO2-EOR Demonstration

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Introduction

To evaluate potential risks to Underground Sources of Drinking Water (USDWs) due to CO_2 leakage, a response surface methodology (RSM) based on a generic TOUGHREACT geochemical model is developed to quantify risks due to CO_2 intrusion. The case study example is the Ogallala aquifer overlying the Farnsworth unit (FWU). The main objectives of this study are to: (1) understand how CO_2 leakage is likely to influence geochemical processes in aquifer sediments; (2) quantify the potential risks to the Ogallala groundwater aquifer associated with changes in groundwater chemistry due to CO_2 leakage from the FWU; and (3) identify water chemistry factors as markers for early detection criteria.

Methodology

Simulation of cement hydration

A batch simulation of cement hydration was conducted for 100 years, to obtain the equilibrium wellbore cement composition in the field environment.

Primary chemical equations in this simulation:

$$(CaO)_3 \cdot A_2O_3 + 3CaSO_4 \cdot 2H_2O + 26H_2O \rightarrow (CaO)_6 \cdot Al_2O_3 \cdot (SO_3)_3$$
$$(CaO)_6 \cdot Al_2O_3 \cdot (SO_3)_3 \cdot (H_2O)_{32} + 2(CaO)_3 \cdot Al_2O_3 + 22H_2O \rightarrow 3(CaO)_4 \cdot Al_2O_3 \cdot SO_3 \cdot (H_2O)_{18}$$
$$(CaO)_3 \cdot SiO_2 + H_2O \rightarrow CSH + Ca(OH)_2$$
$$(CaO)_2 \cdot SiO_2 + H_2O \rightarrow CSH + Ca(OH)_2$$
$$(CaO)_4 \cdot Al_2O_3 \cdot Fe_2O_3 + 3CaSO_4 \cdot 2H_2O + 21H_2O \rightarrow (CaO)_6 \cdot Al_2O_3 \cdot (SO_3)_3 \cdot (H_2O)_{32} + Fe_2O_3 \cdot (H_2O)_3$$

Simulation of CO_2 leakage flux through wellbores

A vertical 1-D simulation was conducted for 100 years, calibrated with the mineralogy result of the cement hydration model. A dual-permeability continuum was developed to simulated fracture and matrix.. The uncertainties of leakage flux were quantified by RSM.

Table: Hydrogeological parameters

Property	Value	Property	Value
Reservoir		**USDW aquifer**	
Thickness	30 m	Thickness	100 m
Permeability	4.52×10^{-14} m^2	Permeability	5.0×10^{-13} m^2
Porosity	0.1453	Porosity	0.30
Rock density	2650 kg/m^3	Rock density	2600 kg/m^3
Salinity	0.06	Salinity	0.00035
Pressure	300-350 bar		
CO_2 saturation	0.1-0.9		
Cement		**Fracture**	
Permeability	5.0×10^{-20} m^2	Permeability	1.0×10^{-14} m^2
Porosity	0.08	Porosity	0.40
Rock density	2400 kg/m^3	Rock density	2400 kg/m^3
		Fracture proportion	0.01-0.1

Quantification of the risks with CO_2 leakage into the USDW

- Model setup: 2-D radial modal.

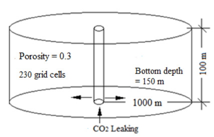

Table: Selection of the initial water chemistry

Name	Concentration (mg/L)	Name	Concentration (mg/L)
H^+	pH 7.73	Cu^{2+}	0.014
NO_3^-	15.21	Pb^{2+}	8.7×10^{-4}
$H_2AsO_4^-$	0.0024 (as As)	$HSeO_3^-$	0.003 (as Se)
Cd^{2+}	3.44×10^{-5}	Ag^+	3.61×10^{-5}
$Cr(OH)_2^+$	0.002 (as Cr)	Zn^{2+}	0.45
Mn^{2+}	0.0077	TDS	570

Table: Independent parameters for simulations of CO_2 leaking into USDW aquifer

Parameter name	Low (-1)	Mid (0)	High (+1)	Distribution
Permeability: m^2	10^{-14}	10^{-13}	10^{-12}	Lognormal
Leaking rate: $kg/(s \cdot m^2)$	10^{-21}	10^{-19}	10^{-17}	Lognormal
CEC: meq/100g	1	6.5	12	Uniform
Absorbent SSA	1	50.5	100	Uniform

Results

Cement hydration

With the consumption of alite, belite, ferrite and aluminate, CSH, portlandite and ettringite precipitate as main products.

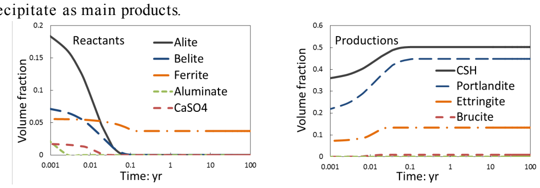

Figure: Composition changes during cement hydration

CO_2 leakage flux through wellbores

Results suggest a probability > 90% that any leakage would be between 10^{-14} – 10^{-10} $kg/(m^2 \cdot year)$. This leakage rate is far less than previous estimates. We determined that these resulting small flux values are due to: (1) reactions between CO_2 and portlandite ($Ca(OH)_2$) consume CO_2; (2) porosity decreases due to precipitation of $CaCO_3$, which further degrades the leakage pathway.

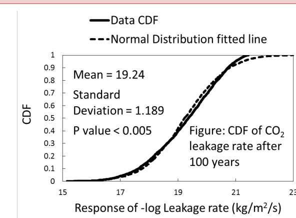

Figure: CDF of CO_2 leakage rate after 100 years

Risk assessment of CO_2 leakage into the Ogallala USDW

The coefficient of determination (R^2) between simulation results and the responses of the regression (RSM) model for most water indices of interest exceeded 0.9, suggesting that the resulting trained ROMs are effective for representing full-scale (non-ROM) simulation results.

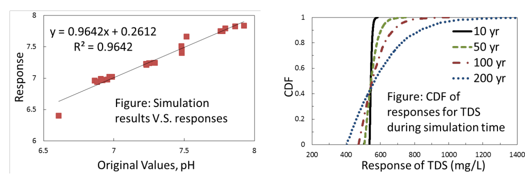

Figure: Simulation results V.S. responses

Figure: CDF of responses for TDS during simulation time

Conclusions

- Probability > 90% that the leakage rate is between 10^{-14} – 10^{-10} $kg/(m^2 \cdot year)$.
- Simulated small CO_2 leakage rate is attributed to CO_2 reaction with portlandite ($Ca(OH)_2$) in the wellbore cement; this reaction consumes CO_2 and further decreases fracture porosity, degrading the CO_2 pathway.
- Within the range of simulated CO_2 leakage rates, trace metal concentrations could be twice as much as the initial value after 200 years, for the "worst case" scenario. However, all resulting simulated trace metal concentrations, even for the worst case scenario, are less than 1/5 of the MCL limit, suggesting that the risk of such contamination to the Ogallala groundwater quality is not significant.
- Water quality at 100, 500 and 1000 m away from the leakage pathway reflects the slight impact after 200 years, suggesting that the monitoring wells in place today will be capable of detecting significant leakage.
- TDS and nitrate are suggested markers for early detection.

Simulated water quality results

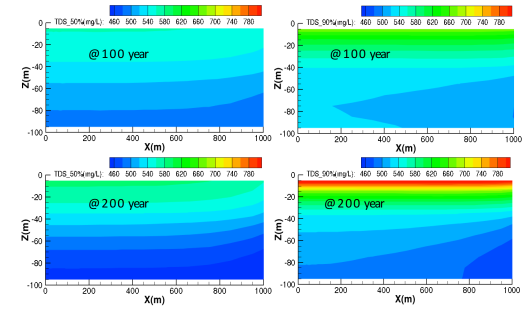

Figure: TDS distribution with 50^{th} and 90^{th} percentile

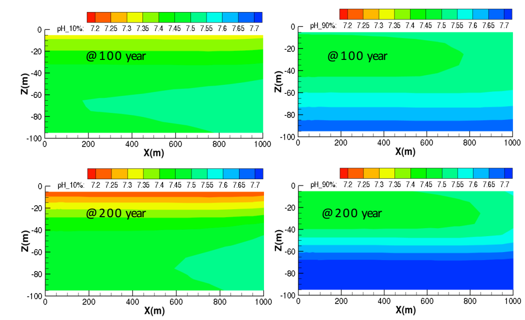

Figure: pH distribution with 10^{th} and 90^{th} percentile

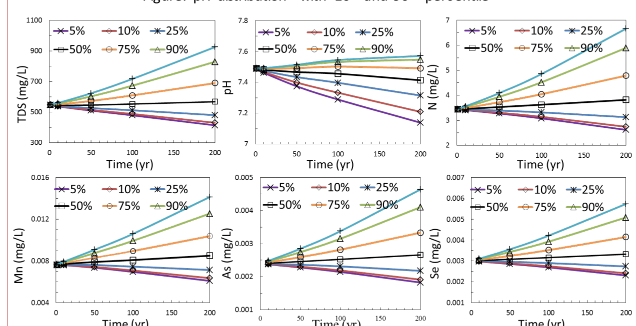

Figure: Selection of simulated water quality changes over time at current FWU monitoring wells

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