

Memorandum

To: Travis Hurst, CTV

Date: April 12, 2023

From: Chris Wolf, P.G. and Beth Salvas, P.G.

Subject: CTV IV Geochemical Modeling

1. Introduction

Carbon TerraVault Holdings, LLC (CTV) has requested that Daniel B. Stephens & Associates, Inc. (DBS&A) perform geochemical modeling for a proposed CTV IV carbon sequestration project in the [REDACTED] to help understand chemical reactions during carbon dioxide (CO₂) storage. For this project, [REDACTED] is the Upper Injection Zone and [REDACTED] is the Lower Injection Zone. Information used to perform the modeling described in this memorandum was obtained from the CTV Class VI permit application materials and other data provided by CTV.

Geochemical modeling was conducted to evaluate the compatibility of the injectate with groundwater and rocks or sediments composing the aquifer system. 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 based on chemical equilibrium conditions (Parkhurst and Appelo, 2013).

2. Geochemistry for CTV IV Storage Project

Four geologic units were considered during this evaluation:

- [REDACTED] Upper Confining Zone
- Upper Injection Zone
- [REDACTED] Internal barrier
- Lower Injection Zone

The [REDACTED] consists of marine deposited claystone with shale and siltstone. The Upper Injection Zone consists of thick sands deposited as a fluvial-deltaic sequence, and is predominantly composed of quartz and feldspar minerals. The [REDACTED] consists of marine deposited claystone interbedded with siltstone. The Lower Injection Zone consists of marine deposited sands, and is predominantly composed of quartz and feldspar minerals.

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 in the rocks may dissolve into solution or form new minerals. Important reactions that have occurred in the Upper and Lower Injection Zones include the following:

- Precipitation and dissolution of cements and authigenic minerals, consisting of various minerals including quartz, clays, potassium feldspar (K-feldspar), albite and oligoclase feldspars, amphibole, apatite, and pyrite
- Dissolution of feldspars, quartz, lithic fragments
- Formation of feldspar and quartz overgrowths
- Precipitation of illite, chlorite, and other clays

2.1 Upper Injection Zone Fluid Geochemistry

Data from a water sample for the Upper Injection Zone were provided (Table 1). The sample results include a complete suite of major ions and pH, so they were used for the geochemical modeling. With a calculated total dissolved solids (TDS) concentration greater than 13,000 parts per million (ppm), the Upper Injection Zone groundwater is considered brackish.

The net charge of a water sample may be calculated using the cation and anion analytical results. Because 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 sample was calculated in PHREEQC at 0.01 percent.

2.2 Lower Injection Zone Fluid Geochemistry

Data from a water sample for the Lower Injection Zone were provided (Table 1). The sample results include a mostly complete suite of major ions and pH, so they were used for the geochemical modeling. With a calculated TDS concentration greater than 14,000 ppm, the

Lower Injection Zone groundwater is considered brackish. The charge balance for the sample was calculated in PHREEQC at -0.13 percent.

2.3 CTV IV Storage Project Mineralogy

Mineralogy for the upper confining unit in [REDACTED] was evaluated using Fourier transform infrared spectroscopy (FTIR) and x-ray diffraction (XRD) to determine the bulk and clay mineralogy of core samples. The mineralogy identified by FTIR and XRD is typically dominated by quartz and feldspar minerals and layered illite and smectite clay minerals. Based on the analyses, 21 to 34 percent of the shale unit consists of clay minerals (Table 2).

Mineralogy for the Upper Injection Zone was evaluated using XRD to determine the bulk and clay mineralogy of core samples. The Upper Injection Zone consists of fluvial-deltaic sands, and is composed predominantly of quartz and feldspar minerals (Table 2). The amount of clay minerals varies from 9 to 44 percent, and they are mostly kaolinite, chlorite, and illite minerals.

Mineralogy for the internal barrier in the [REDACTED] was evaluated using FTIR and XRD to determine the bulk and clay mineralogy of core samples. The [REDACTED] consists of marine deposited claystone interbedded with siltstone, and the mineralogy identified by FTIR and XRD is typically dominated by quartz and feldspar minerals and layered illite and smectite clay minerals. Based on the analyses, 36 to 58 percent of the shale unit consists of clay minerals (Table 2).

Mineralogy for the Lower Injection Zone was evaluated using XRD to determine the bulk and clay mineralogy of core samples. The Lower Injection Zone consists of marine deposited sands, and is composed predominantly of quartz and feldspar minerals (Table 2). The amount of clay minerals varies from 8 to 24 percent, and they are mostly chlorite, illite and mica minerals.

2.4 Injectate Chemistry

For the geochemical modeling, two scenarios of different chemical compositions for the carbon dioxide injectate were developed (Table 3). The compositions were normalized to 100 percent 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 from the geochemical analysis because ethane gas is not in the model database. The normalized chemistry for Scenarios 1 and 2 was modeled for the CTV IV storage project.

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 its components in groundwater (Appelo and Postma, 2005). Mineral dissolution-precipitation reactions directly impact the aqueous chemistry. In general, as minerals dissolve, the concentrations in groundwater increase and when minerals precipitate, the 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 carbon dioxide injection. The mineral, gas, and aqueous phases were assumed to be in chemical equilibrium.

Based on the available injectate gas compositions, the ideal gas law and Raoult's Law were used to calculate the gas composition in moles. The initial and final pressures of 90.7 and 119.1 atmospheres (atm), respectively, were used to calculate the partial pressures of the injectate components for the upper injection zone. The initial and final pressures of 129.8 and 136.8 atm, respectively, were used to calculate the partial pressures of the injectate components for the Lower Injection Zone.

A reservoir temperature of 41°C was used for the upper injection zone and a reservoir temperature of 49°C was used for the lower injection 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, pressures, and temperatures 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. At the CTV IV site, the geologic formations are predominantly composed of 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.

3.2 Saturation Indices

Saturation indices (SIs) were calculated that represent whether a particular mineral (e.g., calcite) 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 changed 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 or FTIR 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

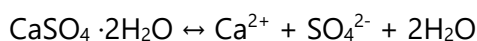
IAP = ion activity product

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:



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

Interpreting the results of the SI calculation is straightforward:

- SI > 0 indicates that mineral is supersaturated in solution and may precipitate onto aquifer matrix
- SI = 0 indicates that mineral is at chemical equilibrium with the water
- 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 for the upper and lower injection zones (Table 1) that were entered as received in ppm for elemental concentrations and standard units for pH.

In order to model the geochemistry of the clay minerals identified by XRD or FTIR for the Upper Injection Zone, an aluminum (Al) concentration was calculated in PHREEQC by equilibrating the provided water chemistry with the most abundant aluminosilicate clay mineral, chlorite at 41°C and 90.7 atm. The modeled aqueous aluminum concentration was used in subsequent modeling at 0.0006 ppm for the Upper Injection Zone. This concentration is reasonable for a sandstone aquifer at the neutral pH values in this zone.

For the Lower Injection Zone, in order to model the geochemistry of the clay minerals identified by XRD or FTIR, aluminum (Al), potassium (K), and phosphate (PO₄) concentrations were calculated in PHREEQC by equilibrating the provided water chemistry with the most abundant clay mineral, illite, and the phosphate mineral, hydroxylapatite at 49°C and 129.8 atm. The modeled aqueous concentrations were used in subsequent modeling at 0.60 ppm aluminum, 0.23 ppm potassium, and 0.04 ppm phosphate for the Lower Injection Zone. These concentrations are reasonable for a sandstone aquifer at the neutral pH values in this zone.

For input into PHREEQC model, the mineralogy of the upper and lower injection zones and of [REDACTED] (Table 2) were converted to moles per liter (mol/L) using porosity and bulk density values as follows:

- Upper Confining Zone: Porosity of 28.5 percent and 2.18 average bulk density
- Upper Injection Zone: Porosity of 31.4 percent and 2.13 average bulk density
- Lower Injection Zone: Porosity of 30.4 percent and 2.15 average bulk density
- Internal barrier: Porosity of 28.3 percent and 2.18 average bulk density

The converted values for mineralogy that were input into PHREEQC are in shown Table 4. When not initially present, the carbonate minerals calcite, dolomite, and siderite were included as equilibrium minerals in the model runs.

Average temperature provided for the upper injection zone is 41°C at the CTV IV site with an initial average pore volume pressure of 90.7 atm, which is expected to increase to 119.1 atm by project completion. The amount of carbon dioxide in 1 liter of gas at 90.7 atm and 41°C based on ideal gas law ($PV = nRT$) is 3.524 moles, and the amount of gas in 1 liter increases to 4.626 moles at 119.1 atm.

For the Lower Injection Zone, the average temperature provided is 49°C at the CTV IV site with an initial average pore volume pressure of 129.8 atm, which is expected to increase to 136.8 atm by project completion. The amount of carbon dioxide in 1 liter of gas at 129.8 atm and 49°C based on ideal gas law ($PV = nRT$) is 4.913 moles, and the amount of gas in 1 liter increases to 5.176 moles at 136.8 atm.

5. Geochemical Modeling Results and Discussion

Model results showing the changes in mineralogy designated as equilibrium phases in PHREEQC are presented for CTV IV in Table 5 for the Upper Injection Zone, Table 6 for [REDACTED], Table 7 for the Lower Injection Zone, and Table 8 for [REDACTED]. Model results are presented in Tables 9 and 10 for the water chemistry based on the equilibrium phases in the Upper and Lower Injection Zones, respectively. The modeling steps were as follows:

- Upper Injection Zone

- ◇ Upper Injection Zone: Use the upper injection zone groundwater sample and equilibrate with selected mineralogy data set for the Upper Injection Zone (Table 4) with Scenario 1 injectate chemistry at initial and final reservoir pressures
- ◇ [REDACTED] Use the model results for upper injection zone at final reservoir pressure and equilibrate with selected upper confining zone mineralogy data set (Table 4) with Scenario 1 injectate chemistry at final reservoir pressure
- ◇ [REDACTED] Use the model results for upper injection zone at final reservoir pressure and equilibrate with selected [REDACTED] mineralogy data set (Table 4) with Scenario 1 injectate chemistry at final reservoir pressure
- ◇ Repeat both steps using the Scenario 2 injectate chemistry
- Lower Injection Zone
 - ◇ Lower Injection Zone: Use the lower injection zone groundwater sample and equilibrate with selected mineralogy data set for the Lower Injection Zone (Table 4) with Scenario 1 injectate chemistry at initial and final reservoir pressures
 - ◇ [REDACTED] Use the model results for lower injection zone at final reservoir pressure and equilibrate with selected [REDACTED] mineralogy data set (Table 4) with Scenario 1 injectate chemistry at final reservoir pressure
 - ◇ Repeat both steps using the Scenario 2 injectate chemistry

Equilibrium geochemical modeling of the injection of carbon dioxide indicates that changes in mineralogy and aqueous chemistry are likely to occur, but overall, both 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 pyrite are present in relatively smaller amounts compared to the silicate minerals.

Although the model indicates minerals will dissolve and precipitate, the net change in mass is minimal. Based on molar mass for the Upper Injection Zone, there is a small increase of 0.6 to 1.3 percent in the Upper Injection Zone, a minimal decrease of 0.5 percent in the Upper Confining Zone, and a small increase of 0.6 percent in the internal barrier.

For the Lower Injection Zone, there is a small increase of 3 percent in the Lower Injection Zone and a small increase of 1.1 percent in the internal barrier. The amount of porosity in the Upper and Lower Injection Zones, the internal barrier, and the Upper Confining Zone are 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 in the groundwater.

Based on the modeling, the following reactions are expected to occur in the Upper Injection Zone (Table 5):

- Amphibole (modeled as tremolite mineral) is not stable and dissolves, releasing calcium, magnesium, and silica to solution.
- In Scenario 2, methane gas is slightly reactive with the minerals present in the formation.
- Quartz is relatively stable and tends to precipitate, removing silica and oxygen from solution.
- Illite and chlorite (modeled as chamosite-7A mineral) tend to dissolve, releasing iron, silica, and aluminum into solution.
- Pyrite tends to dissolve, releasing iron and sulfur into solution.

Based on the modeling, the following reactions are expected to occur in the Upper Confining Zone in [REDACTED] (Table 6):

- Anorthite is not stable and dissolves, releasing sodium, calcium, aluminum, and silica to solution.
- Methane gas is not stable, and dissolves into solution.
- Albite, K-feldspar, and kaolinite, are relatively stable and tend to precipitate in the models, removing calcium, sodium, silica, aluminum, iron, magnesium, oxygen, and potassium from solution.
- Smectite tends to dissolve in the models, and releases calcium, silica, aluminum, iron, magnesium, and oxygen into solution.

Based on the modeling, the following reactions are expected to occur in the Lower Injection Zone (Table 7):

- Apatite (modeled as the hydroxylapatite mineral) is stable with little dissolution.
- Quartz, K-feldspar, and kaolinite are relatively stable and tend to precipitate in the models, removing silica, aluminum, oxygen, and potassium from solution.

- Chlorite and illite are not stable and dissolve, releasing iron, magnesium, aluminum, potassium, and silica to solution.
- Calcite, dolomite, and siderite precipitate, removing calcium, magnesium, iron, and carbonate from solution.
- Pyrite is relatively stable, and dissolves slightly under Scenario 1.

Based on the modeling, the following reactions are expected to occur in the internal barrier of the [REDACTED] (Table 8):

- Quartz, albite, K-feldspar, and kaolinite are relatively stable and tend to precipitate in the models, removing sodium, silica, iron, aluminum, oxygen, and potassium from solution.
- Calcite, chlorite, and smectite are not stable and dissolve, releasing calcium, iron, magnesium, aluminum, potassium, sodium, carbonate, and silica to solution.
- Dolomite and siderite precipitate, removing calcium, magnesium, iron, and carbonate from solution.
- Pyrite is relatively stable, and dissolves slightly under Scenarios 1 and 2.

Based on the model results, the CO₂ gas in the injectate will form carbonate minerals, dissolve into solution, or remain in a gas phase. The formation of carbonate minerals can be an important mechanism to remove and immobilize carbon dioxide from solution through incorporation in the mineral phase. Several carbonate minerals like calcite, dolomite, and Dawsonite [NaAl(CO₃)(OH)₂] have positive SI values, indicating that these carbonate minerals are likely to become saturated in groundwater and precipitate during CO₂ injection.

Based on the equilibrium modeling, the aqueous chemistry results are provided in Table 9 (Upper Injection Zone) and Table 10 (Lower Injection Zone). Results indicate the following:

- Carbon dioxide will dissolve into solution, and is included in the 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 ion, sodium bicarbonate, calcium bicarbonate ion, magnesium bicarbonate ion, iron bicarbonate ion, calcium sulfate, and calcium carbonate.
- The pH values ranged from 6.6 to 7.3 at the CTV IV site.

- The pe remains negative for the Upper and Lower Injection Zones and for the internal barrier, indicating reducing conditions. For the upper barrier the pe becomes positive, indicating oxidizing conditions.
- The calcium in solution includes the following ions and complexes: calcium, calcium bicarbonate, calcium chloride, and calcium carbonate.

Based on the geochemical equilibrium modeling, the injection of carbon dioxide at the CTV IV site into the Upper and Lower Injection Zones does not cause significant reactions that will affect the injection or containment of the gas.

References

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Tables

Table 1. Baseline Geochemistry for the CTV IV Storage Project, Upper and Lower Injection Zones

Analyte	Concentration (ppm ^a)	
	Upper Injection Zone 6/4/1980	Lower Injection Zone 2/9/1990
Boron	72.2	—
Bicarbonate	1,449	1,635
Calcium	61.5	100
Chloride	6,867	7,120
Iron	8.2	—
Magnesium	8.9	14
Potassium	75	—
pH (s.u.)	8.32	7.97
Silica	12.8	—
Sodium	5,054	5,235
Sulfate	295	310
Total dissolved solids	13,889	14,415

^a Unless otherwise noted

ppm = Parts per million

— = Not determined

s.u. = Standard units

Table 2. Mineralogy of the CTV IV Storage Project

Depth (feet)	Test Type	Mineralogical Content (%)																		
		Quartz	Plagioclase	K-feldspar	Albite	Oligoclase	Andesine	Labrodorite	Calcite	Amphibole	Glauconite	Apatite	Pyrite	Sepiolite	Kaolinite	Chlorite	Illite and Mica	Smectite	Illite - Smectite and Mixed Layer Clays	Total Clay
4,442.5	FTIR	26.0	—	17.0	14.0	0.0	11.0	—	1.0	—	—	—	—	—	5.0	3.0	—	—	23.0	31.0
4,454.5	FTIR	30.0	—	15.0	8.0	15.0	6.0	—	0.0	—	—	—	—	—	2.0	6.0	—	—	18.0	26.0
4,476.5 ^a	FTIR	30.0	—	18.0	13.0	4.0	6.0	—	0.0	—	—	—	—	—	5.0	9.0	—	—	15.0	29.0
4,480.5	FTIR	26.0	—	20.0	13.0	0.0	10.0	—	0.0	—	—	—	—	—	0.0	6.0	—	—	25.0	31.0
4,498.5	FTIR	34.0	—	19.0	13.0	0.0	13.0	—	0.0	—	—	—	—	—	1.0	2.0	—	—	18.0	21.0
4,500.5	FTIR	28.0	—	19.0	0.0	19.0	0.0	—	0.0	—	—	—	—	—	0.0	12.0	—	—	22.0	34.0
4,425.5	XRD	35.0	25.0	15.0	—	—	—	—	—	—	—	—	—	—	5.0	5.0	5.0	10.0	—	25.0
4,622.0	XRD	42.2	18.7	10.7	—	—	—	—	0.0	—	—	—	0.6	—	9.4	3.4	4.5	—	10.5	27.8
4,905.0	XRD	34.9	20.7	10.2	—	—	—	—	0.7	—	—	—	1.1	—	15.2	5.8	5.8	—	5.5	32.3
5,247	XRD	27.8	—	16.2	34.0	—	0.0	0.0	—	0.0	—	0.8	0.0	0.0	3.6	17.0	0.0	1.1	—	21.7
5,249	XRD	17.0	—	32.7	6.5	—	0.0	0.0	—	0.0	—	—	0.0	0.0	34.9	0.0	8.4	0.5	—	43.8
6,400	XRD	40.3	—	17.1	0.0	—	3.6	29.2	—	0.2	—	—	0.0	0.0	5.2	4.0	0.4	0.0	—	9.6
6,466	XRD	36.3	—	12.6	0.2	—	0.0	36.6	—	0.6	—	—	0.7	0.0	2.7	5.4	5.0	0.0	—	13.0
6,532	XRD	34.2	—	24.1	0.0	—	31.0	0.0	—	1.1	—	—	0.5	—	2.9	2.0	4.2	—	—	9.1
6,598 ^b	XRD	33.9	—	22.0	0.0	—	34.5	0.0	—	0.2	—	—	0.2	0.0	3.6	5.4	0.1	0.0	—	9.2
8,828 ^c	FTIR	23.0	—	9.0	12.0	0.0	9.0	—	3.0	—	0.0	—	1.0	—	12.0	5.0	—	—	26.0	43.0
8,830	XRD	30.0	17.0	11.0	—	—	—	—	0.0	—	—	—	4.0	—	3.4	14.4	6.1	14.1	—	38.0
8,909	FTIR	20.0	—	13.0	10.0	0.0	10.0	—	0.0	—	2.0	—	2.0	—	5.0	3.0	—	—	35.0	43.0
8,937	FTIR	20.0	—	8.0	7.0	0.0	5.0	—	0.0	—	0.0	—	2.0	—	14.0	6.0	—	—	38.0	58.0
8,939	XRD	24.0	18.0	11.0	—	—	—	—	1.0	—	—	—	3.0	—	3.0	15.5	7.7	16.8	—	43.0
8,940	FTIR	23.0	—	12.0	14.0	0.0	15.0	—	0.0	—	0.0	—	0.0	—	4.0	5.0	—	—	27.0	36.0
8,942	FTIR	23.0	—	10.0	9.0	0.0	6.0	—	0.0	—	0.0	—	2.0	—	12.0	5.0	—	—	33.0	50.0
9,439	FTIR	20.0	—	9.0	7.0	0.0	7.0	—	0.0	—	0.0	—	1.0	—	0.0	5.0	—	—	51.0	56.0
9,441	FTIR	21.0	—	12.0	10.0	0.0	9.0	—	2.0	—	0.0	—	3.0	—	0.0	0.0	—	—	43.0	43.0
7,104	XRD	39.9	—	6.5	0.0	—	27.4	0.0	—	0.0	—	—	1.2	1.3	5.7	8.5	9.5	0.0	—	23.7
7,136	XRD	42.8	—	8.7	0.0	—	39.6	0.0	—	—	—	—	0.5	0.0	1.4	4.7	2.4	0.0	—	8.5
7,146 ^d	XRD	37.5	—	11.1	34.2	—	—	—	—	—	—	5.3	1.1	—	1.8	1.3	7.7	—	—	10.8

^a Most likely mineral composition for ██████████ selected for modeling

^b Most likely mineral composition for Upper Injection Zone selected for modeling

^c Most likely mineral composition for ██████████ selected for modeling

^d Most likely mineral composition for Lower Injection Zone selected for modeling

— = Not detected

Table 3. Estimated Compositions for Carbon Dioxide Injectate

Gas	Mass Fraction (original composition)	Mass Fraction (normalized model input)
<i>Injectate Scenario 1</i>		
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
<i>Injectate Scenario 2</i>		
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 IV Storage Project

PHREEQC Mineral	Chemical Formula	Molar Mass (g/mol)	[REDACTED]		Input for Upper Inj Zone ^b		[REDACTED]		Input for Lower Injection Zone ^d	
			%	mol/L	%	mol/L	%	mol/L	%	mol/L
Quartz	SiO ₂	60.08	30	38.19	33.9	38.34	23	29.53	37.5	44.10
K-Feldspar	KAlSi ₃ O ₈	278.33	18	4.95	22.0	5.37	9	2.49	11.1	2.82
Albite (includes Andesine)	NaAlSi ₃ O ₈	263.02	19	5.53	34.5	8.90	21	6.16	34.2	9.19
Anorthite (for Oligoclase)	Na _{0.8} Ca _{0.2} Al _{1.2} Si _{2.8} O ₈	265.42	4	1.15	—	—	0	0	—	—
Calcite	CaCO ₃	100.09	0	0	—	—	3	2.31	—	—
Tremolite (for Amphibole)	Ca ₂ Mg ₅ (Si ₈ O ₂₂)(OH) ₂	812.37	—	—	0.2	0.02	—	—	—	—
Hydroxylapatite (for Apatite)	Ca ₅ (OH)(PO ₄) ₃	509.12	—	—	—	—	—	—	5.3	0.74
Pyrite	FeS ₂	119.98	—	—	0.2	0.12	1	0.64	1.1	0.65
Kaolinite	Al ₂ Si ₂ O ₅ (OH) ₄	258.16	5	1.48	3.6	0.95	12	3.59	1.8	0.49
Chamosite-7A (for chlorite)	Fe ₂ Al ₂ SiO ₅ (OH) ₄	664.18	9	1.04	5.4	0.55	5	0.58	1.3	0.14
Illite	K _{0.6} Mg _{0.25} Al _{1.8} Al _{0.5} Si _{3.5} O ₁₀ (OH) ₂	389.34	—	—	0.1	0.02	—	—	7.7	1.40
Smectite	Ca _{0.02} Na _{0.15} K _{0.2} Fe _{0.29} Fe _{0.16} Mg _{0.9} Al _{1.25} Si _{3.75} ·12 H ₂ O	549.07	15	2.09	—	—	26	3.65	—	—

^a Mineral composition selected for [REDACTED] at 4476.5 feet depth with 28.5% average porosity and 2.18 average bulk density.

^b Mineral composition selected for Upper Injection Zone at 6598 feet depth with 31.4% average porosity and 2.13 average bulk density.

^c Mineral composition selected for [REDACTED] at 8828 feet depth with 28.3% average porosity and 2.18 average bulk density.

^d Mineral composition selected for Lower Injection Zone at 7146 feet depth with 30.4% average porosity and 2.15 average bulk density.

g/mol = Grams per mole

mol/L = Moles per liter

Table 5. Mineralogical Changes Based on Equilibrium Geochemical Modeling for Upper Injection Zone with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Sample	Injection Zone at 6,598 feet						Injection Zone at 6,598 feet					
Injection Chemistry	Scenario 1						Scenario 2					
Pressure (atm)	90.7			119.1			90.7			119.1		
Albite	8.90	6.84	-2.06	8.90	5.82	-3.08	8.90	6.81	-2.09	8.90	5.79	-3.11
CH ₄ (g)	—	—	—	—	—	—	0.004	0.001	-0.003	0.005	0.002	-0.003
CO ₂ (g)	3.49	0	-3.49	4.58	0	-4.58	3.52	0	-3.52	4.62	0	-4.62
Calcite	0	0	0	0	0	0	0	0	0	0	0	0
Chamosite-7A	0.55	0	-0.55	0.55	0	-0.55	0.55	0	-0.55	0.55	0	-0.55
Dolomite	0	0.04	0.04	0	0.04	0.04	0	0.04	0.04	0	0.04	0.04
H ₂ S(g)	0.00004	0	-0.00004	0.00005	0	-0.00005	0.001	0	-0.001	0.001	0	-0.001
Illite	0.02	0	-0.02	0.02	0	-0.02	0.02	0	-0.02	0.02	0	-0.02
K-Feldspar	5.37	5.38	0.01	5.37	5.38	0.01	5.37	5.38	0.01	5.37	5.38	0.01
Kaolinite	0.95	2.56	1.60	0.95	3.06	2.11	0.95	2.57	1.62	0.95	3.08	2.13
N ₂ (g)	0.04	0.04	-0.0001	0.05	0.05	-0.0001	—	—	—	—	—	—
Pyrite	0.12	0.12	0.00003	0.12	0.12	0.00004	0.12	0.12	0.002	0.12	0.12	0.002
Quartz	38.34	42.06	3.73	38.34	44.09	5.75	38.34	42.12	3.78	38.34	44.16	5.83
SO ₂ (g)	0.00007	0	-0.00007	0.00009	0	-0.00009	—	—	—	—	—	—
Siderite	0	1.11	1.11	0	1.11	1.11	0	1.10	1.10	0	1.10	1.10
Tremolite	0.02	0	-0.02	0.02	0	-0.02	0.02	0	-0.02	0.02	0	-0.02

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. Mineralogical Changes Based on Equilibrium Geochemical Modeling for [REDACTED] with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)					
	Initial	Final	Delta	Initial	Final	Delta
<i>Sample</i>	<i>Confining Zone at 4,476.5 feet</i>			<i>Confining Zone at 4,476.5 feet</i>		
<i>Injection Chemistry</i>	<i>Scenario 1</i>			<i>Scenario 2</i>		
<i>Pressure (atm)</i>	<i>119.1</i>			<i>119.1</i>		
Albite	5.53	5.99	0.47	5.53	5.98	0.46
Anorthite	1.15	0	-1.15	1.15	0	-1.15
CH ₄ (g)	—	—	—	0.005	0	-0.005
CO ₂ (g)	4.58	0	-4.58	4.62	0	-4.62
Calcite	0	0	0	0	0	0
Chamosite-7A	1.04	0	-1.04	1.04	0	-1.04
Dolomite	0	1.18	1.18	0	1.18	1.18
H ₂ S(g)	0.00005	0	-0.00005	0.001	0	-0.001
K-Feldspar	4.95	5.21	0.26	4.95	5.21	0.26
Kaolinite	1.48	4.12	2.64	1.48	4.13	2.65
N ₂ (g)	0.05	0.05	0.000004	—	—	—
Quartz	38.19	38.95	0.76	38.19	38.98	0.79
SO ₂ (g)	0.00009	0	-0.00009	—	—	—
Siderite	0	2.45	2.45	0	2.50	2.50
Smectite-low-Fe-Mg	2.09	0.79	-1.30	2.09	0.79	-1.30

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. Mineralogical Changes Based on Equilibrium Geochemical Modeling for Lower Injection Zone with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Sample	Injection Zone at 7,146 feet						Injection Zone at 7,146 feet					
Injection Chemistry	Scenario 1						Scenario 2					
Pressure (atm)	129.8			136.8			129.8			136.8		
Albite	9.19	5.86	-3.33	9.19	5.84	-3.35	9.19	5.86	-3.33	9.19	5.84	-3.35
CH ₄ (g)	—	—	—	—	—	—	0.005	0.002	-0.003	0.005	0.002	-0.003
CO ₂ (g)	4.86	0.63	-4.23	5.12	0.88	-4.25	4.91	0.70	-4.21	5.17	0.94	-4.23
Calcite	0	0.06	0.06	0	0.06	0.06	0	0.07	0.07	0	0.07	0.07
Chamosite-7A	0.14	0	-0.14	0.14	0	-0.14	0.14	0	-0.14	0.14	0	-0.14
Dolomite	0	0.35	0.35	0	0.35	0.35	0	0.35	0.35	0	0.35	0.35
H ₂ S(g)	0.00005	0.08	0.08	0.00005	0.08	0.08	0.001	0	-0.001	0.001	0	-0.001
Hydroxylapatite	0.74	0.65	-0.08	0.74	0.65	-0.08	0.74	0.65	-0.08	0.74	0.65	-0.08
Illite	1.40	0	-1.40	1.40	0	-1.40	1.40	0	-1.40	1.40	0	-1.40
K-Feldspar	2.82	3.65	0.83	2.82	3.65	0.83	2.82	3.65	0.83	2.82	3.65	0.83
Kaolinite	0.49	3.49	2.99	0.49	3.49	3.00	0.49	3.49	2.99	0.49	3.49	3.00
N ₂ (g)	0.05	0.05	-0.0001	0.05	0.05	-0.0001	—	—	—	—	—	—
Pyrite	0.65	0.60	-0.04	0.65	0.60	-0.05	0.65	0.65	0.002	0.65	0.65	0.002
Quartz	44.10	50.63	6.53	44.10	50.66	6.56	44.10	50.63	6.53	44.10	50.66	6.56
SO ₂ (g)	0.0001	0	-0.0001	0.0001	0	-0.0001	—	—	—	—	—	—
Siderite	0	0.32	0.32	0	0.32	0.32	0	0.27	0.27	0	0.27	0.27

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. Mineralogical Changes Based on Equilibrium Geochemical Modeling for [REDACTED] with Scenario 1 and Scenario 2 Injectates

Mineral	Mineralogical Content (mol/L)											
	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta	Initial	Final	Delta
Sample	Confining Zone at 8,828 feet			Confining Zone at 8,828 feet			Confining Zone at 8,828 feet			Confining Zone at 8,828 feet		
Reservoir	Upper Injection Zone			Upper Injection Zone			Lower Injection Zone			Lower Injection Zone		
Injection Chemistry	Scenario 1			Scenario 2			Scenario 1			Scenario 2		
Pressure (atm)	119.1			119.1			136.8			136.8		
Albite	6.16	8.86	2.70	6.16	8.83	2.67	6.16	8.33	2.17	6.16	8.29	2.13
CH ₄ (g)	—	—	—	0.005	0	−0.005	—	—	—	0.005	0	−0.005
CO ₂ (g)	4.58	0	−4.58	4.62	0	−4.62	5.12	0	−5.12	5.17	0	−5.17
Calcite	2.31	0	−2.31	2.31	0	−2.31	2.31	0	−2.31	2.31	0	−2.31
Chamosite-7A	0.58	0	−0.58	0.58	0	−0.58	0.58	0	−0.58	0.58	0	−0.58
Dolomite	0	2.39	2.39	0	2.39	2.39	0	2.39	2.39	0	2.39	2.39
H ₂ S(g)	0.00005	0	−0.00005	0.001	0	−0.001	0.00005	0	−0.00005	0.001	0	−0.001
K-Feldspar	2.95	3.68	0.73	2.95	3.68	0.73	2.95	3.68	0.73	2.95	3.68	0.73
Kaolinite	3.59	4.73	1.15	3.59	4.75	1.16	3.59	5.00	1.41	3.59	5.02	1.43
N ₂ (g)	0.05	0.05	−0.000003	—	—	—	0.05	0.05	−0.000003	—	—	—
Pyrite	0.64	0.60	−0.04	0.64	0.60	−0.04	0.64	0.60	−0.04	0.64	0.60	−0.04
Quartz	29.53	31.21	1.68	29.53	31.28	1.75	29.53	32.28	2.75	29.53	32.36	2.83
SO ₂ (g)	0.00009	0	−0.00009	—	—	—	0.0001	0	−0.0001	—	—	—
Siderite	0	2.85	2.85	0	2.84	2.84	0	2.85	2.85	0	2.84	2.84
Smectite-low-Fe-Mg	3.65	0	−3.65	3.65	0	−3.65	3.65	0	−3.65	3.65	0	−3.65

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 the Upper Injection Zone with Scenario 1 and Scenario 2 Injectates

Constituent	Concentration (mg/L ^a)							
Geologic Zone	Upper Injection Zone at 6,598 feet				Shale at 4,476.5 feet		at 8,828 feet	
Injection Chemistry	Scenario 1		Scenario 2		Scenario 1	Scenario 2	Scenario 1	Scenario 2
Pressure (atm)	90.7	119.1	90.7	119.1	119.1		119.1	
Al ³⁺	0.000660	0.000510	0.000655	0.000507	0.000504	0.000500	0.00127	0.00121
B ³⁺	73.2	73.2	73.2	73.2	73.2	73.2	73.2	73.2
TIC	102,323	150,338	103,908	152,363	140,304	142,152	118,387	122,612
Ca ²⁺	0.000322	0.000461	0.000324	0.000465	0.000464	0.000438	0.00000541	0.00000578
Cl ⁻	6,962	6,962	6,962	6,962	6,962	6,962	6,962	6,962
Fe ²⁺	1.35	1.71	1.36	1.72	11,572	8,958	0.661	0.691
K ⁺	98.9	126	99.6	127	116	118	48.7	50.9
Mg ²⁺	1,506	1,506	1,506	1,506	1,271	1,377	23,440	23,440
N ₂	7.81	7.64	—	—	7.40	—	7.80	—
Na ⁺	52,532	75,821	53,153	76,649	69,568	70,671	26,278	27,887
SO ₄ ²⁻	304	305	0.00740	0.00809	319	96.060	8,330	7,454
SiO ₂	5.11	4.95	5.10	4.94	4.75	4.75	5.27	5.25
TDS (sum)	163,815	235,147	165,709	237,687	230,197	230,413	183,533	188,485
pH (s.u.)	7.0	6.9	7.0	6.9	6.9	6.9	7.3	7.3
pe (unitless)	-3.3	-3.1	-3.9	-3.8	11	11	-3.5	-3.5

Italics indicate HS⁻ not SO₄²⁻

^a Unless otherwise noted

mg/L = Milligrams per liter

atm = Atmospheres

TDS = Total dissolved solids

s.u. = Standard units

Table 10. Modeled Equilibrium Aqueous Concentrations for the Lower Injection Zone with Scenario 1 and Scenario 2 Injectates

Constituent	Concentration (mg/L ^a)					
Geologic Zone	Lower Injection Zone at 7,146 feet				at 8,828 feet	
Injection Chemistry	Scenario 1		Scenario 2		Scenario 1	Scenario 2
Pressure (atm)	129.8	136.8	129.8	136.8	136.8	
Al ³⁺	0.000693	0.000691	0.000696	0.000694	0.00100	0.00099
TIC	139,732	140,216	140,832	141,360	132,206	135,727
Ca ²⁺	7.51	7.52	7.48	7.48	0.00002	0.00002
Cl ⁻	7,225	7,225	7,225	7,225	7,225	7,225
Fe ²⁺	2.12	2.12	2.12	2.12	1.18	1.20
K ⁺	196	196	195	195	111	112
Mg ²⁺	0.276	0.277	0.275	0.275	21,930	21,930
N ₂	7.05	7.05	—	—	7.24	—
Na ⁺	81,867	82,212	81,867	82,212	44,991	45,888
PO ₄ ³⁻	23,315	23,429	23,629	23,752	23,429	23,752
SO ₄ ²⁻	1,372	1,419	0.0350	0.0352	9,445	7,454
SiO ₂	6.30	6.30	6.31	6.31	6.58	6.58
TDS (sum)	253,730	254,720	253,763	254,760	239,352	242,095
pH (s.u.)	6.6	6.6	6.6	6.6	6.9	6.9
pe (unitless)	-2.8	-2.8	-3.5	-3.5	-3.1	-3.1

^a Unless otherwise noted

mg/L = Milligrams per liter

atm = Atmospheres

TDS = Total dissolved solids

s.u. = Standard units