Memorandum

To: Siraj Moopen, CRC **Date:** July 31, 2024

From: Chris Wolf and Brad Bessinger

Subject: CTV VI Geochemical Modeling

1. Introduction

For a proposed carbon sequestration project CTV VI, CRC has requested Daniel B. Stephens & Associates, Inc. (DBS&A) to perform geochemical modeling to help understand chemical reactions during carbon dioxide (CO_2) storage. Information used to perform the modeling described below was provided by CRC.

Geochemical modeling was conducted to evaluate the compatibility of the injectate with groundwater and rocks composing the injection zone and confining zone. The intent of the modeling is to identify the major potential reactions that may affect injection or containment (U.S. EPA, 2013).

Geochemical modeling using the PHREEQC (pH-REdox-Equilibrium) software was used to calculate the behavior of minerals and changes in aqueous chemistry and mineralogy based on chemical equilibrium conditions (Parkhurst and Appelo, 2013).

This technical memorandum describes the site conditions and modeling results for CTV VI (Tables 1 through 12). There are a series of four Injection Zones that are, from the deepest to shallowest: Claimed as PBI Claimed as PBI A "reaction path" approach was used for the modeling that allowed chemical equilibrium between the minerals and groundwater of each injection zone followed by reactions with the CO_2 injectate. Each Injection Zone was reacted sequentially from deepest to shallowest with the final solution in the Claimed as PBI allowed to react with Claimed as PBI confining unit. This sequence was modeled using two injectate chemistries.

Based on the geochemical equilibrium modeling, the injection of carbon dioxide at the CTV VI site does not cause significant reactions that will affect the injection or containment of the gas.

2. Geochemistry for CTV VI Storage Project

While rocks are buried in the earth's crust, chemical reactions between the rocks and groundwater are termed weathering or diagenesis, which involves the dissolution of minerals into groundwater and precipitation of minerals from solution. Reactions are driven by fluid movement, temperature, and pressure changes due to burial depth and compaction. Over time, minerals and cements may dissolve and form new minerals. Important reactions that typically occur in clastic sedimentary rocks include the following:

- Precipitation and dissolution of cements and authigenic minerals consisting of various minerals including quartz, clays, potassium feldspar (K-feldspar), plagioclase feldspar, siderite, gypsum, and pyrite
- Dissolution of feldspars, quartz, lithic fragments
- Formation of feldspar and quartz overgrowths
- Precipitation or dissolution of illite, kaolinite and other clays

2.1 Injection Zone Fluid Geochemistry

Data were used from water samples collected in the Injection Zones and the Confining Zone in CTV VI (Table 1). These samples had a complete suite of major ions and pH, so they were used for the geochemical modeling. With total dissolved solids (TDS) concentrations greater than 20,000 parts per million (ppm), the groundwater samples are considered brackish.

The net charge of a water sample may be calculated using the results for the cation and anion data. Based on the fact that water has a net neutral charge, the sum of the cation and anion charges should be zero. Variations due to sampling and analyses often cause the calculated value to vary, and a value within 5 percent of neutral is considered a "good" balance. The charge balance for the water samples used for the modeling were "balanced" in the PHREEQC simulations.

2.2 Injection Zone and Confining Zone Mineralogy

Mineralogy was evaluated using x-ray diffraction (XRD) to determine the bulk and clay mineralogy of core samples. Analyses were available for the Claimed as PBI and Claimed as PBI Claimed as PBI The Claimed as PBI was modeled using the Claimed as PBI data, and the Claimed as PBI were modeled using data for an equivalent unit in the Claimed as PBI

At CTV VI, mineralogy of the injection zones is dominated by quartz and feldspars, with about <8 percent clay mineral content (Table 2). The Confining Zone is dominated by clay minerals including kaolinite, chlorite, illite, and layered illite/smectite, with lesser amounts of quartz and feldspar. The Confining Zone was modeled with 48.1 percent clay minerals.

2.3 Injectate Chemistry

Chemical compositions for the carbon dioxide injectate were divided into two scenarios of different compositions (Table 3). The chemistry for Scenario 1 and Scenario 2 was modeled at CTV VI.

3. Equilibrium Geochemical Modeling

When modeling groundwater geochemistry, the water chemistry, gas chemistry, and mineralogy are used to constrain the model because mineral solubility controls the concentrations of a mineral's elemental components in groundwater (Appelo and Postma, 2005). Mineral dissolution-precipitation reactions directly impact the aqueous chemistry. In general, as minerals dissolve the elemental concentrations in groundwater increase and when minerals precipitate the elemental concentrations in groundwater decrease. Chemical equilibrium indicates that congruent reactions will appear balanced between reactants and products with no apparent change in the chemical system.

The PHREEQC model was used to evaluate potential changes to mineralogy and aqueous composition in the subsurface due to CO_2 injection. The mineral, gas, and aqueous phases were assumed to be in chemical equilibrium.

Based on the available injectate gas compositions, PHREEQC was used to calculate the partial pressures and mole fractions of the injectate components.

The reservoir temperatures varied by depth, with the greatest value of 89°C in the deepest Injection Zone and the lowest value of 57°C within the Confining Zone.

3.1 Geochemical Database

For reactions involving water and minerals, the equilibrium relationship between products and reactant activities (concentrations) can be calculated using known values for parameters like Gibb's energy found in thermodynamic databases (Zhu and Anderson, 2002). Thermodynamic values for these calculations are compiled in databases from several entities including the

U.S. Geological Survey (USGS) and Lawrence Livermore National Laboratory. A database developed at the Lawrence Livermore National Laboratory (LLNL.dat) was used for this evaluation. The LLNL.dat database includes a temperature range for the thermodynamic data provided from 0 to 300°C. This database is appropriate for the groundwater concentrations, pressure, and temperature used in the modeled scenarios.

When modeling saline waters, the Pitzer database (Parkhurst and Appelo, 2013) is often used, but it has thermodynamic data for a limited number of minerals including calcite, dolomite, gypsum, and quartz. The Injection Zones and Confining Zone include minerals that are not included in the Pitzer database, so the LLNL.dat database was used because it also includes smectite, illite, pyrite and the minerals listed in Table 2.

For the injection gases, methane is included in the database as a gas and aqueous phase, but ethane is not included as a gas phase. The ethane gas portion of the injection chemistry was not modeled. The mass fractions were normalized excluding the ethane.

3.2 Saturation Indices

Saturation indices (SIs) were calculated that represent whether a particular mineral (e.g., calcite or gypsum) is in chemical equilibrium with the groundwater. SI calculations are used to predict if a mineral is likely to precipitate or dissolve in the groundwater and if these reactions change the concentrations of dissolved elements.

Chemical equilibrium was assumed for the reactions in the model. Equilibrium modeling sets the saturation indices to a zero (0) value for a given mineral. Minerals used in the modeling scenarios are based on those detected using XRD and their relative abundances. The assumption of chemical equilibrium allows dissolution and precipitation reactions to be quantified in the model.

The formula for calculating saturation indices (SI) is as follows:

$$SI = \frac{IAP}{K_{sp}} \quad (1)$$

where SI = saturation index
IAP = ion activity product
K_{sp} = solubility product

Using gypsum as an example (Clark, 2015), the ion activity product of gypsum (IAP_{gypsum}) is the product of the activity (a, activity is approximately equal to concentration in dilute solutions) of calcium (Ca) and sulfate (SO_4):

$$IAP = a_{Ca^{2+}} \times a_{SO_4{}^{2-}} \quad (2)$$

The solubility product, K_{sp}, is an indication of the relative solubility of a mineral in water. A value less than zero (<0) indicates that the mineral will dissolve and contribute ions to solution and may result in a relatively high activity or concentration. A value greater than zero (>0) indicates that the mineral has a low solubility, may precipitate from solution, and will not contribute many ions to the solution. For the mineral gypsum, the K_{sp} based on the dissociation reaction of gypsum in water is:

$$CaSO_4 \cdot 2H_2O \leftrightarrow Ca^{2+} + SO_4{}^{2-} + 2H_2O$$

$$K_{sp} = \frac{a_{Ca^{2+}} + a_{SO_4{}^{2-}} + a_{H_2O}}{a_{gypsum}} = 10^{-4.60} \quad (3)$$

Interpreting the results of the SI calculation is straightforward:

- Log SI > 0 indicates that mineral is supersaturated in solution and may precipitate onto aquifer matrix or pore space.
- Log SI = 0 indicates that mineral is at chemical equilibrium with the water.
- Log SI < 0 indicates that mineral is undersaturated in solution and may dissolve from aquifer matrix.

Due to potential systematic errors introduced during sampling and analysis, results within the range of ±0.5 of zero are typically considered in or near chemical equilibrium.

4. Geochemical Model Input

To construct the equilibrium models in PHREEQC, site-specific data were used as input including water chemistry, mineralogy, temperature, and pressure.

Data include the water chemistry data for the Injection Zones (Table 1), which were entered as received in parts per million (ppm) for elemental concentrations and standard units for pH.

For input into PHREEQC, the mineralogy in Table 2 was converted to a molar volume in moles per liter (mol/L) using porosity and bulk density values as follows:

- Injection Zone 1: rock density of 2.13 kilograms per liter (kg/L) and porosity of 30.8 percent
- Injection Zone 2: rock density of 2.16 kg/L and porosity of 29.3 percent
- Injection Zone 3: rock density of 2.23 kg/L and porosity of 25.9 percent
- Injection Zone 4: rock density of 2.28 kg/L and porosity of 22.3 percent
- Confining Zone: rock density of 2.07 kg/L and porosity of 26.4 percent

The converted values for mineralogy that were input into PHREEQC are shown in Table 4.

- Injection Zone 1: Pressure of 154.5 to 173.3 atmospheres (atm)
- Injection Zone 2: Pressure of 205.2 to 208.1 atm
- Injection Zone 3: Pressure of 259.4 to 288.6 atm
- Injection Zone 4: Pressure of 297.8 to 329.3 atm
- Upper Confining Zone: Pressure of 137.2 atm

5. Geochemical Modeling Results and Discussion

Model results showing the changes in mineralogy designated as equilibrium phases in PHREEQC are presented for CTV VI in Tables 5 through 8 for the Injection Zones and the Confining Zone. Model results are presented in Tables 9 through 12 for the water chemistry based on the equilibrium phases. The modeling steps were as follows:

- Injection Zones: Use the Injection Zone groundwater data and equilibrate with zone mineralogy dataset for the Injection Zone and carbon dioxide at given reservoir pressures and temperature. Models were run using each injectate composition and reacted with the zone above.
- Confining Zone: Use the model results for Injection Zone 1 and equilibrate with the Confining Zone mineralogy dataset and carbon dioxide at final reservoir pressure. Models were run using each injectate composition.

Equilibrium geochemical modeling of the injection of carbon dioxide indicate that changes in mineralogy and aqueous chemistry are likely to occur but, overall, all geologic units are

composed dominantly of silicate minerals such as quartz and feldspar that are not expected to be highly reactive during carbon dioxide sequestration. More reactive minerals like calcite and dolomite are present in relatively smaller amounts compared to the silicate minerals.

Although the model indicates that minerals will dissolve and precipitate, the net change in mass is minimal. Based on the mineralogical changes, there tends to be a small change in the overall mass calculated by the model. Within the Injection Zones, precipitation of minerals is occurring and ranges from 2 to 6.8 percent of the molar mass. For the Confining Zone, dissolution of minerals is occurring and is about 0.6 percent of the molar mass. Overall, the porosity within the Injection Zones and Confining Zone is not expected to be significantly impacted by mineral dissolution and precipitation reactions during carbon dioxide sequestration.

The TDS concentration is predicted to increase as dissolved aqueous species increase from the injection gases dissolving into the groundwater.

Based on the modeling, the following reactions are expected to occur:

- Dissolution of feldspars and calcite and the precipitation of quartz and siderite.
- Smectite and/or kaolinite dissolution resulting in the precipitation of illite.
- Chlorite (chamosite) when initially present is not stable and dissolves, releasing iron, aluminum, and silica to solution.
- Feldspars dissolve, releasing cations like sodium, calcium, aluminum and silica to solution, likely contributing to calcite and clay mineral formation.
- Albite tends to be a stable feldspar mineral but does dissolve in some scenarios.
- Pyrite tends to dissolve, releasing iron and sulfate to solution.

For all geologic units, the formation of carbonates like calcite, dolomite, or siderite was predicted to occur in several model scenarios. The formation of carbonate minerals can be an important mechanism to remove and immobilize carbon dioxide from solution through incorporation of CO_2 in the mineral phase. The CO_2 gas in the injectate will form carbonate minerals, dissolve into solution, or remain in a gas phase.

Results of equilibrium modeling indicate the following:

- Carbon dioxide will dissolve into solution and is included in total inorganic carbon (TIC), which also includes bicarbonate and carbonate species. Results indicate that when carbon

dioxide is dissolved in solution, the following dissolved species will occur as the following ions and complexes: carbon dioxide, bicarbonate, sodium bicarbonate, calcium bicarbonate, and magnesium bicarbonate.

- The pH values tend to be slightly acidic to slightly alkaline.
- The Eh is maintained as reducing conditions for the model runs.
- The calcium in solution includes the following ions and complexes: calcium, calcium bicarbonate, and calcium sulfate complex.

Based on the geochemical equilibrium modeling, the injection of carbon dioxide at the CTV VI site does not cause significant reactions that will affect the injection or containment of the gas.

References

Appelo, C.A.J. and D. Postma. 2005. *Geochemistry, groundwater and pollution*. 2nd Edition. Balkema, Rotterdam.

Clark, I. 2015. *Groundwater geochemistry and isotopes*. 1st edition. CRC Press. <https://doi.org/10.1201/b18347>.

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U.S. Environmental Protection Agency (U.S. EPA). 2013. *Geologic sequestration of carbon dioxide, Underground Injection Control (UIC) Program Class VI well site characterization guidance*. EPA 816-R-13-004. Available at <https://www.epa.gov/uic/final-class-vi-guidance-documents>.

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Tables

Table 1. Baseline Geochemistry for the CTV VI Storage Project

Analyte	Concentration (ppm [a])		
	Claimed as PBI [redacted]	Claimed as PBI	Claimed as PBI
	6/8/1985	6/8/1985	6/8/1985
UWI	Claimed as PBI	[redacted]	[redacted]
Well Name	Claimed as PBI	[redacted]	[redacted]
Aluminum	NA	NA	NA
Alkalinity (as $CaCO_3$)	150	110	110
Boron	28	58	72
Barium	NA	NA	NA
Bicarbonate (as $CaCO_3$)	190	140	110
Calcium	1,500	400	460
Chloride	18,100	11,900	12,400
Iron	3.8	0.11	0.46
Potassium	110	35	35
Magnesium	310	67	29
Manganese	NA	NA	NA
Sodium	9,400	7,200	7,450
pH (s.u.)	7.2	7.4	7.5
Sulfide	5	5	5
Sulfate	5	5.5	14
Silica	NA	NA	NA

[a] Unless otherwise noted
NA = Not analyzed
ppm = Parts per million
s.u. = Standard units

Table 2. Mineralogy of the CTV VI Storage Project Injection and Confining Zones

Claimed as PBI

Depth (feet)	Test Type	Mineralogical Content (%)												
		Quartz	Opal CT	Plagioclase	K-Feldspar	Calcite	Dolomite	Pyrite	Barite	Kaolinite	Chlorite	Illite	Illite-Smectite and Mixed Layer Clays	Total Clay
7,581.1	XRD	18.5	—	12.7	5.1	0.0	0.0	4.7	0.0	13.4	3.7	15.7	26.3	59.1
7,587.1	XRD	21.8	—	15.3	6.3	0.0	0.0	5.9	—	9.3	3.4	14.9	23.1	50.7
7,590.1	XRD	17.0	—	10.6	4.6	0.0	0.0	7.7	—	16.6	3.6	15.0	24.8	60.0
7,608.2	XRD	19.0	—	10.7	5.4	0.8	0.0	7.1	—	23.4	3.4	11.0	19.2	57.0
6,011.4	XRD	19.1	5.5	16.1	5.1	4.6	1.0	4.3	—	2.3	2.1	21.2	18.7	44.3
6,014.1	XRD	10.7	10.4	13.1	4.5	0.0	0.4	5.5	—	3.0	3.0	23.2	26.3	55.5
6,023.8	XRD	23.2	3.9	18.7	7.3	0.3	0.7	4.0	—	2.9	1.8	14.9	22.2	41.8
6,030.4	XRD	9.1	20.9	11.7	4.8	0.0	0.0	4.6	—	1.6	1.6	14.9	30.9	49.0
6,036.1	XRD	29.1	6.1	20.6	7.3	0.0	1.2	4.7	—	2.1	1.1	11.2	16.7	31.1
6,048.1	XRD	20.6	3.1	16.6	5.9	0.0	0.8	4.3	—	8.2	1.1	15.4	24.1	48.8
8,200.0	XRD	32.0	0.0	35.0	22.0	0.0	0.0	4.0	0.0	2.5	0.8	2.7	1.1	7.0
8,612.0	XRD	36.0	—	33.0	20.0	—	—	2.0	—	3.5	0.9	4.2	0.4	9.0
8,751.0	XRD	36.0	—	33.0	20.0	—	—	—	1.0	3.4	0.7	3.9	2.0	10.0
4,304.0	XRD	42.9	—	14.1	11.9	0.0	0.0	5.8	—	20.2	2.4	1.9	0.8	25.3

[a] Average mineral composition for Claimed as PBI selected for modeling.
[b] Average mineral composition for Claimed as PBI selected for modeling Claimed as PBI
[c] Most likely mineral composition for modeling Claimed as PBI
— = Not detected

Table 3. Estimated Compositions for Carbon Dioxide Injectate

Gas	Mass Faction (original composition)	Mass Fraction (normalized model input)
Injectate Scenario 1		
Carbon dioxide	0.9921253	0.99352
Nitrogen	0.0064308	0.00644
Hydrogen sulfide	0.0000078	0.00001
Sulfur dioxide plus sulfur trioxide	0.0000295	0.00003
Total	0.9985934	1.00
Injectate Scenario 2		
Carbon dioxide	0.9988419	0.9995
Methane	0.0003863	0.0004
Ethane	0.0005330	—
Hydrogen sulfide	0.0001394	0.0001
Total	0.9999007	1.00

Note: The original compositions were normalized to 100% for use as model input. For Scenario 1, the sulfur dioxide plus sulfur trioxide fraction was input as sulfur dioxide in the model. For Scenario 2, the ethane component was excluded as ethane gas is not in the model database.

Table 4. Mineralogy Input for PHREEQC Selected for CTV VI Storage Project

PHREEQC Mineral	Chemical Formula	Molar Mass (g/mol)	Input for [redacted]		Input for [redacted]		Input for [redacted]		Input for [redacted]		Input for [redacted]	
			%	mol/L	%	mol/L	%	mol/L	%	mol/L	%	mol/L
Quartz	SiO_2	60.08	26.2	32.27	42.9	42.51	42.9	45.66	34.3	43.24	34.3	52.66
K-Feldspar	$KAlSi_3O_8$	278.33	5.4	1.45	11.9	2.55	11.9	2.73	20.4	5.56	20.4	6.78
Plagioclase (assumed albite)	$NaAlSi_3O_8$	263.02	14.1	3.97	14.1	3.19	14.1	3.43	33.3	9.59	33.3	11.68
Calcite	$CaCO_3$	100.09	0.6	0.41	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Dolomite	$CaMg(CO_3)_2$	184.40	0.4	0.16	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Rhodochrosite	$MnCO_3$	114.95	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Siderite	$FeCO_3$	115.86	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00	0.0	0.00
Pyrite	FeS_2	119.98	5.1	3.15	5.8	2.88	5.8	3.09	3.0	1.87	3.0	2.28
Barite	$BaCO_3$	258.16	0.0	0.00	0.0	0.00	0.0	0.00	0.5	0.15	0.5	0.18
Kaolinite	$Al_2Si_2O_5(OH)_4$	258.16	8.0	2.29	20.2	4.66	20.2	5.00	3.1	0.91	3.1	1.10
Chamosite-7A (for chlorite)	$Fe_2Al_2SiO_5(OH)_4$	664.18	2.4	0.27	2.4	0.22	2.4	0.23	0.8	0.09	0.8	0.11
Illite	$K_{0.6}Mg_{0.25}Al_{1.8}Al_{0.5}Si_{3.5}O_{10}(OH)_2$	389.34	15.2	2.89	1.9	0.29	1.9	0.31	3.6	0.70	3.6	0.85
Smectite-low-Fe-Mg	$Ca_{0.02}Na_{0.15}K_{0.2}Fe_{0.29}Fe_{0.16}Mg_{0.9}Al_{1.25}Si_{3.75}{\cdot}12H_2O$	549.07	22.5	3.02	0.8	0.09	0.8	0.09	1.1	0.16	1.1	0.19

g/mol = Grams per mole
mol/L = Moles per liter

Table 5. Mineralogy Changes Based on Equilibrium Geochemical Modeling for Injection Zone 4 Claimed as PBI [redacted] with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Claimed as PBI			[redacted]			[redacted]			[redacted]		
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Injection Chemistry	*Scenario 1*						*Scenario 2*					
Pressure (atm)	*329*			*289*			*329*			*289*		
$CH_4(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$CO_2(g)$	0.00	9.56	9.56	0.00	0.00	0.00	0.00	9.67	9.67	0.00	0.00	0.00
$H_2S(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$N_2(g)$	0.00	0.11	0.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$SO_2(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Albite	11.65	10.97	–0.68	9.56	9.76	0.20	11.65	10.98	–0.67	9.56	9.76	0.20
Barite	0.17	0.18	0.01	0.14	0.15	0.00	0.17	0.17	0.00	0.14	0.15	0.01
Calcite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Chamosite-7A	0.05	0.00	–0.05	0.04	0.00	–0.04	0.05	0.00	–0.05	0.04	0.00	–0.04
Dolomite	0.00	0.02	0.02	0.00	0.00	0.00	0.00	0.02	0.02	0.00	0.00	0.00
Illite	0.00	1.29	1.29	0.00	1.31	1.31	0.00	1.30	1.30	0.00	1.31	1.31
Kaolinite	1.77	1.29	–0.48	1.46	0.47	–0.98	1.77	1.28	–0.49	1.46	0.47	–0.98
K-Feldspar	7.24	6.54	–0.69	5.94	5.23	–0.71	7.24	6.54	–0.70	5.94	5.23	–0.71
Pyrite	2.28	2.28	0.00	1.88	1.87	0.00	2.28	2.29	0.00	1.88	1.87	0.00
Quartz	52.18	54.38	2.20	42.85	43.14	0.29	52.18	54.36	2.18	42.85	43.14	0.29
Rhodochrosite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Siderite	0.00	0.30	0.30	0.00	0.25	0.25	0.00	0.30	0.30	0.00	0.25	0.25
Smectite	0.43	0.00	–0.43	0.35	0.00	–0.35	0.43	0.00	–0.43	0.35	0.00	–0.35

Negative (–) delta value indicates that mineral or gas dissolves into solution, while positive (+) delta value indicates that mineral precipitates from solution.
mol/L = Moles per liter atm = Atmospheres

Table 6. Mineralogy Changes Based on Equilibrium Geochemical Modeling for Injection Zone 3 Claimed as PBI [redacted] with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Claimed as PBI			[redacted]			[redacted]			[redacted]		
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Injection Chemistry	*Scenario 1*						*Scenario 2*					
Pressure (atm)	*289*			*208*			*289*			*208*		
$CH_4(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$CO_2(g)$	0.00	8.20	8.20	0.00	0.00	0.00	0.00	8.29	8.29	0.00	0.00	0.00
$H_2S(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$N_2(g)$	0.00	0.10	0.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$SO_2(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Albite	9.56	8.67	–0.90	3.41	3.74	0.33	9.56	8.67	–0.89	3.41	3.74	0.33
Barite	0.14	0.15	0.00	0.00	0.00	0.00	0.14	0.14	0.00	0.00	0.00	0.00
Calcite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Chamosite-7A	0.04	0.00	–0.04	0.21	0.00	–0.21	0.04	0.00	–0.04	0.21	0.00	–0.21
Dolomite	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00
Illite	0.00	0.87	0.87	0.00	0.83	0.83	0.00	0.87	0.87	0.00	0.83	0.83
Kaolinite	1.46	1.40	–0.06	5.25	4.69	–0.56	1.46	1.39	–0.06	5.25	4.69	–0.56
K-Feldspar	5.94	5.49	–0.45	2.90	2.44	–0.46	5.94	5.49	–0.46	2.90	2.44	–0.46
Pyrite	1.88	1.87	0.00	3.09	3.09	0.00	1.88	1.88	0.00	3.09	3.09	0.00
Quartz	42.85	45.34	2.49	45.49	45.00	–0.49	42.85	45.33	2.48	45.50	44.99	–0.51
Rhodochrosite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Siderite	0.00	0.25	0.25	0.00	0.51	0.51	0.00	0.24	0.24	0.00	0.51	0.51
Smectite	0.35	0.00	–0.35	0.18	0.00	–0.18	0.35	0.00	–0.35	0.18	0.00	–0.18

Negative (–) delta value indicates that mineral or gas dissolves into solution, while positive (+) delta value indicates that mineral precipitates from solution.
mol/L = Moles per liter atm = Atmospheres

Table 7. Mineralogy Changes Based on Equilibrium Geochemical Modeling for Injection Zone 2 Claimed as PBI [redacted] with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Claimed as PBI			[redacted]			[redacted]			[redacted]		
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Injection Chemistry	*Scenario 1*						*Scenario 2*					
Pressure (atm)	*208*			*173*			*208*			*173*		
$CH_4(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
$CO_2(g)$	0.00	4.88	4.88	0.00	0.00	0.00	0.00	4.94	4.94	0.00	0.00	0.00
$H_2S(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$N_2(g)$	0.00	0.07	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$SO_2(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Albite	3.41	2.06	–1.35	3.18	3.55	0.37	3.41	2.06	–1.35	3.18	3.55	0.37
Barite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Calcite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Chamosite-7A	0.21	0.00	–0.21	0.20	0.00	–0.20	0.21	0.00	–0.21	0.20	0.00	–0.20
Dolomite	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00
Illite	0.00	0.00	0.00	0.00	0.68	0.68	0.00	0.00	0.00	0.00	0.68	0.68
Kaolinite	5.25	6.23	0.98	4.89	4.41	–0.48	5.25	6.24	0.99	4.89	4.41	–0.48
K-Feldspar	2.90	2.94	0.03	2.70	2.33	–0.37	2.90	2.94	0.04	2.70	2.33	–0.37
Pyrite	3.09	3.09	0.00	2.88	2.88	0.00	3.09	3.09	0.00	2.88	2.88	0.00
Quartz	45.49	48.36	2.88	42.36	41.77	–0.58	45.50	48.40	2.90	42.36	41.80	–0.56
Rhodochrosite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Siderite	0.00	0.50	0.50	0.00	0.47	0.47	0.00	0.50	0.50	0.00	0.47	0.47
Smectite	0.18	0.00	–0.18	0.17	0.00	–0.17	0.18	0.00	–0.18	0.17	0.00	–0.17

Negative (–) delta value indicates that mineral or gas dissolves into solution, while positive (+) delta value indicates that mineral precipitates from solution.
mol/L = Moles per liter atm = Atmospheres

Table 8. Mineralogy Changes Based on Equilibrium Geochemical Modeling for Injection Zone 1 Claimed as PBI [redacted] with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Claimed as PBI			[redacted]			[redacted]			[redacted]		
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Injection Chemistry	*Scenario 1*						*Scenario 2*					
Pressure (atm)	*173*			*137*			*173*			*137*		
$CH_4(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
$CO_2(g)$	0.00	3.12	3.12	0.00	0.00	0.00	0.00	3.17	3.17	0.00	0.00	0.00
$H_2S(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$N_2(g)$	0.00	0.06	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
$SO_2(g)$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Albite	3.18	1.04	–2.14	3.81	5.71	1.90	3.18	1.03	–2.15	3.81	5.72	1.91
Barite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Calcite	0.00	0.00	0.00	0.40	0.00	–0.40	0.00	0.00	0.00	0.40	0.00	–0.40
Chamosite-7A	0.20	0.00	–0.20	0.08	0.00	–0.08	0.20	0.00	–0.20	0.08	0.00	–0.08
Dolomite	0.00	0.01	0.01	0.16	0.59	0.44	0.00	0.01	0.01	0.16	0.59	0.44
Illite	0.00	0.00	0.00	0.00	5.74	5.74	0.00	0.00	0.00	0.00	5.73	5.73
Kaolinite	4.89	6.25	1.36	4.58	0.00	–4.58	4.89	6.25	1.36	4.58	0.00	–4.58
K-Feldspar	2.70	2.73	0.03	3.02	0.02	–3.00	2.70	2.73	0.03	3.02	0.02	–3.00
Pyrite	2.88	2.88	0.00	3.15	3.13	–0.02	2.88	2.88	0.00	3.15	3.13	–0.02
Quartz	42.36	46.80	4.44	30.68	31.44	0.76	42.36	46.82	4.46	30.68	31.44	0.76
Rhodochrosite	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Siderite	0.00	0.47	0.47	0.00	1.18	1.18	0.00	0.47	0.47	0.00	1.18	1.18
Smectite	0.17	0.00	–0.17	3.84	1.63	–2.21	0.17	0.00	–0.17	3.84	1.63	–2.22

Negative (–) delta value indicates that mineral or gas dissolves into solution, while positive (+) delta value indicates that mineral precipitates from solution.
mol/L = Moles per liter atm = Atmospheres

Table 9. Modeled Equilibrium Aqueous Concentrations for Injection Zone 4 Claimed as PBI with Scenario 1 and Scenario 2 Injectates

Parameter	Concentration (mg/L [a]) [b]							
	Claimed as PBI		[redacted]		[redacted]		[redacted]	
	Initial	Final	Initial	Final	Initial	Final	Initial	Final
Injection Chemistry	*Scenario 1*				*Scenario 2*			
Pressure (atm)	*329*		*289*		*329*		*289*	
Temperature (°C)	88.9	88.9	80.4	88.9	88.9	88.9	80.4	88.9
pH (s.u.)	6.79	6.35	6.93	6.4	6.79	6.35	6.93	6.4
Eh (mV)	–265	–208	–266	–208	–265	–239	–266	–241
TDS	21,800	89,400	20,900	73,700	21,800	90,900	20,900	74,300
Aluminum	0.0125	0.00551	0.00983	0.00612	0.0125	0.00556	0.00983	0.00618
Barium	748	1.3	649	0.627	748	1340	649	837
Bicarbonate	77.7	49,600	78.2	37,800	77.7	50,500	78.2	38,600
Boron	74.3	74.6	59.7	73.7	74.3	74.6	59.7	73.7
Calcium	283	0.00113	246	0.00159	283	0.0011	246	0.00153
Chloride	12,800	12,800	12,300	12,700	12,800	12,800	12,300	12,700
Iron	1.06	1.06	1.12	0.935	1.06	1.05	1.12	0.924
Magnesium	6.26	1,120	6.63	721	6.26	1,090	6.63	684
Potassium	85.8	262	67.7	228	85.8	259	67.7	224
Sodium	7,650	25,000	7,470	21,300	7,650	24,700	7,470	21,100
Sulfate	0.244	439	0.24	774	0.244	0.426	0.24	0.577
Sulfide	0.0035	0.0194	0.00211	0.0156	0.0035	0.0531	0.00211	0.0445
Silica	43.1	42.9	35.8	42.9	43.1	42.9	35.8	42.9

[a] Unless otherwise noted.

[b] Values rounded to 3 significant figures.

mg/L = Milligrams per liter
atm = Atmospheres
s.u. = Standard units
mV = Millivolts
TDS = Total dissolved solids

Table 10. Modeled Equilibrium Aqueous Concentrations for Injection Zone 3 Claimed as PBI with Scenario 1 and Scenario 2 Injectates

Parameter	Concentration (mg/L [a]) [b]							
	Claimed as PBI		[redacted]		[redacted]		[redacted]	
	Initial	Final	Initial	Final	Initial	Final	Initial	Final
Injection Chemistry	*Scenario 1*				*Scenario 2*			
Pressure (atm)	*289*		*208*		*289*		*208*	
Temperature (°C)	80.4	80.4	68.3	80.4	80.4	80.4	68.3	80.4
pH (s.u.)	6.93	6.42	7.13	6.51	6.93	6.42	7.13	6.52
Eh (mV)	–266	–206	–342	–210	–266	–235	–327	–241
TDS	20,900	114,000	20,600	79,600	20,900	116,000	20,600	80,800
Aluminum	0.00983	0.0038	0.00657	0.00457	0.00983	0.00382	0.00657	0.00461
Barium	649	1.79	14	0.839	649	1,290	14	978
Bicarbonate	78.2	68500	1.88	43,000	78.2	69,500	1.82	43,900
Boron	59.7	60.7	66.6	59.7	59.7	60.6	66.6	59.7
Calcium	246	0.000527	370	0.000938	246	0.000517	370	0.000907
Chloride	12,300	12,400	12,500	12,300	12,300	12,400	12,500	12,200
Iron	1.12	1.2	1.21	0.976	1.12	1.19	1.21	0.967
Magnesium	6.63	2170	13.1	986	6.63	2140	11.9	960
Potassium	67.7	243	49.8	190	67.7	241	49.9	188
Sodium	7,470	29,900	7,600	22,500	7,470	29,800	7,600	22,300
Sulfate	0.24	345	2.52×10^{-9}	545	0.24	0.476	9.22×10^{-8}	0.467
Sulfide	0.00211	0.0139	0.0128	0.0104	0.00211	0.0359	0.00762	0.029
Silica	35.8	35.5	26.6	35.5	35.8	35.5	26.6	35.5

[a] Unless otherwise noted.
[b] Values rounded to 3 significant figures.

mg/L = Milligrams per liter
atm = Atmospheres
s.u. = Standard units
mV = Millivolts
TDS = Total dissolved solids

Table 11. Modeled Equilibrium Aqueous Concentrations for Injection Zone 2 Claimed as PBI with Scenario 1 and Scenario 2 Injectates

Parameter	Concentration (mg/L [a]) [b]							
	Claimed as PBI		[redacted]		[redacted]		[redacted]	
	Initial	Final	Initial	Final	Initial	Final	Initial	Final
Injection Chemistry	*Scenario 1*				*Scenario 2*			
Pressure (atm)	*208*		*173*		*208*		*173*	
Temperature (°C)	68.3	68.3	57	68.3	68.3	68.3	57	68.3
pH (s.u.)	7.13	6.52	7.33	6.6	7.13	6.52	7.33	6.6
Eh (mV)	–342	–203	–335	–206	–327	–241	–320	–209
TDS	20,600	164,000	20,600	129,000	20,600	164,000	20,600	129,000
Aluminum	0.00657	0.00213	0.00446	0.00248	0.00657	0.00212	0.00445	0.00248
Barium	14	2.69	10.7	1.29	14	14.5	10.7	2.91
Bicarbonate	1.88	105,000	13.1	79,500	1.82	106,000	13	80,200
Boron	66.6	69.4	66.6	68.3	66.6	69.4	66.6	68.3
Calcium	370	0.000281	374	0.000259	370	0.000281	374	0.000256
Chloride	12,500	13,000	12,400	12,800	12,500	13,000	12,400	12,800
Iron	1.21	1.46	1.38	1.23	1.21	1.47	1.38	1.23
Magnesium	13.1	3,840	14.5	3,260	11.9	3,840	13.3	3,280
Potassium	49.8	218	36	180	49.9	218	36	180
Sodium	7,600	41,000	7,600	32,300	7,600	41,100	7,600	32,400
Sulfate	2.52×10^{-9}	224	7.77×10^{-9}	416	9.22×10^{-8}	0.0271	2.65×10^{-7}	185
Sulfide	0.0128	0.00792	0.00504	0.00658	0.00762	0.0288	0.00305	0.00741
Silica	26.6	26.4	19.6	26.4	26.6	26.4	19.6	26.4

[a] Unless otherwise noted.
[b] Values rounded to 3 significant figures.

mg/L = Milligrams per liter
atm = Atmospheres
s.u. = Standard units
mV = Millivolts
TDS = Total dissolved solids

Table 12. Modeled Equilibrium Aqueous Concentrations for Injection Zone 1 Claimed as PBI with Scenario 1 and Scenario 2 Injectates

Parameter	Concentration (mg/L [a]) [b]							
	Claimed as PBI							
	Initial	Final	Initial	Final	Initial	Final	Initial	Final
Injection Chemistry	*Scenario 1*				*Scenario 2*			
Pressure (atm)	*173*		*137*		*173*		*137*	
Temperature (°C)	57	57	53.1	57	57	57	53.1	57
pH (s.u.)	7.33	6.61	7.26	7.08	7.33	6.6	7.26	7.08
Eh (mV)	–335	–196	–331	–222	–320	–234	–331	–222
TDS	20,600	23,6000	31,900	105,000	20,600	237,000	31,900	106,000
Aluminum	0.00446	0.00114	0.00298	0.00226	0.00445	0.00114	0.00298	0.00226
Barium	10.7	2.36	35.5	0.139	10.7	11.4	35.5	0.15
Bicarbonate	13.1	158,000	22.4	61,600	13	159,000	22.4	62,400
Boron	66.6	70.9	30	65.4	66.6	70.9	30	65.4
Calcium	374	0.000314	1,340	3.86×10^{-5}	374	0.000315	1,340	3.75×10^{-5}
Chloride	12,400	13,300	19,400	12,200	12,400	13,300	19,400	12,200
Iron	1.38	1.81	3.31	0.637	1.38	1.81	3.31	0.637
Magnesium	14.5	3,640	34.8	5,910	13.3	3,640	34.8	6,000
Potassium	36	204	46.2	88.9	36	204	46.2	89
Sodium	7,600	61,200	10,900	21,800	7,600	61,500	10,900	21,800
Sulfate	7.77×10^{-9}	215	1.01×10^{-9}	3210	2.65×10^{-7}	0.0198	1.01×10^{-9}	3,010
Sulfide	0.00504	0.00411	0.00372	0.00274	0.00305	0.0156	0.00372	0.00279
Silica	19.6	19.3	17.4	19.6	19.6	19.3	17.4	19.6

[a] Unless otherwise noted.
[b] Values rounded to 3 significant figures.

mg/L = Milligrams per liter
atm = Atmospheres
s.u. = Standard units
mV = Millivolts
TDS = Total dissolved solids