Applying Geochemical Signals and Statistical Tools to Ensure CO_2 Storage Through Water Monitoring

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Carbon Sequestration

Importance of Monitoring

- Ensures CO_2 storage
- Protects valuable assets
- Provides assurance to community

Geochemical Monitoring

- Sampling reservoir fluid through existing infrastructure
- Employing developed tools to observe relevant reactions
- Provides source attribution, distinguish between different types of geologic fluids, like deep and shallow formation fluid.

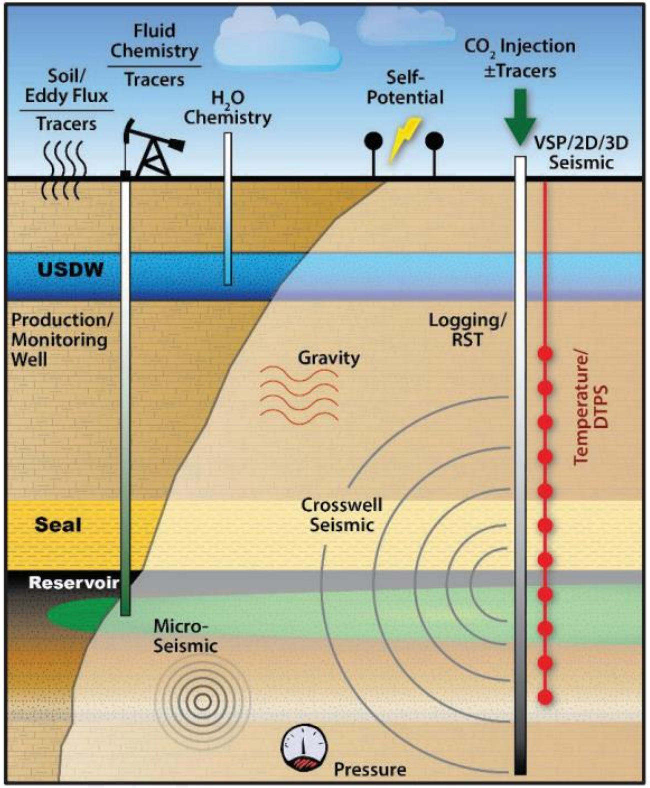


Figure from Balch et al., 2017

Field Studies

Samples

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

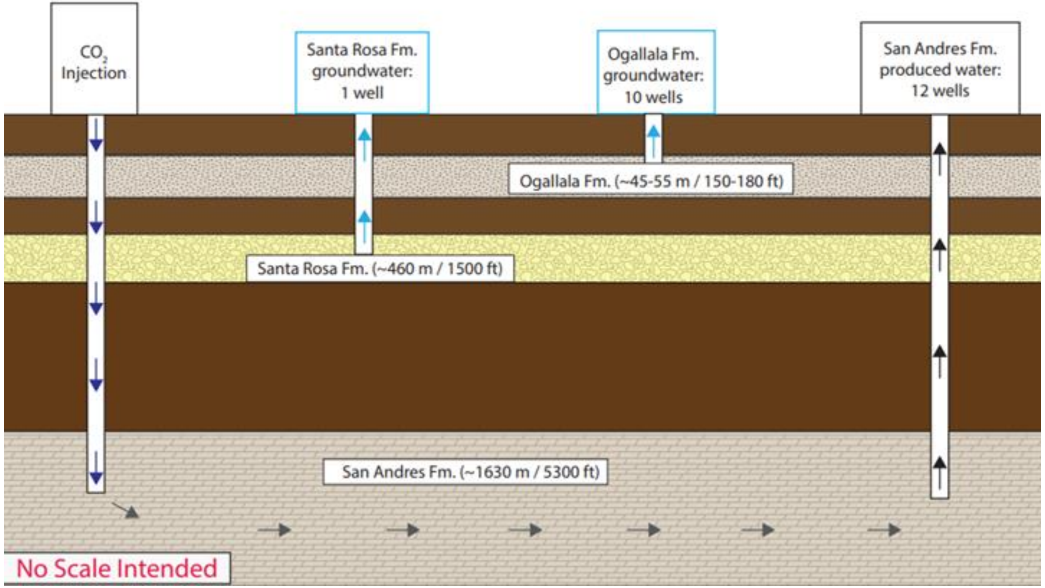
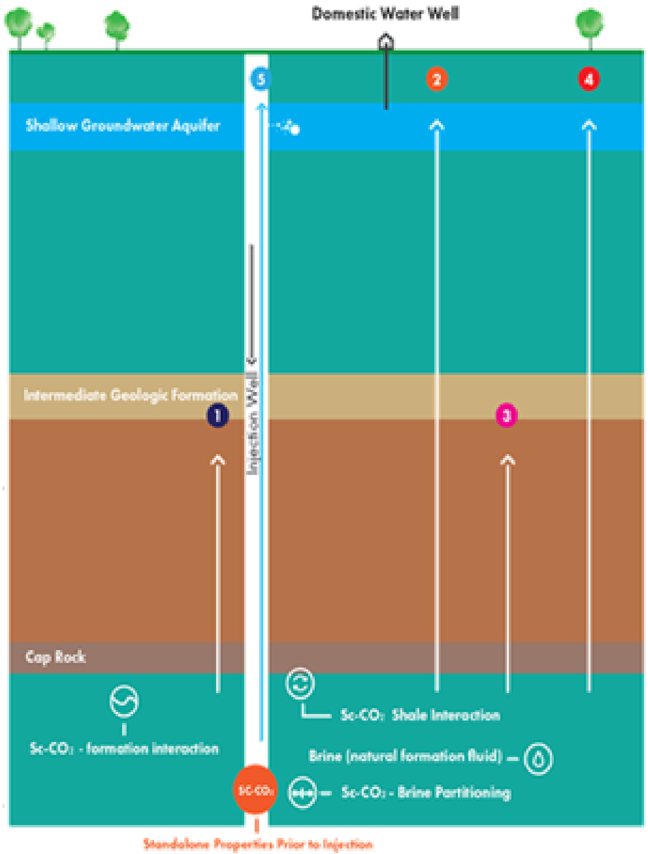


Figure from Miller et al., 2022

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)



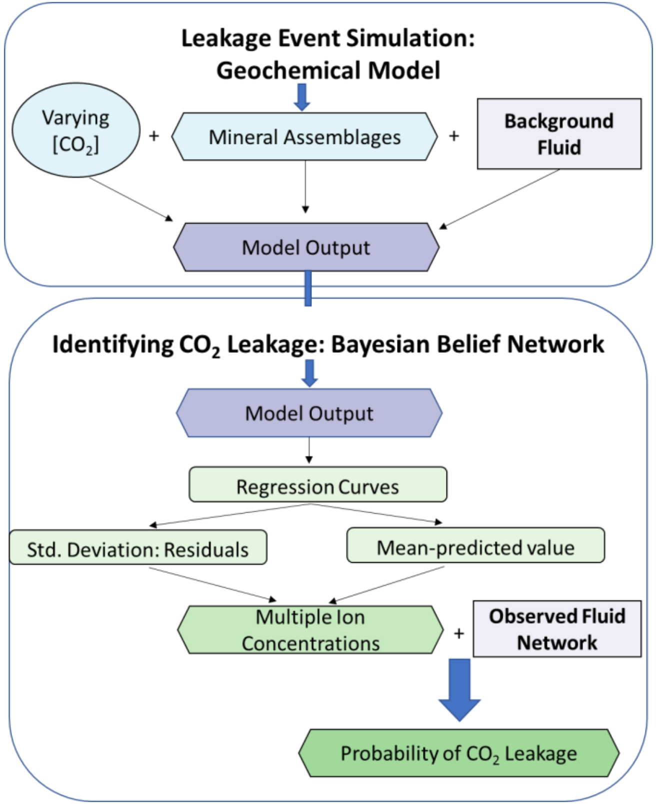
Leakage Pathways

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

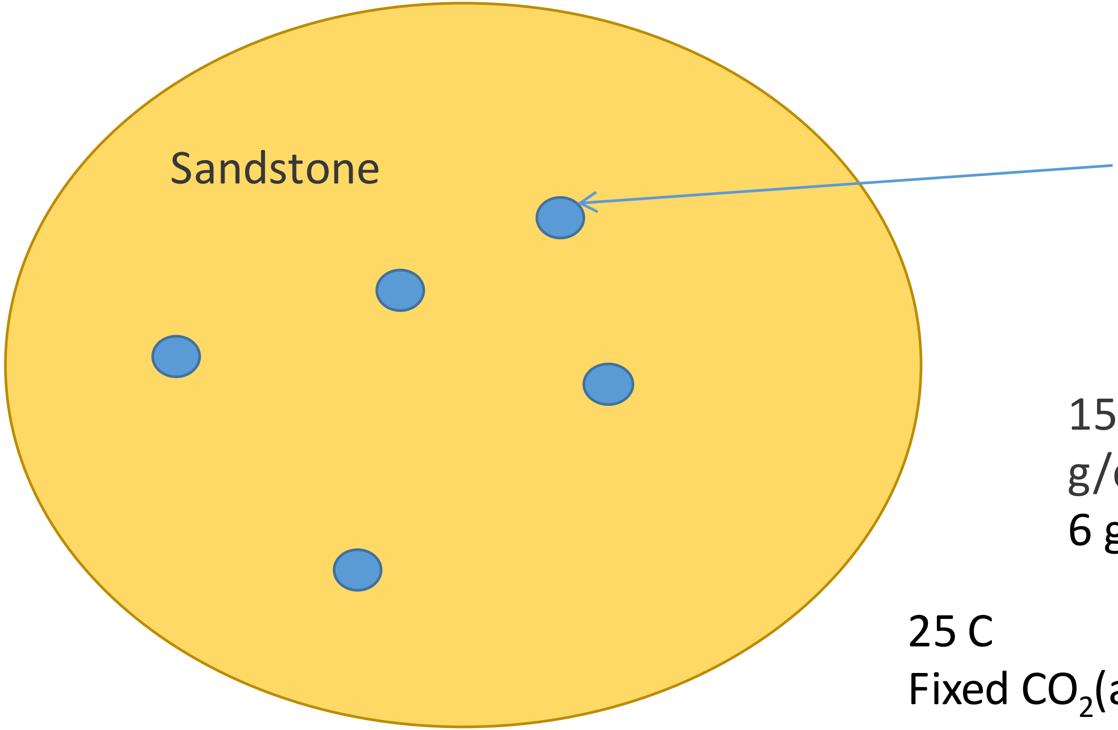
1) Assess fluid chemistry and mineral compositions of monitoring formation
2) Simulate leakage events with a geochemical model
3) Identify CO_2 leakage with a Bayesian Belief Network (BBN)



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



Pore space filled with reservoir fluid

Fixed CO2(aq) present in the fluid

15% porosity 100 g rock, 2.5 g/cm^3 density
6 g of water in pores

25 C
Fixed CO_2(aq) from 0.006–0.306 mol/kg

Geochemical Modeling

Mineral variance

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)	ipidolit-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

Reaction time 2 hrs

Reactive surface 1000 cm^2/g

Rate	mol/cm2/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

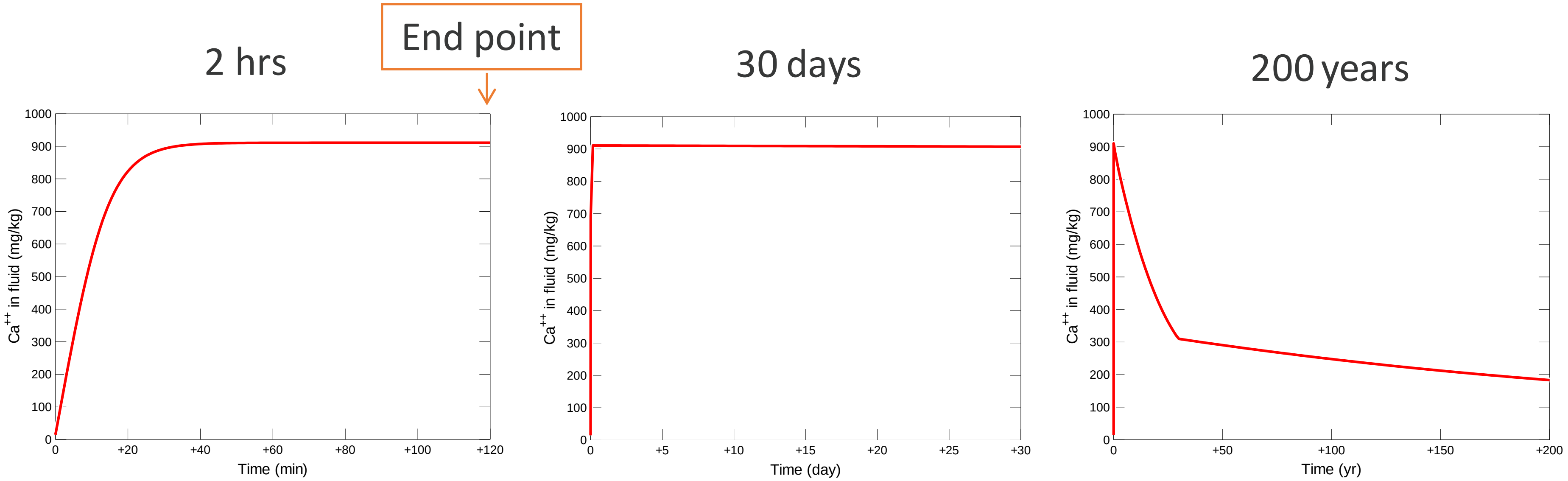
ID	Date	pH	Na	Ca	Mg	K	Cl	SO_4	Br	HCO_3	TDS	Charge balance
			- - - - - - - -					mg/L			- - - - - - - -	
Santa Rosa Fm. groundwater - depth of 460 m												
B1	Jun-13	8.0	1410	26.5	12.6	4.88	440	2200		372	4460	-0.38%
B1	Jan-14	9.1	1090	9.73	9.07	6.12	242	2120		385	3860	-9.02%
B1#	May-14	8.2	1490	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

Ca^{2+} Change over Time

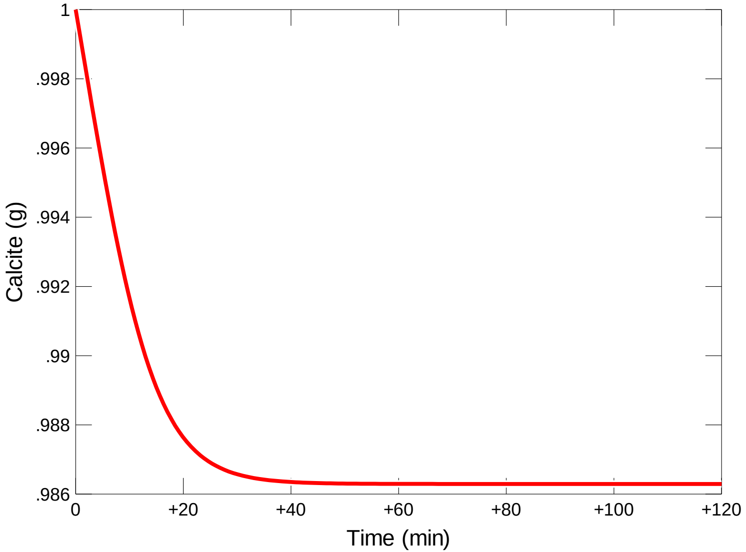
CO_2 = 0.3 mol/kg, Scenario 17, all minor minerals, average fluid



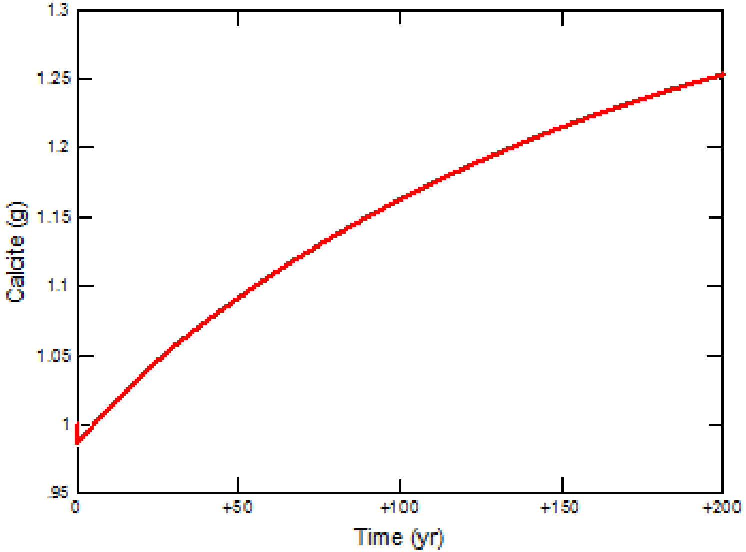
Rapid and significant Ca+ concentration increases only hours after the reaction. The concentration remains at a high level for days, weeks, even months, making it possible to detect this huge increase in a short monitoring period.

Minimal Calcite is Needed

2 hr



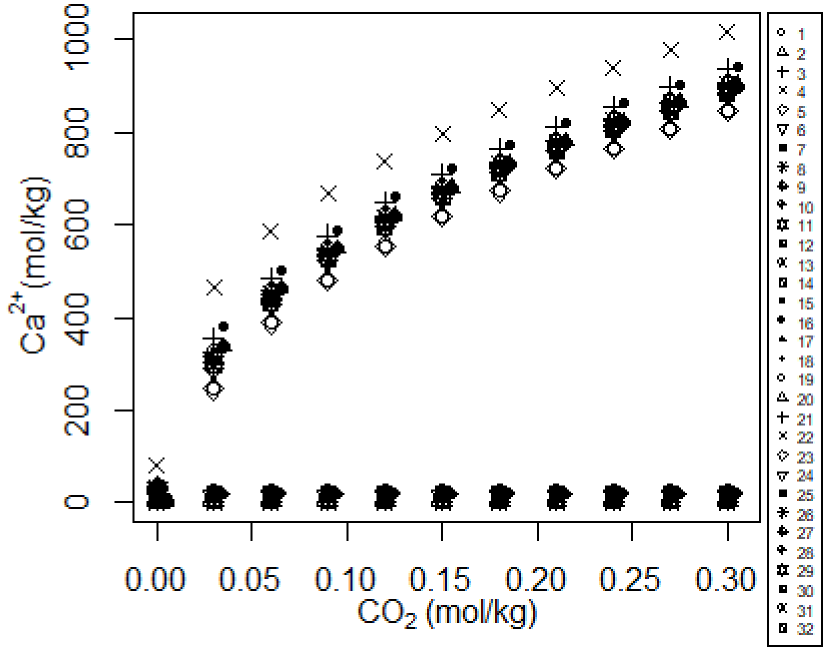
200 years



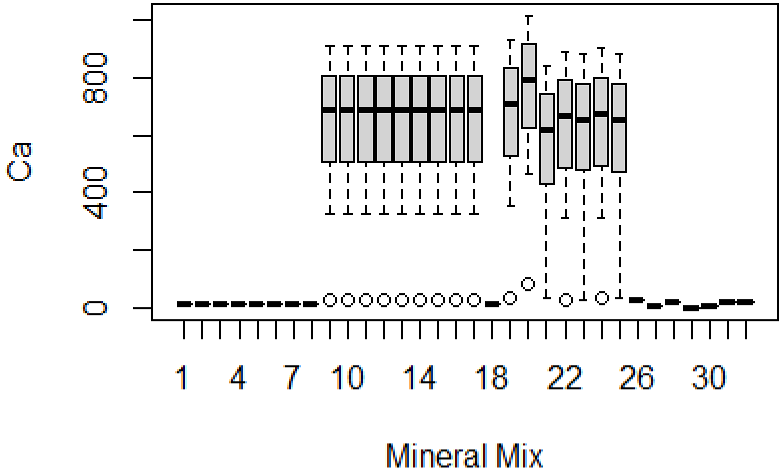
Minimal calcite (<2%) dissolution results in high Ca^{2+} concentration increase.

Calcite reprecipitation due to excessive CO_2 dissolution over time.

Geochemical Model Output Example

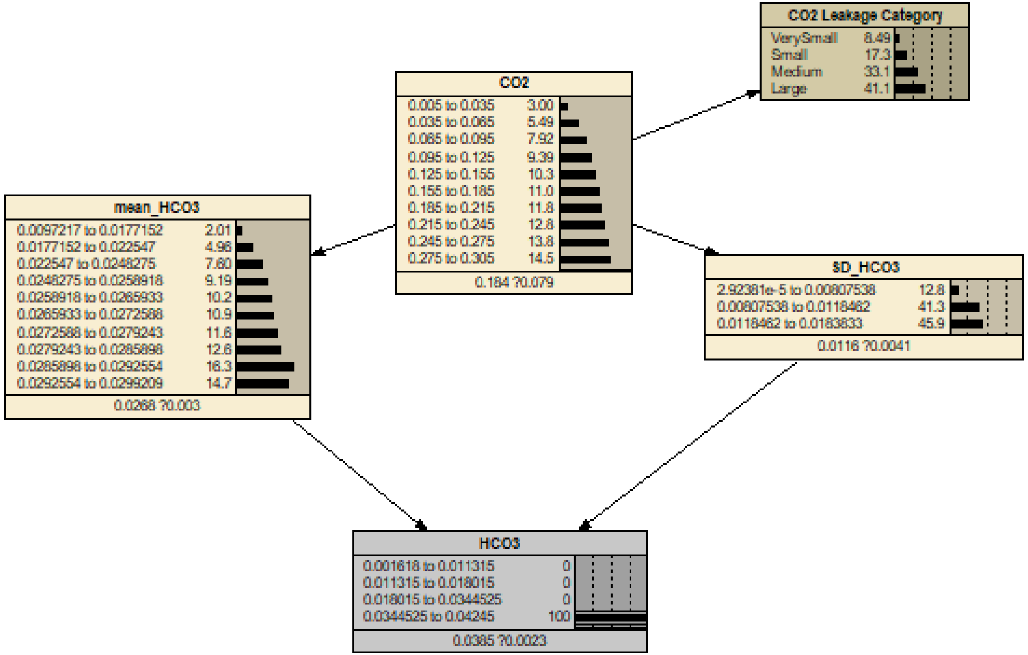


Sc 1-8 no calcite
Sc 9-16 with calcite
Sc 17 all minerals with calcite
Sc 18 all minerals except calcite
Sc 19-25: Sc17 with fluid variance
Sc 26-32: Sc18 with fluid variance



BBN for Leak Detection

- **Upstream node**
  - CO_2 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

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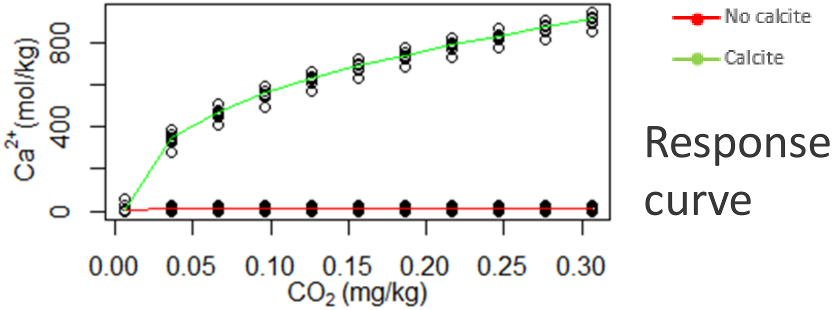
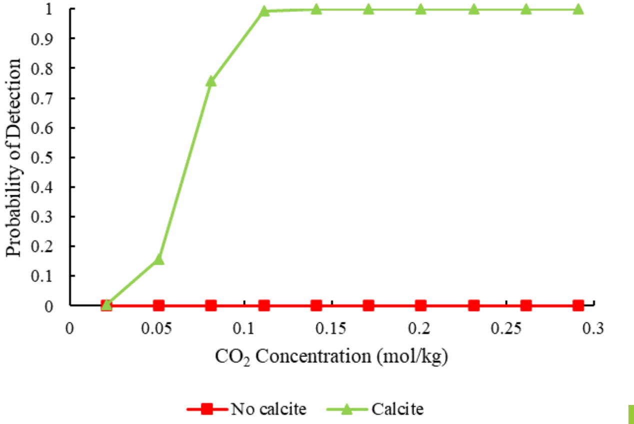
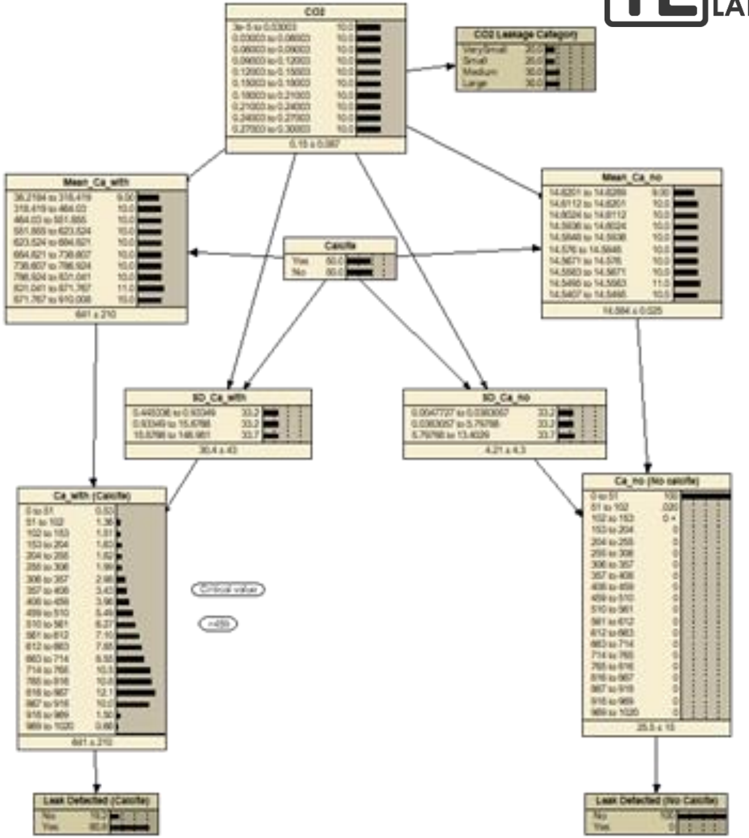
Single index (Ca^{2+}) example

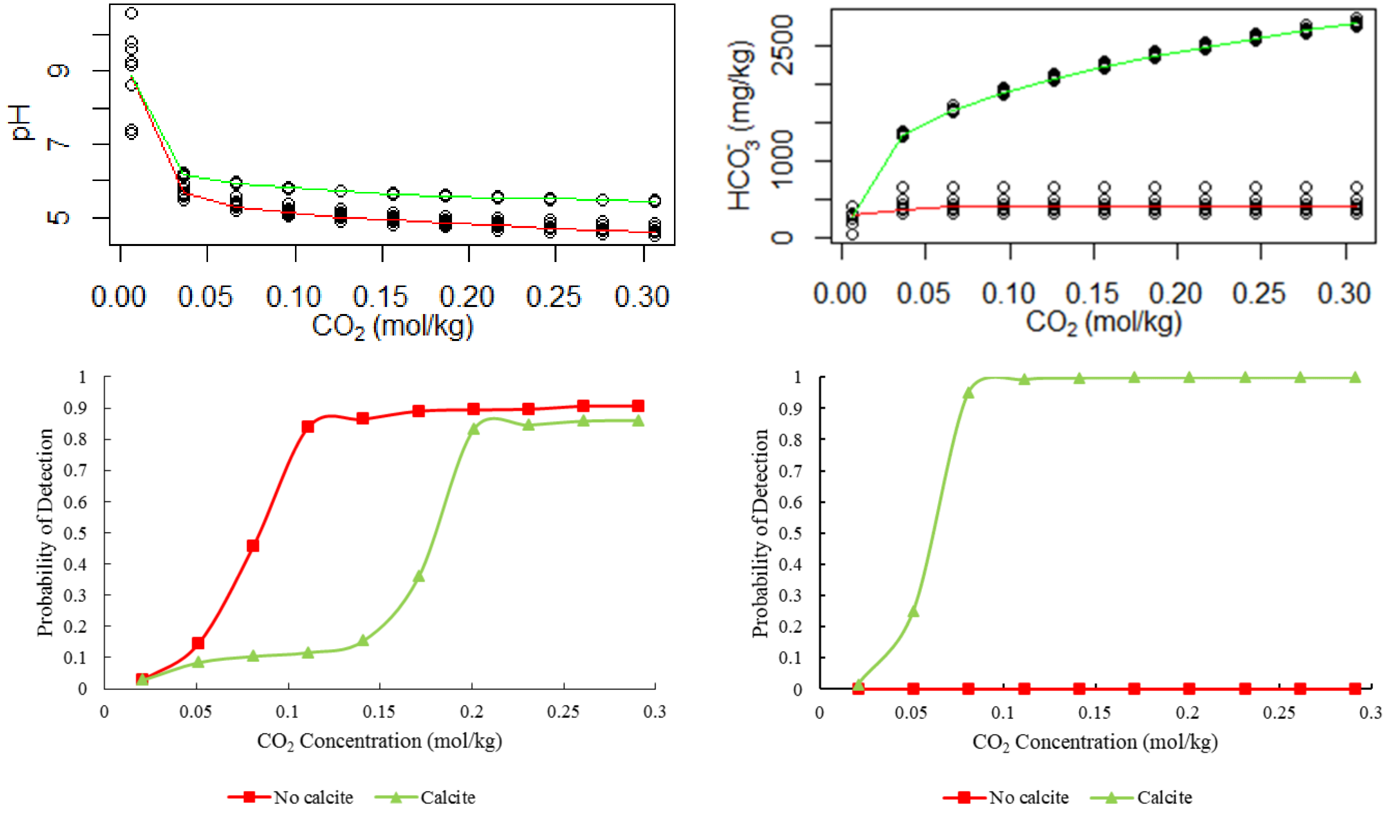


Response curve





Other Indices for Single Index BBN



Ca^{2+}, pH, and HCO3- are chose as indices for BBN.

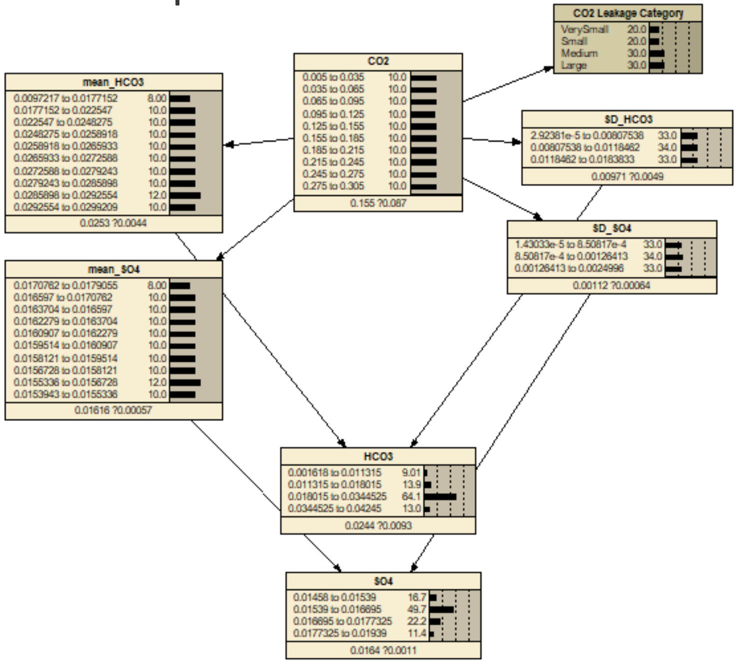
Multi-Index BBN

In progress:

- Combining Ca^{2+}, pH and HCO_3^- for multi-index BBN model and CO_2(leakage) detection.

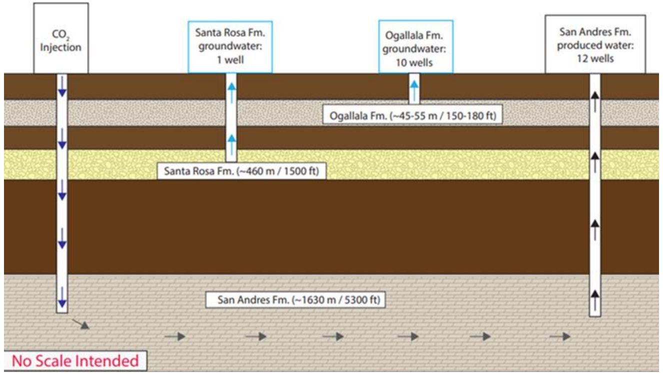
- Manuscript in preparation for Environmental Science & Technology.

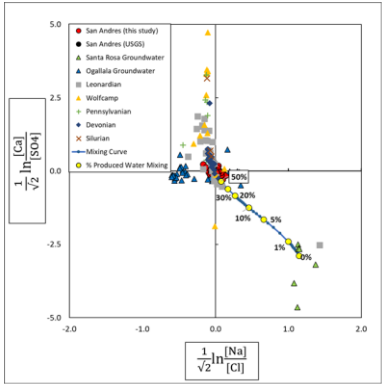
Example:



Conclusions

- **Geochemical monitoring provides insight into groundwaters and target formation reactions**
- **Geochemical-statistical models (GILD) can provide CO_2 leakage detection via robust statistical analysis**
  - The current model applies user input via licensed software and researcher knowledge
  - Goal is to create a standalone version that can be used by groundwater observers





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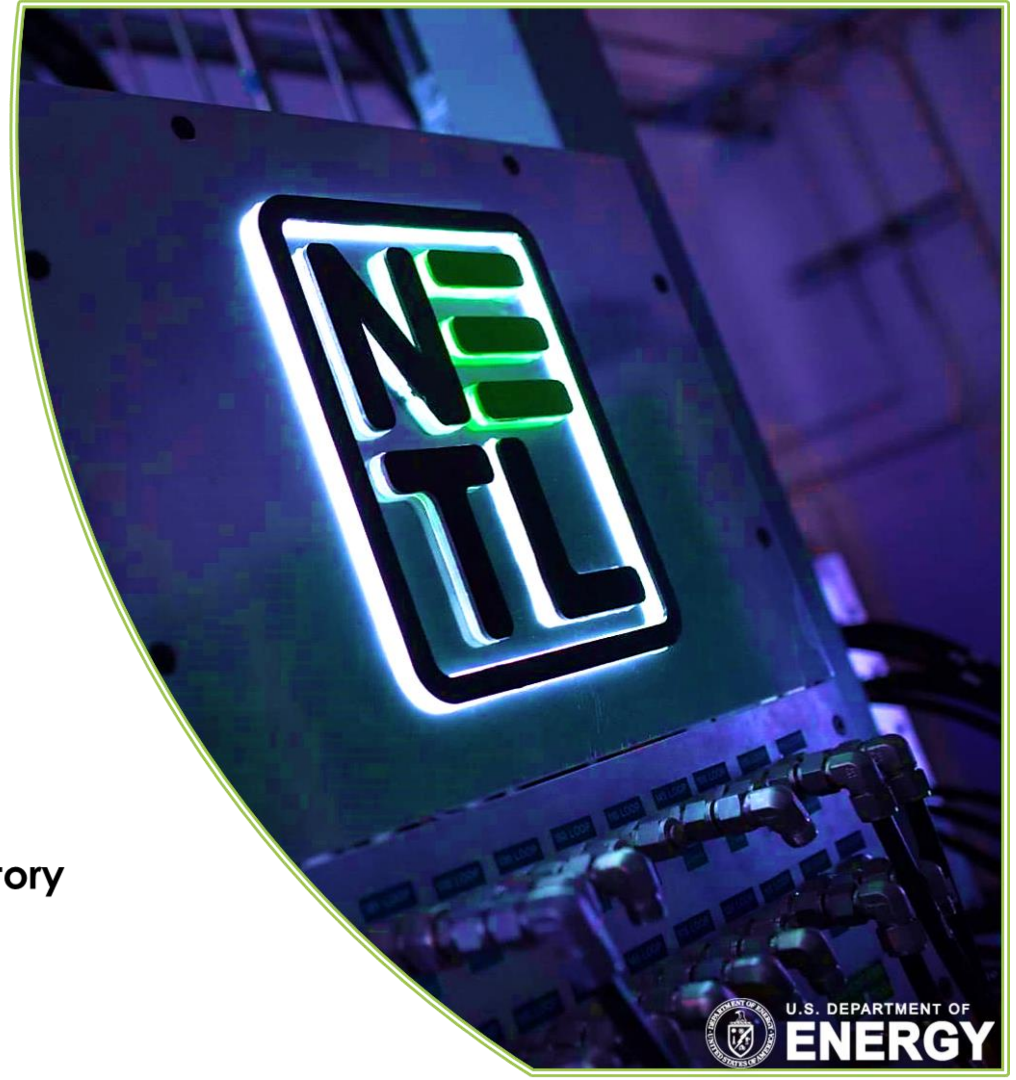
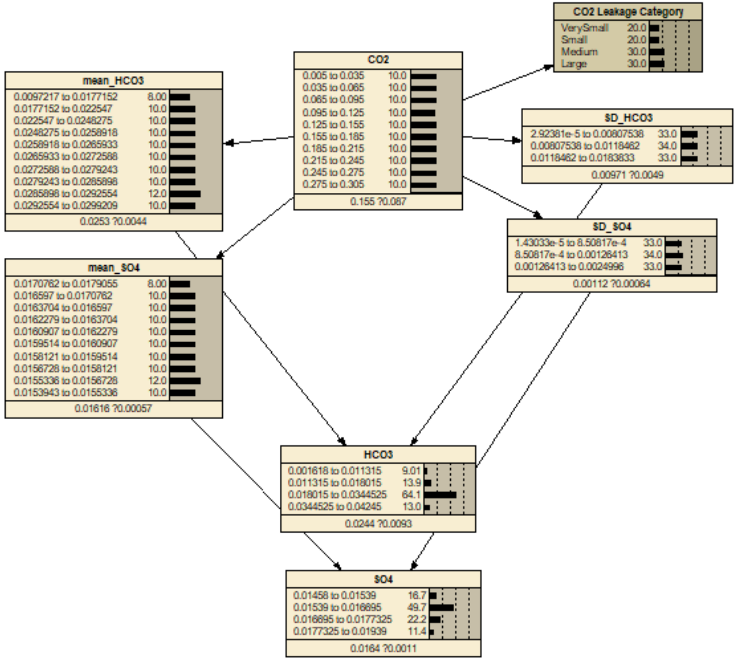
Contact: Wei Xiong, wei.xiong@netl.doe.gov



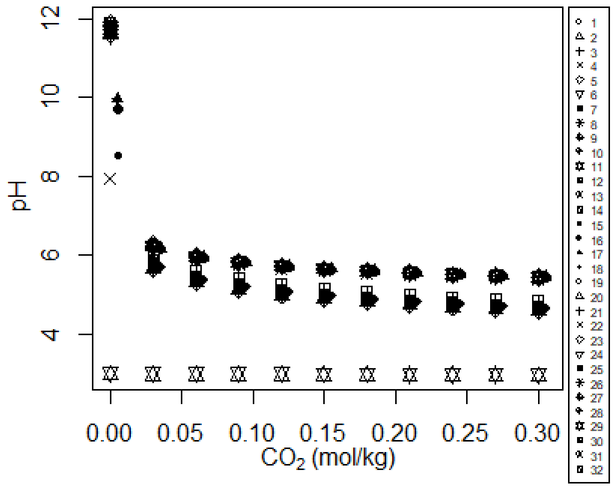
Supplemental Slides

Construction of BBN-Regression Results

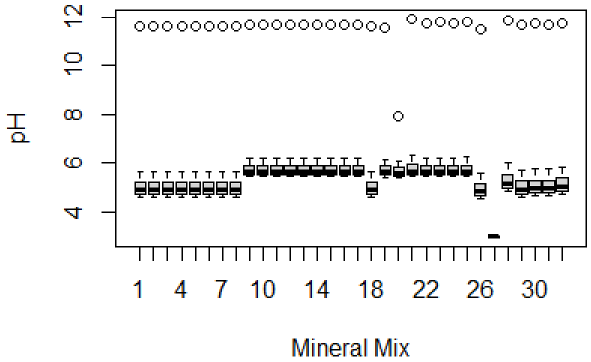
- Mean-predicted value from the response function for each CO_2 level
- SD-standard deviation of residuals (geochemical model output-predicted values)
- Ion concentration-normally distributed with mean and SD



pH

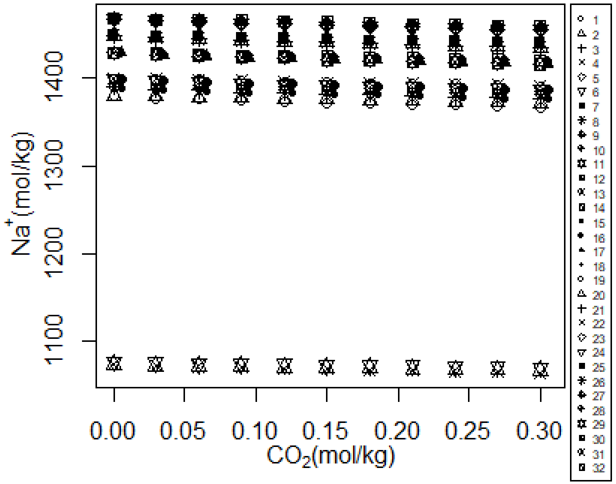


pH
12
10
8
6
4
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO2 (mol/kg)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32

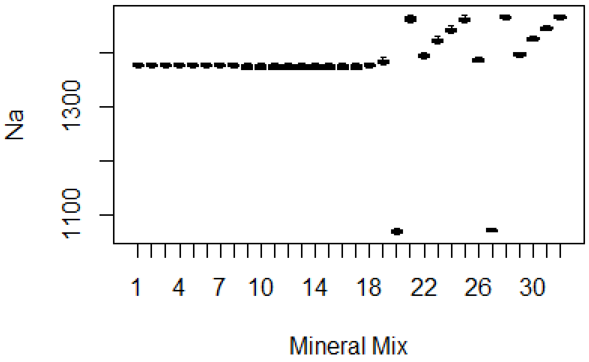


pH
12
10
8
6
4
1
4
7
10
14
18
22
26
30
Mineral Mix

Na

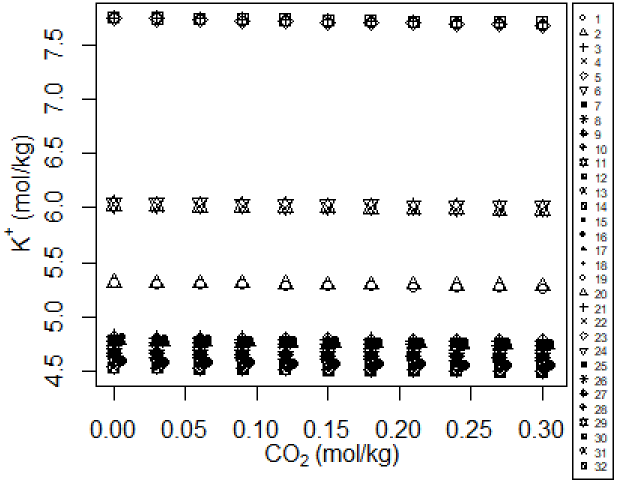


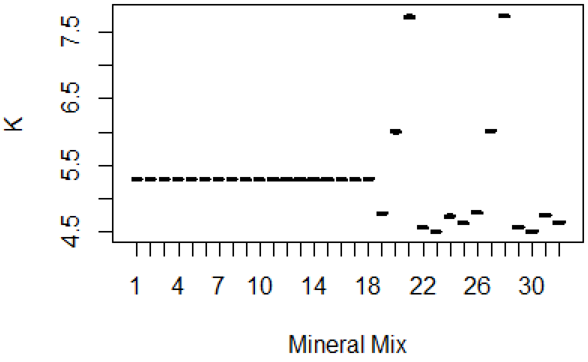
Na+(mol/kg)
1100
1200
1300
1400
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO2(mol/kg)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32



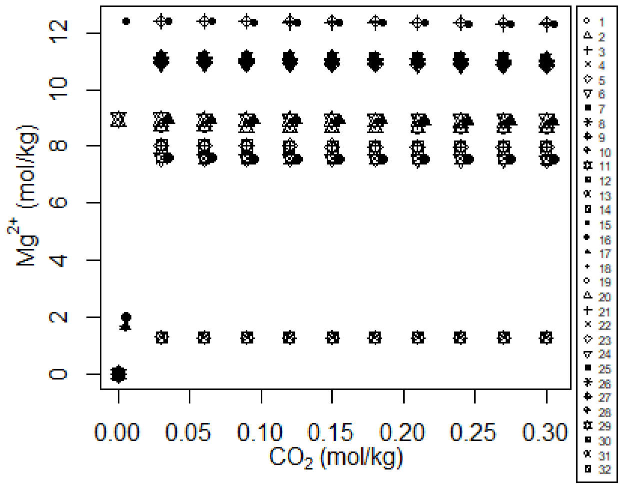
Na
1100
1300
1
4
7
10
14
18
22
26
30
Mineral Mix

K

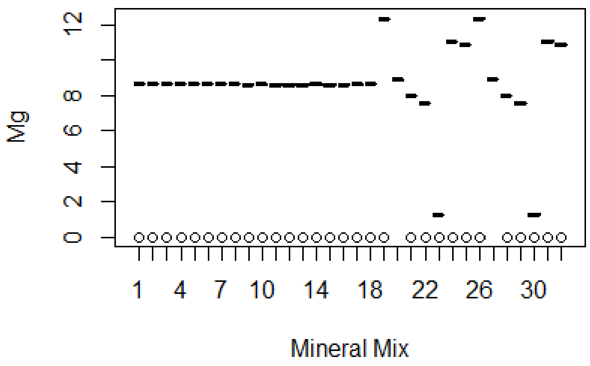

K^+ (mol/kg)
CO_2 (mol/kg)
0.00
0.05
0.10
0.15
0.20
0.25
0.30
4.5
5.0
5.5
6.0
6.5
7.0
7.5


K
Mineral Mix
1
4
7
10
14
18
22
26
30
4.5
5.5
6.5
7.5

Mg

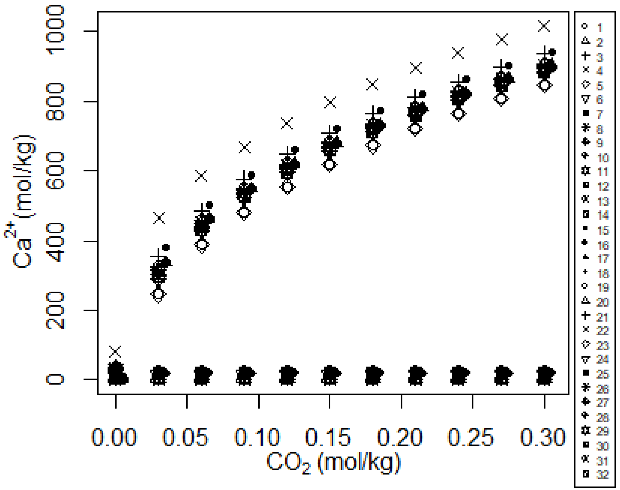


Mg^{2+} (mol/kg)
0
2
4
6
8
10
12
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO_2 (mol/kg)
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32

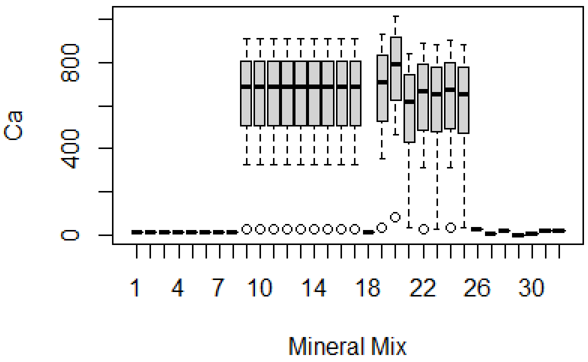


Mg
0
2
4
6
8
12
1
4
7
10
14
18
22
26
30
Mineral Mix

Ca

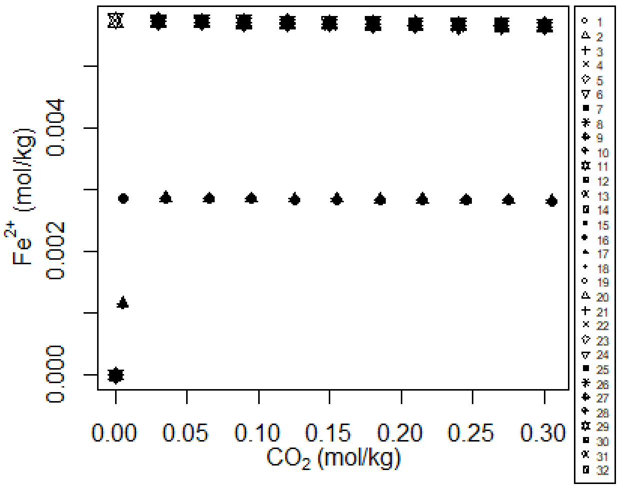


Ca^{2+} (mol/kg)
0
200
400
600
800
1000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO_2 (mol/kg)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32

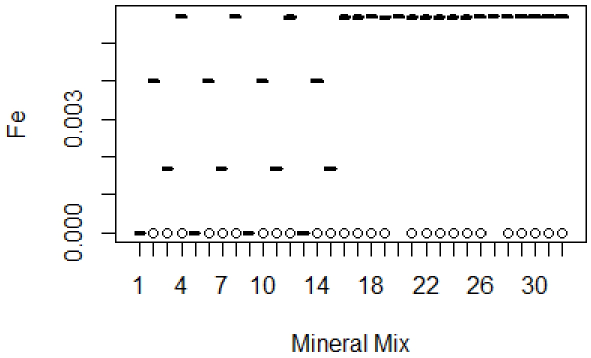


Ca
0
400
800
1
4
7
10
14
18
22
26
30
Mineral Mix

Fe

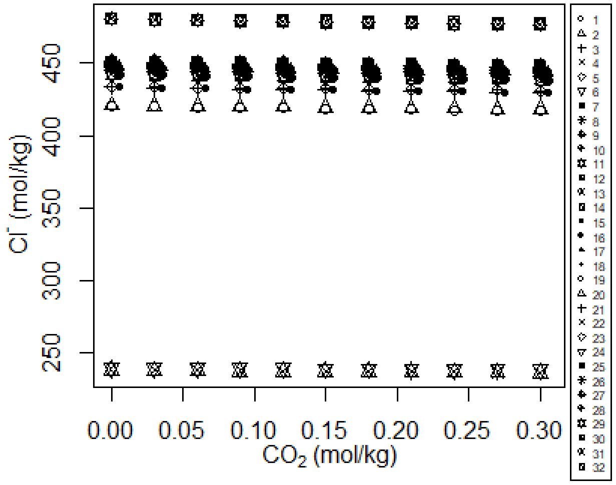


Fe^{2+} (mol/kg)
0.000
0.002
0.004
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO_2 (mol/kg)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32

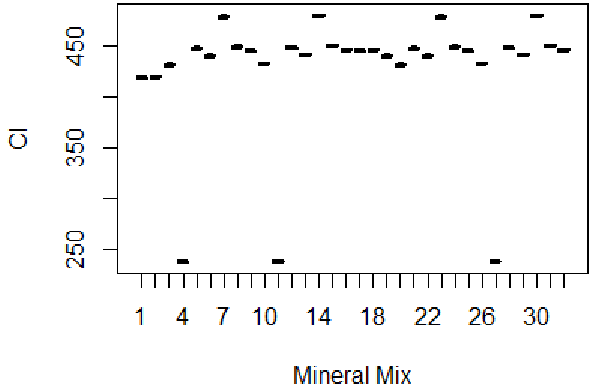


Fe
0.000
0.003
1
4
7
10
14
18
22
26
30
Mineral Mix

Cl

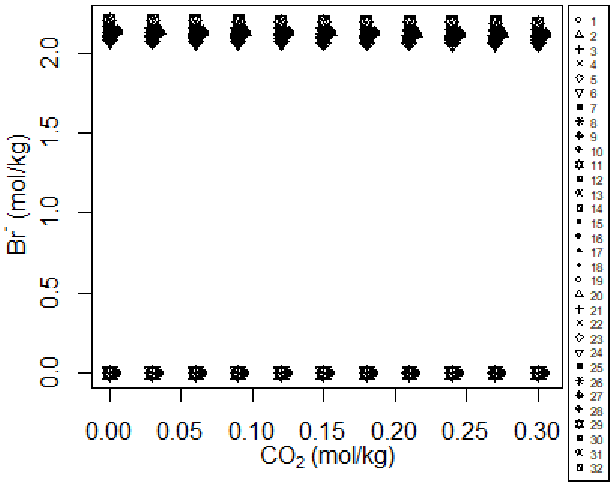


Cl⁻ (mol/kg)
250
300
350
400
450
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO_2 (mol/kg)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32



Cl
250
350
450
1
4
7
10
14
18
22
26
30
Mineral Mix

Br



Br⁻ (mol/kg)
0.0
0.5
1.0
1.5
2.0
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO_2 (mol/kg)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
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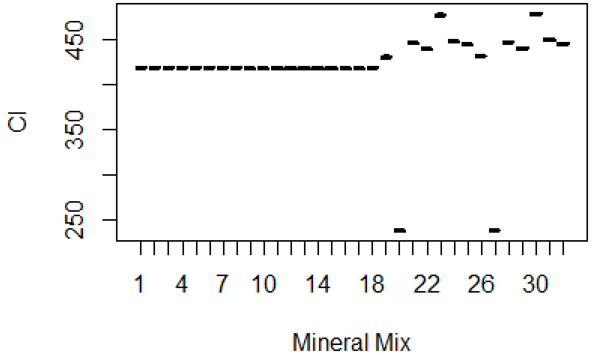
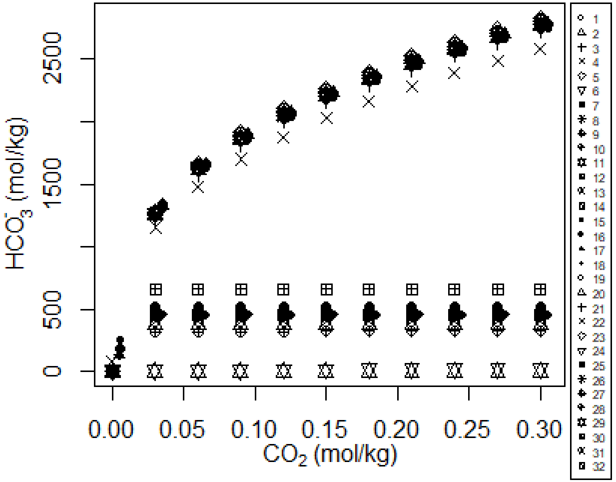
26
27
28
29
30
31
32

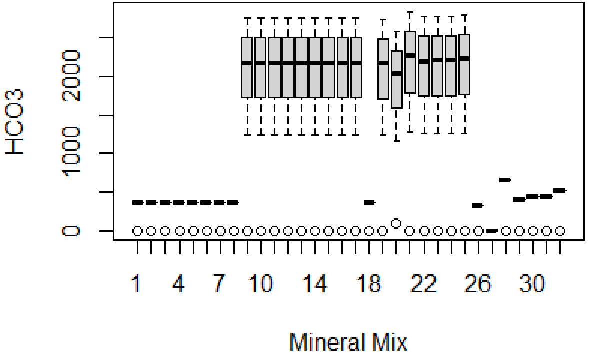


Cl
250
350
450
1
4
7
10
14
18
22
26
30
Mineral Mix

HCO3

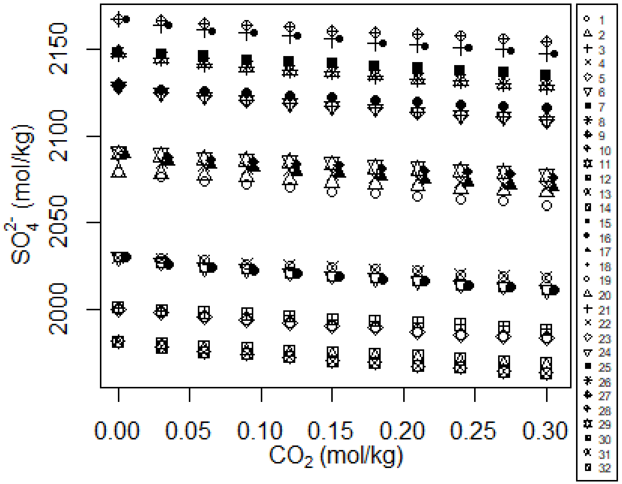


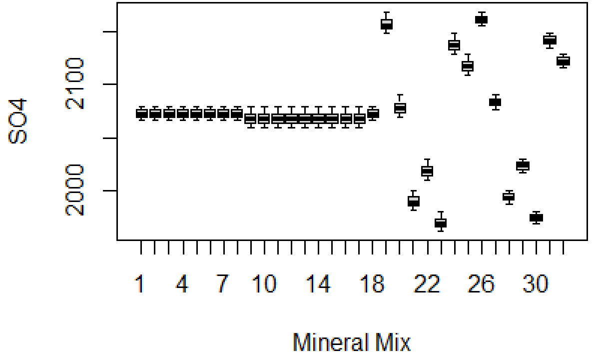
HCO_3^- (mol/kg)
0
500
1500
2500
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO_2 (mol/kg)
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32



HCO3
0
1000
2000
1
4
7
10
14
18
22
26
30
Mineral Mix

SO4


2000
2050
2100
2150
SO_4^{2-} (mol/kg)
0.00
0.05
0.10
0.15
0.20
0.25
0.30
CO_2 (mol/kg)
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32


SO4
2000
2100
1
4
7
10
14
18
22
26
30
Mineral Mix