

Applying Geochemical Signals and Statistical Tools to Ensure CO₂ Storage Through Water Monitoring



Wei Xiong

Research Scientist

Research & Innovation Center



2022 Carbon Management Review Meeting

Aug. 17, 2022

Disclaimer



This project was funded by the United States Department of Energy, National Energy Technology Laboratory, in part, through a site support contract. Neither the United States Government nor any agency thereof, nor any of their employees, nor the support contractor, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Authors



Wei Xiong^{1,2}, Jiaan Wang³, Mitchell Small³, Brian Stewart⁴, Rosemary Capo⁴, Brandon McAdams^{1,2}, J. Alexandra Hakala¹, R. Burt Thomas⁵,
James Gardiner^{1,2}

¹ National Energy Technology Laboratory, Pittsburgh, PA 15236

² NETL Support Contractor, Pittsburgh, PA 15236

³ Carnegie Mellon University, Pittsburgh, PA 15213

⁴ University of Pittsburgh, Pittsburgh, PA 15260

⁵ National Energy Technology Laboratory, Albany, OR 97321

Carbon Sequestration



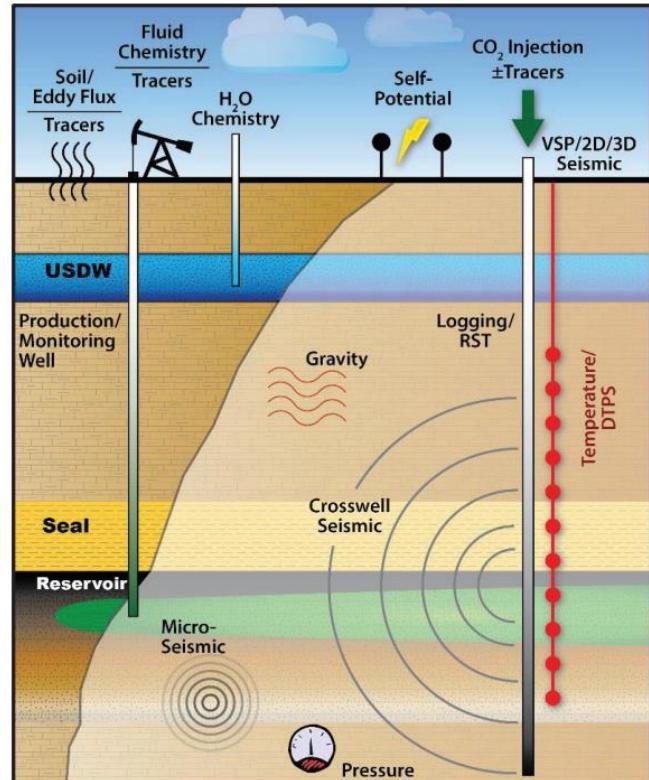
Importance of Monitoring

- Ensures CO₂ storage
- Protects valuable assets
- Provides assurance to the community

Geochemical Monitoring

- Utilizes existing infrastructure
- Employs developed tools
- Provides source attribution

Figure from Balch et al., 2017



Field Studies

Samples

- Ogallala Fm. groundwater
- Santa Rosa Fm. groundwater
- San Andres Fm. produced water

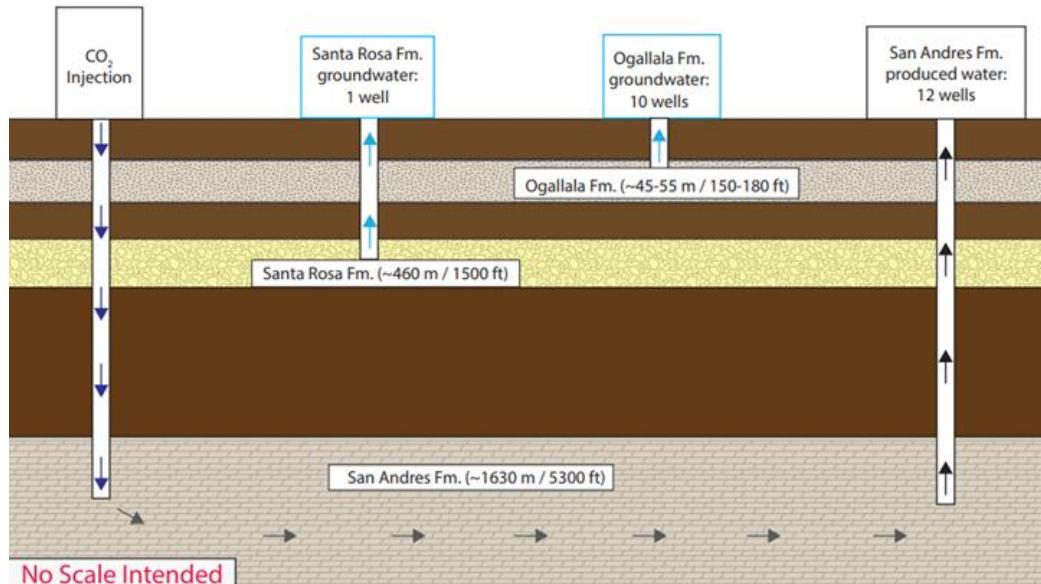


Figure from Miller et al., 2022

Application of Field Results: GILD

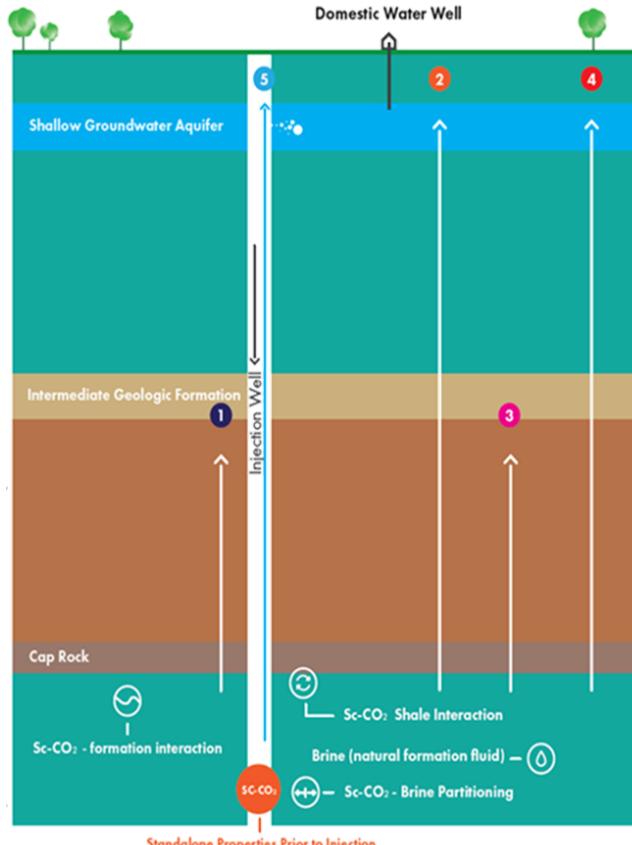


• Problem Definition

- Need for a low-cost, easily implementable monitoring strategy for carbon storage reservoir leak detection

• Proposed Solution

- Geochemically Informed Leak Detection (GILD)



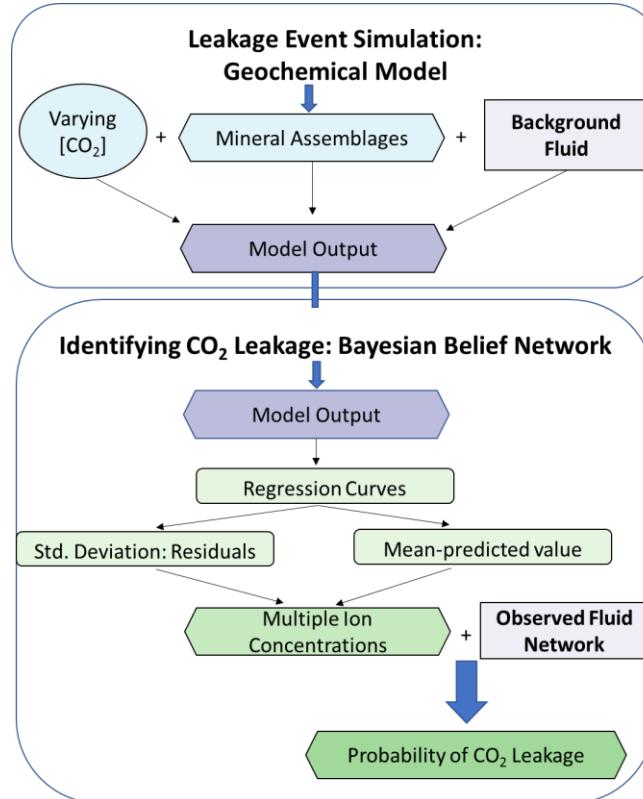
Leakage Pathways

- 1 Wellbore to intermediate formation
- 2 Wellbore to shallow groundwater
- 3 Geologic conduit to intermediate formation
- 4 Geologic conduit to shallow groundwater
- 5 Well to shallow aquifer

GILD Overview

GILD

- 1) Assess fluid chemistry and mineral compositions of monitoring formation
- 2) Simulate leakage events with a geochemical model
- 3) Identify CO₂ leakage with a Bayesian Belief Network (BBN)



Bayesian Belief Network (BBN)

- Decision support tool
- Probabilistic inference from multiple sources of evidence
- Application for leak detection - given monitoring parameters, compute the probabilities of the presence of leakage

Geochemical Modeling



Sandstone minerals: quartz 80 g, kaolinite 10 g, multiple minor minerals

	Carbonate	Feldspar		Mica		Chlorite
No.	Calcite(g)	Albite(g)	Anorthite(g)	Annite(g)	Phlogopite(g)	Ripidolit-14A(g)
1	0	0	1	0	1	0
2	0	0	1	0	1	1
3	0	0	1	1	0	0
4	0	0	1	1	0	1
5	0	1	0	0	1	0
6	0	1	0	0	1	1
7	0	1	0	1	0	0
8	0	1	0	1	0	1
9	1	0	1	0	1	0
10	1	0	1	0	1	1
11	1	0	1	1	0	0
12	1	0	1	1	0	1
13	1	1	0	0	1	0
14	1	1	0	0	1	1
15	1	1	0	1	0	0
16	1	1	0	1	0	1
17	1	1	1	1	1	1
18	0	1	1	1	1	1

Mineral Variance

15% porosity 100 g rock, 2.5 g/cm³ density
6 g of water in pores

25 C

Fixed CO₂(aq) from 0.00003–0.30003 mol/kg

Reaction time 2 hrs

Reactive surface 1000 cm²/g

Rate	mol/cm ² /s
Quartz	1.02E-18
Kaolinite	6.61E-18
Calcite	1.55E-10
Albite	9.12E-17
Anorthite	7.08E-16
Annite	8.51E-18
Phlogopite	3.98E-17
Ripidolit-14A	3.02E-17

Rate constants from Palandri and Kharaka, 2014

Geochemical Modeling



Fluid Variance

Santa Rosa ground water samples

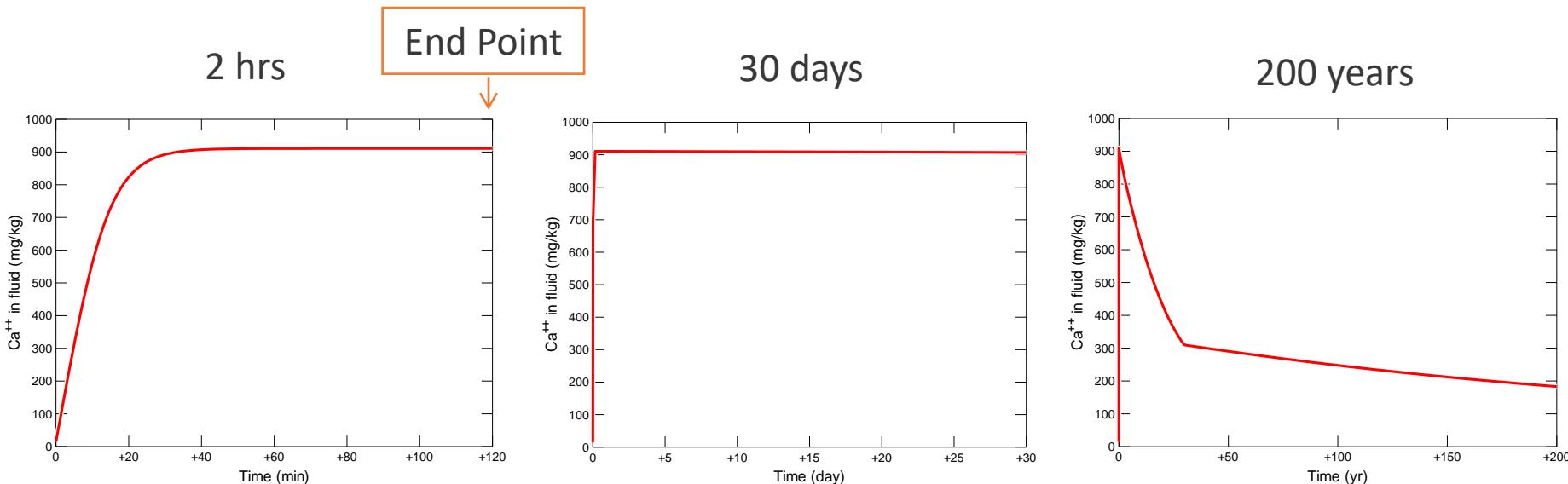
ID	Date	pH	Na	Ca	Mg	K	Cl	SO ₄	Br	HCO ₃	TDS	Charge balance
			----- mg/L -----									
<i>Santa Rosa Fm. groundwater - depth of 460 m</i>												
B1	Jun-13	8.0	1410	26.5	12.6	4.88	440	2200	372	4460	-0.38%	
B1	Jan-14	9.1	1090	9.73	9.07	6.12	242	2120	385	3860	-9.02%	
B1 [#]	May-14	8.2	1490	20.7	8.51	7.87	456	2030	459	4480	3.17%	
B1	Sep-15	8.8	1420	1.21	7.71	4.66	449	2060	2.17	3950	6.17%	
B1	May-16	9.5	1450	3.75	1.32	4.60	488	2010	2.24	389	4350	-0.04%
B1	Nov-16	8.4	1470	21.1	11.3	4.84	458	2180	2.16	205	4350	3.54%
B1	Jul-17	7.7	1490	20.9	11.1	4.73	454	2160	2.11	449	4590	1.55%
Average		8.5	1400	14.8	8.81	5.39	427	2110	2.17	377	4290	0.71%

32 scenarios

17	all minerals	1	1	1	1	1	1
18	all except calcite	0	1	1	1	1	1

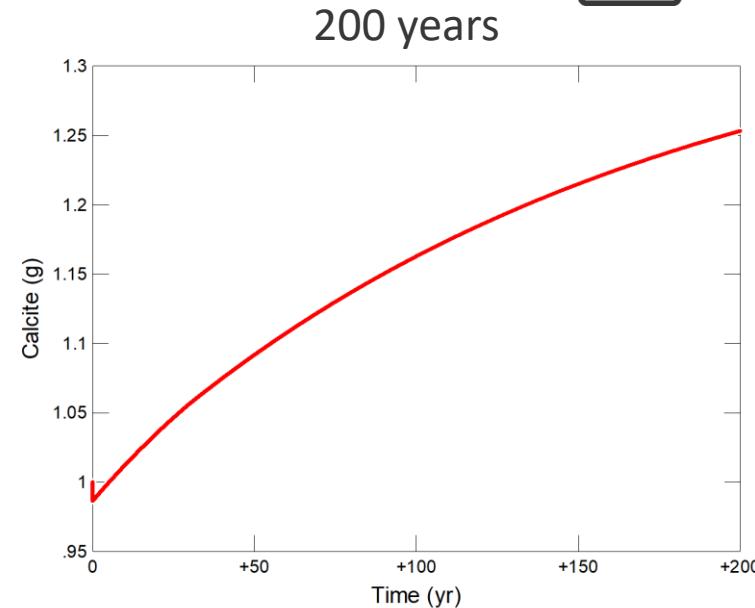
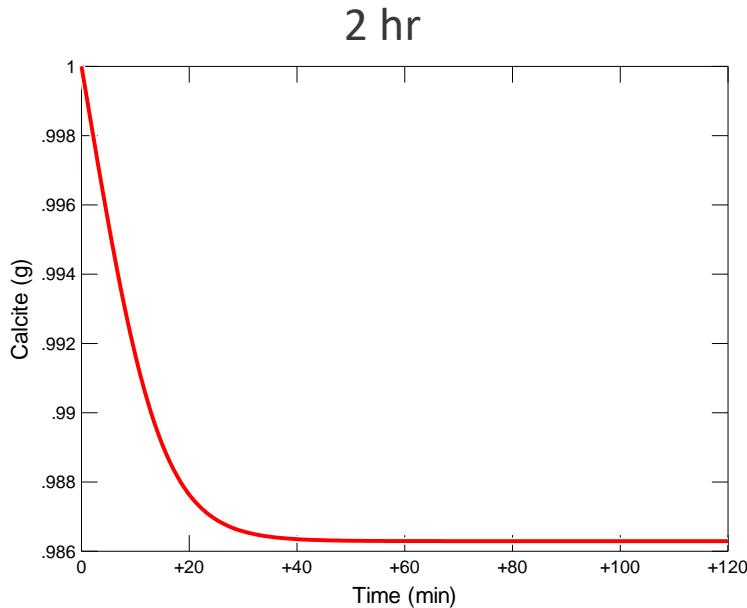
Ca²⁺ Change over Time

CO₂ = 0.30003 mol/kg, Scenario 17, all minor minerals, average fluid



Rapid and significant Ca+ concentration increases only hours after the reaction. The concentration remains at a high level for days, weeks, even months, making it possible to detect this huge increase in a short monitoring period.

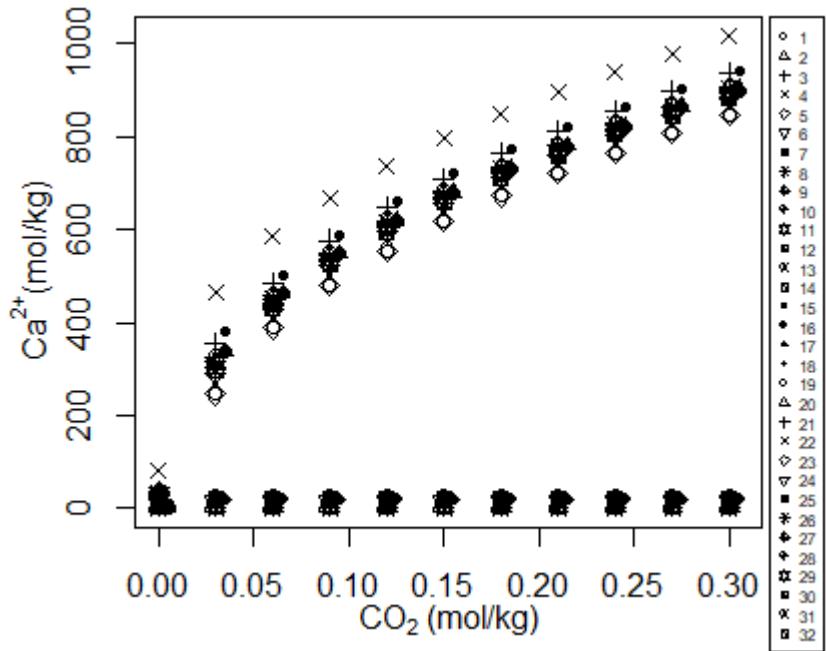
Minimal Calcite is Needed



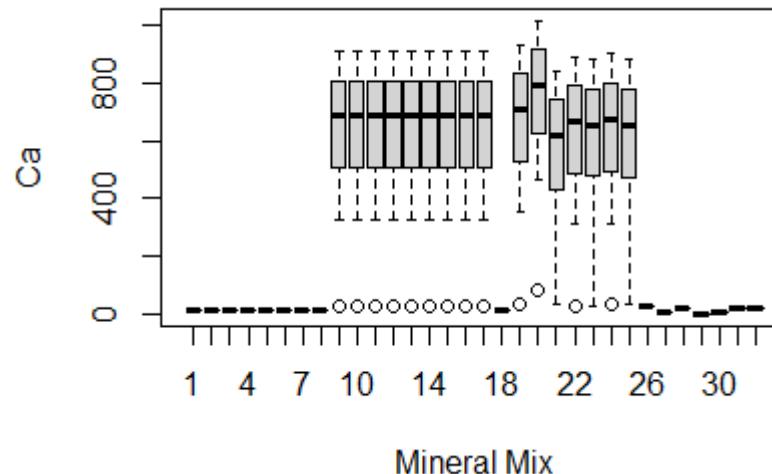
Minimal calcite (<2%) dissolution results in high Ca^{2+} concentration increase.

Calcite reprecipitation due to excessive CO_2 dissolution over time.

Geochemical Model Output Example

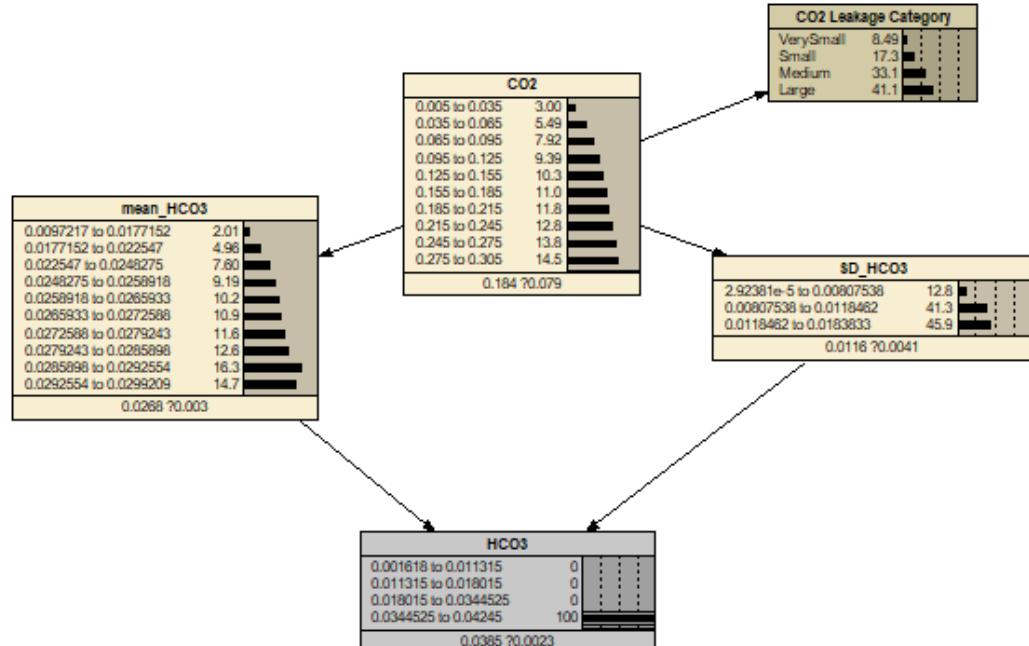


- Sc 1-8 no calcite
- Sc 9-16 with calcite
- Sc 17 all minerals with calcite
- Sc 18 all minerals except calcite
- Sc 19-25: Sc17 with fluid variance
- Sc 26-32: Sc18 with fluid variance



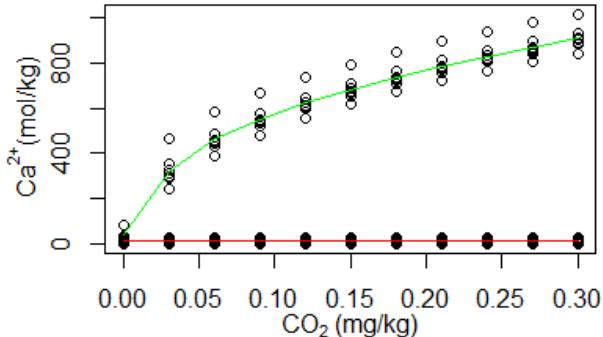
BBN for Leak Detection

- **Upstream node**
 - CO₂ added concentration
- **Arrows**
 - Causal effect
- **Downstream nodes**
 - Monitoring parameters
- **Bars of each node**
 - Probability of a particular range
- **Conditional probability**
 - Probability of downstream given upstream
- **Purpose**
 - Back inference

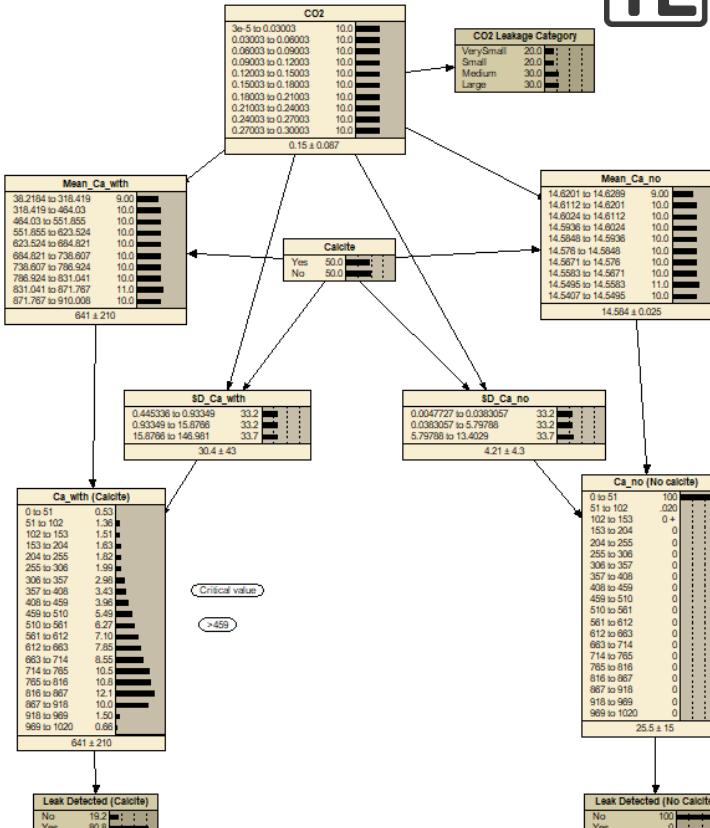
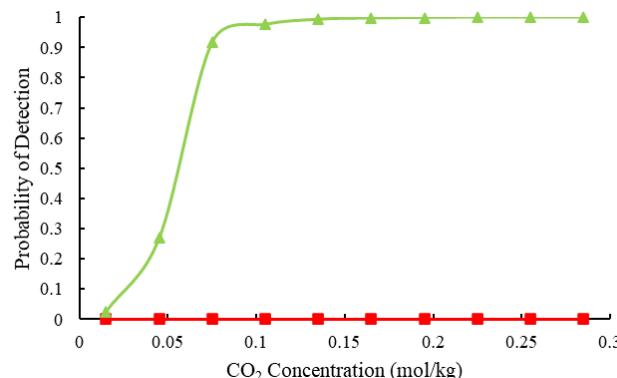


Single-Index BBN Example

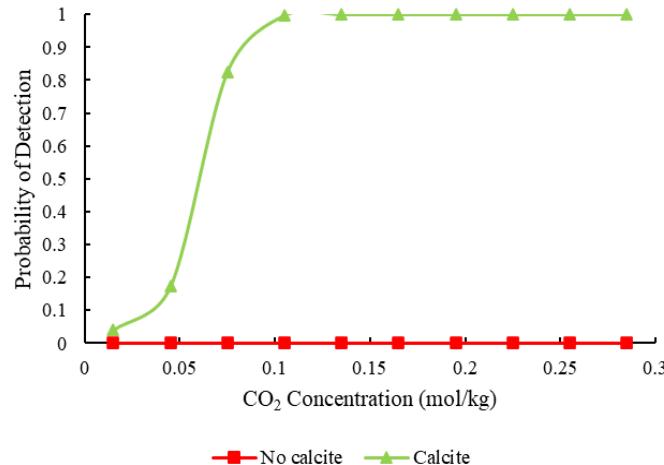
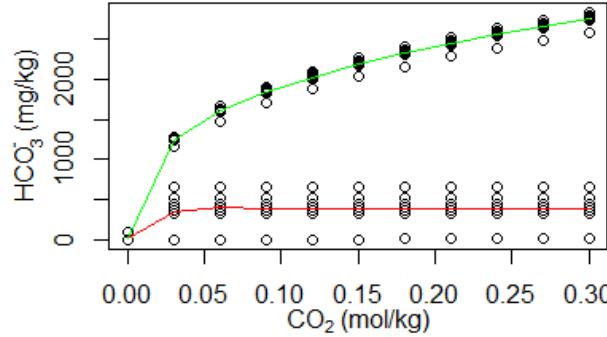
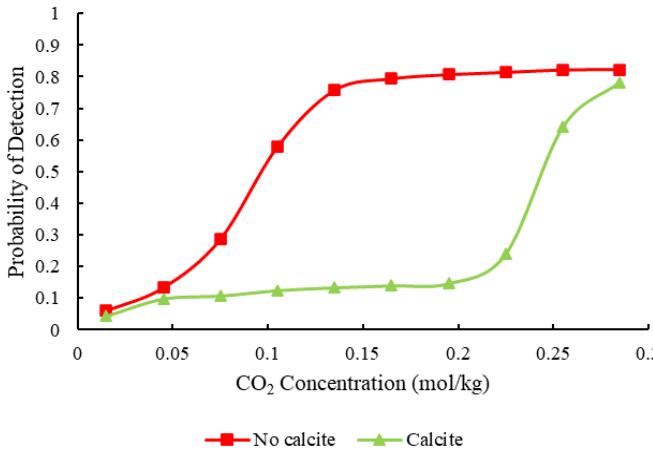
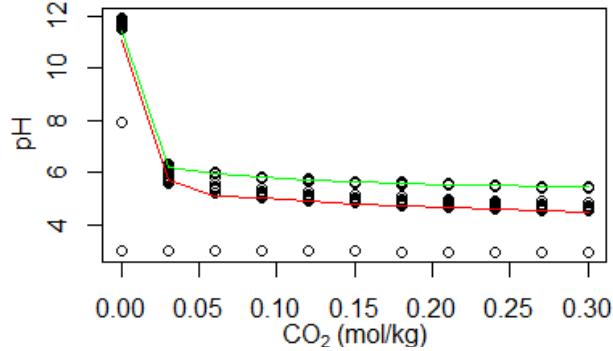
Single-index (Ca^{2+}) example



Response curve



Other Indices for Single-Index BBN



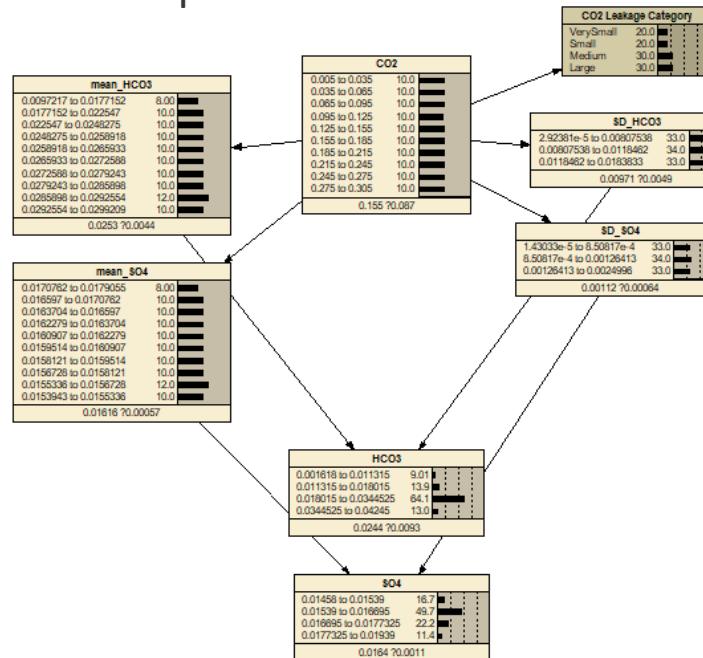
Ca²⁺, pH, and HCO₃⁻ are selected as indices for BBN

Multi-Index BBN

In progress:

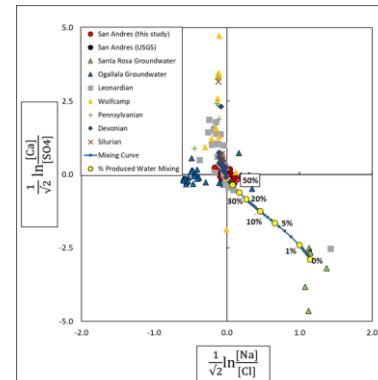
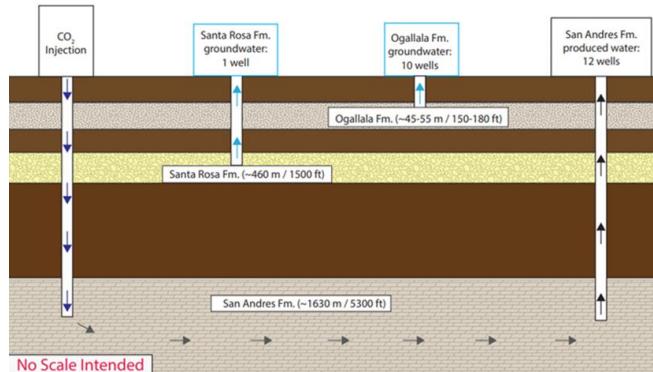
- Combining Ca^{2+} , pH, and HCO_3^- for multi-index BBN model and CO_2 (leakage) detection.
- Manuscript in preparation for *Environmental Science & Technology*.

Example:



Conclusions

- **Geochemical monitoring provides insight into groundwaters and target formation reactions**
 - No significant dissolution of the storage reservoir
 - No produced water migration detected in groundwaters
- **Geochemical-statistical models (GILD) can provide CO₂ leakage detection via robust statistical analysis**
 - The current model applies user input via licensed software and researcher knowledge
 - The goal is to create a standalone version that can be used by groundwater observers



NETL RESOURCES

VISIT US AT: www.NETL.DOE.gov



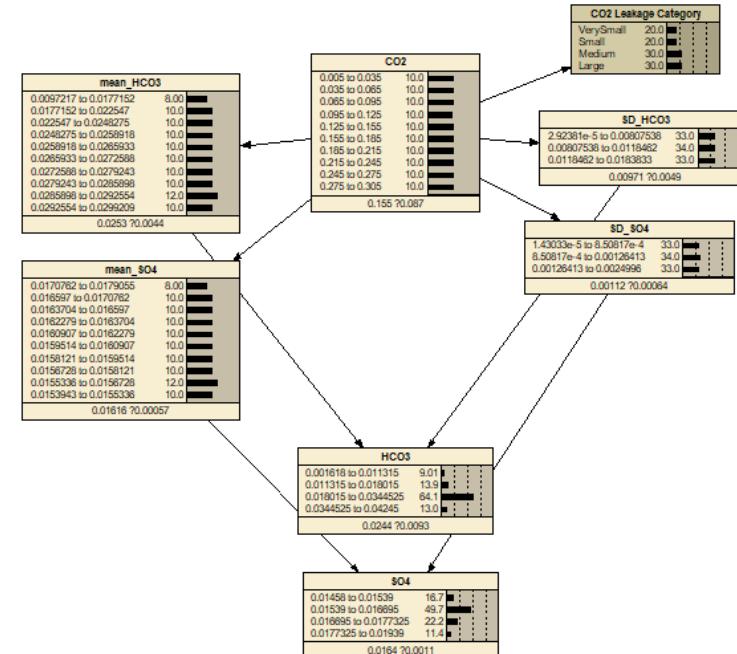
Contact: Wei Xiong, wei.xiong@netl.doe.gov



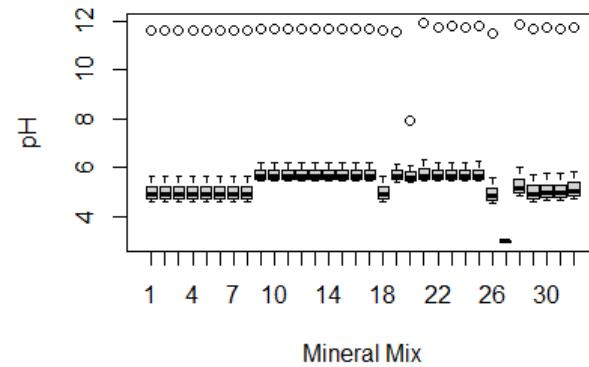
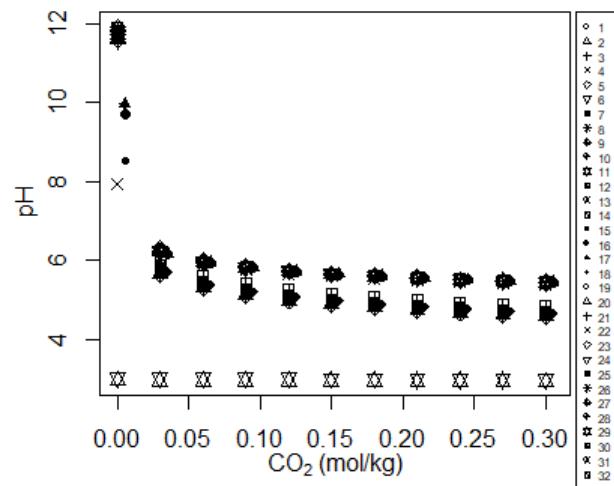
Supplemental Slides

Construction of BBN-Regression Results

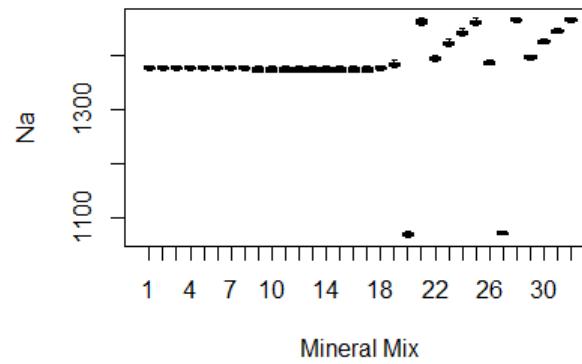
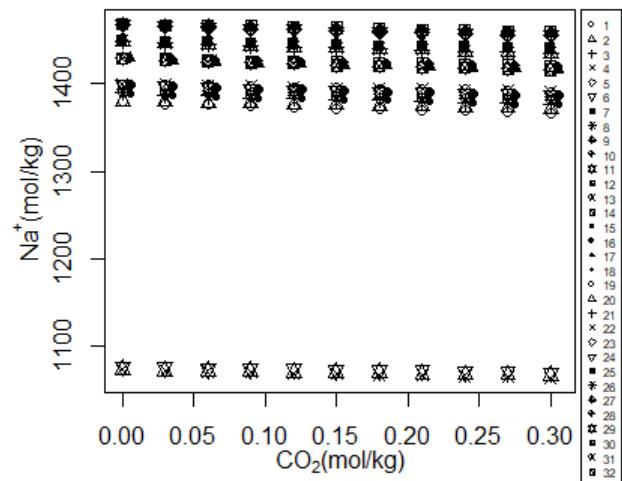
- Mean-predicted value from the response function for each CO_2 level
- SD-standard deviation of residuals (geochemical model output-predicted values)
- Ion concentration-normally distributed with mean and SD



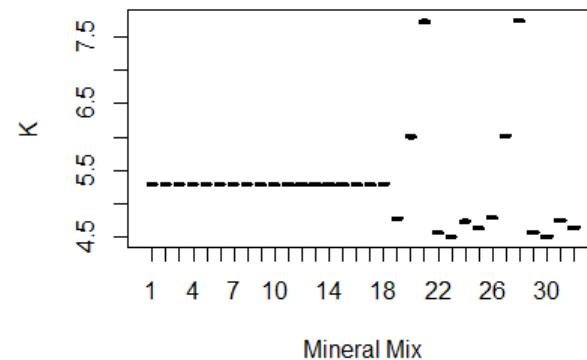
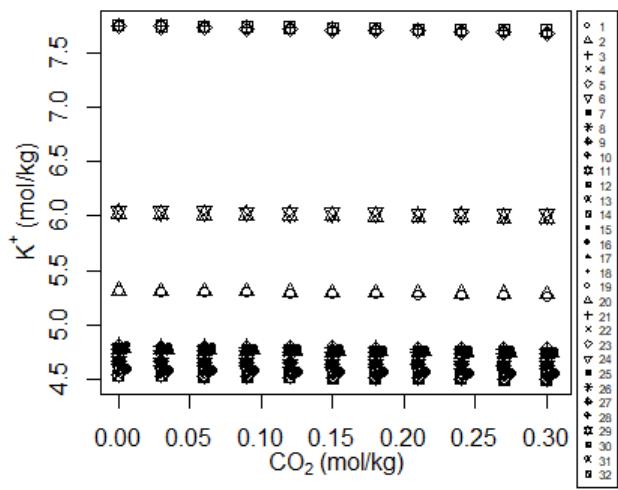
OH



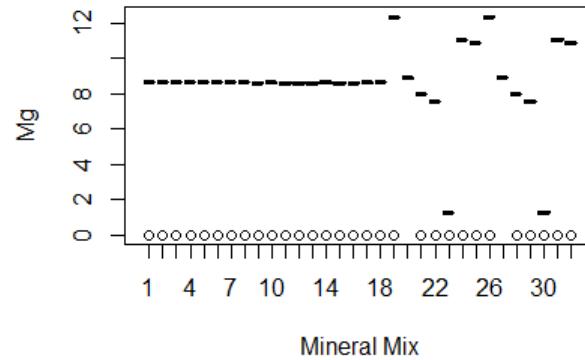
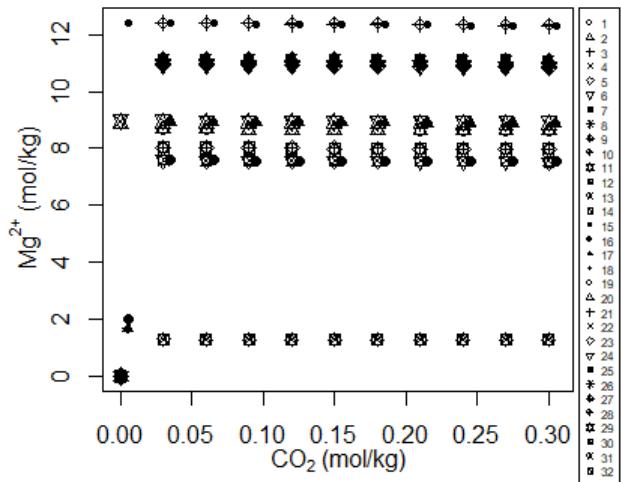
Na



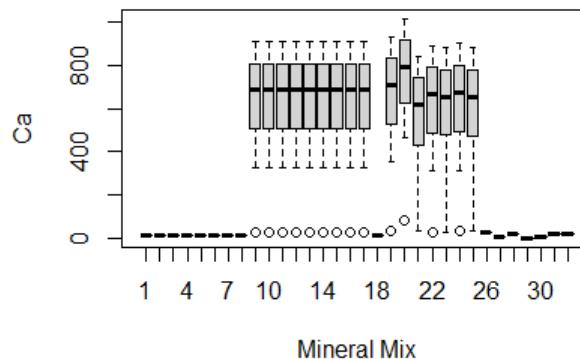
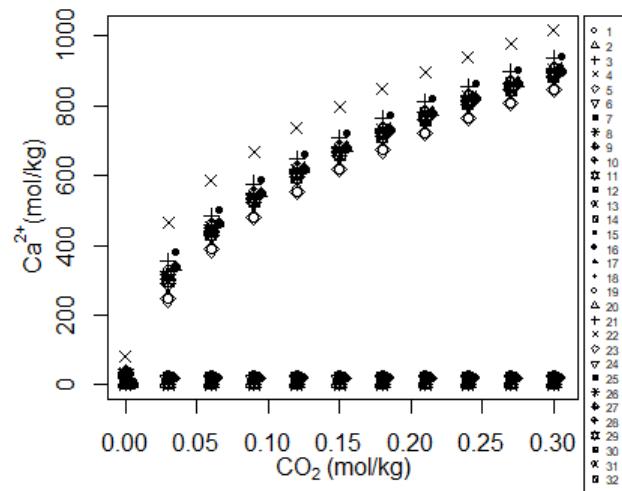
K



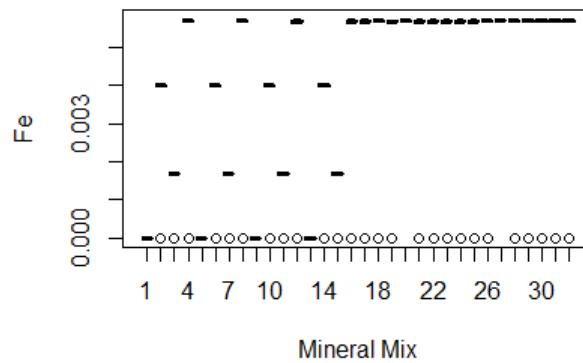
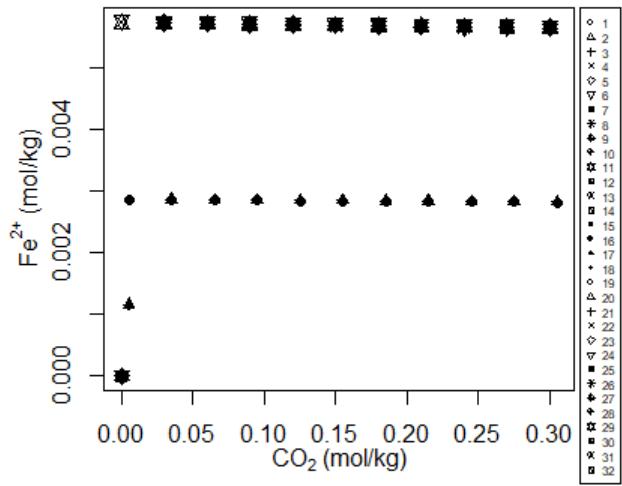
Mg



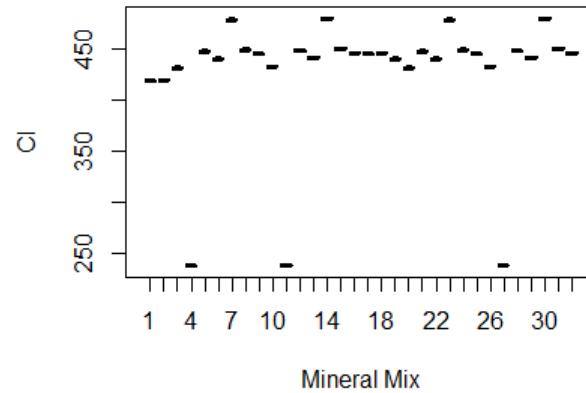
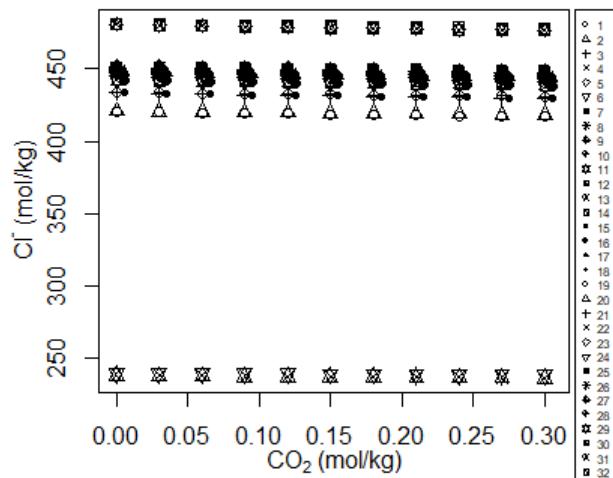
Ca



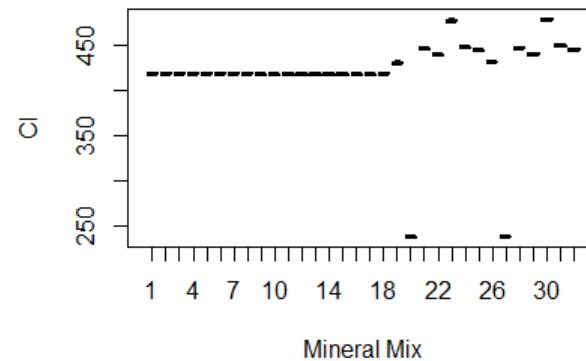
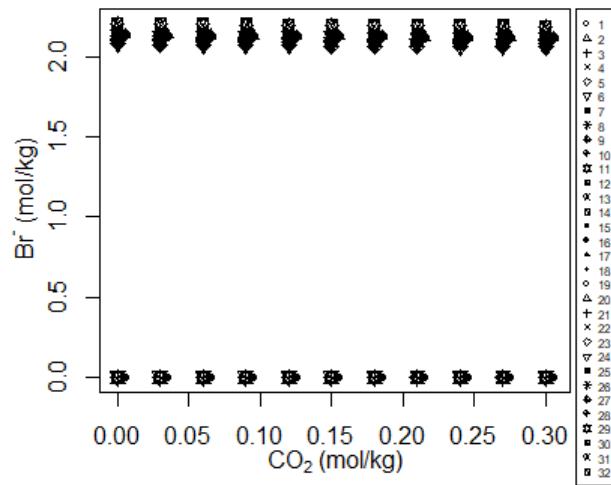
Fe



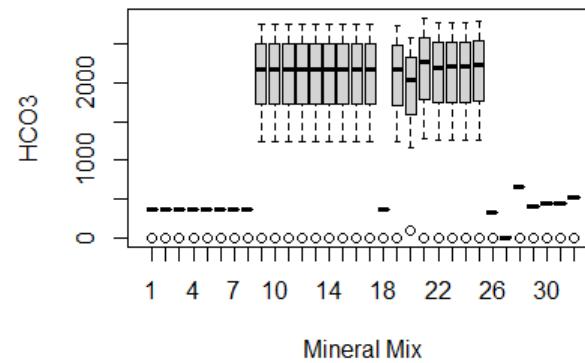
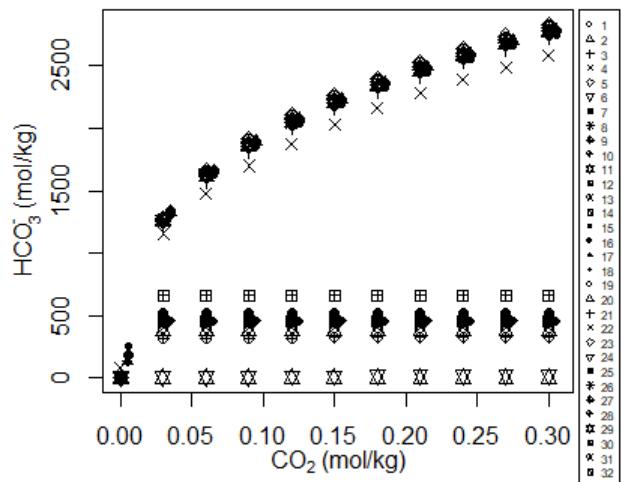
C
|



Br



HCO₃



SO₄

