Prepared for

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DRAFT –

Monitored Natural Attenuation Evaluation

Vermilion Power Plant

North Ash Pond (CCR Unit #910) and Old East Ash Pond (CCR Unit #911) Areas

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TABLE OF CONTENTS

TABLE OF CONTENTS (Continued)

LIST OF TABLES

LIST OF FIGURES

LIST OF APPENDICES

TABLE OF CONTENTS (Continued)

LIST OF ACRONYMS

AVS	acid volatile sulfides
CA	Corrective Action
CAA	Closure Alternatives Analysis
CAAA	Corrective Action Alternatives Analysis
CBR	Closure-by-Removal
CCR	Coal Combustion Residual
CIP	Closure-in-Place
CMA	Corrective Measures Assessment
COCs	Constituents of Concern
CSM	Conceptual Site Model
DMG	Dynegy Midwest Generation, LLC
EPRI	Electric Power Research Institute
GWPS	Groundwater Protection Standards
HCR	Hydrogeologic Site Characterization Report
I.A.C	Illinois Administrative Code
IAEA	International Atomic Energy Agency
IDNR	Illinois Department of Natural Resources
IEPA	Illinois Environmental Protection Agency
ITRC	Interstate Technology Regulatory Council
LGU	Lower Groundwater Unit
LTM	long-term monitoring
MGU	Middle Groundwater Unit
mg/kg	milligrams per kilogram
MNA	Monitored Natural Attenuation
N	normal
NAP	North Ash Pond
OEAP	Old East Ash Pond
OEPA	Ohio Environmental Protection Agency
ORP	Oxidation-Reduction Potential
PMP	Potential Migration Pathway
PRB	permeable reactive barriers
RCRA	Resources Conservation and Recovery Act
SEP	Sequential Extraction Procedure

TABLE OF CONTENTS (Continued)

SIs	Saturation Indices
TDS	Total Dissolved Solids
TOC	Total Organic Carbon
UCU	Upper Confining Unit
USEPA	United States Environmental Protection Agency
VPP	Vermillion Power Plant

1. EXECUTIVE SUMMARY

A monitored natural attenuation (MNA) evaluation was completed to provide input to the corrective measures assessment (CMA) and corrective action alternatives analysis (CAAA) for boron, lithium molybdenum, sulfate, and TDS in groundwater downgradient of the retired North Ash Pond/Old East Ash Pond (NAP/OEAP) impoundment system (the Site) located on Dynegy Midwest Generation, LLC's Vermilion Power Plant property near Oakwood Illinois. Multiple lines of evidence were considered as part of the MNA evaluation to provide information that can be used in the CMA/CAAA to assess whether selection of MNA (together with source control), as either a stand-alone remedial alternative for groundwater or groundwater remedy component.

Characterization of the aquifer solids and geochemical modeling were completed to identify likely chemical attenuation mechanisms for each constituent of concern (COC). Batch attenuation testing was completed to calculate Site-specific partition coefficients for each COC that were used in evaluations of attenuation rate and capacity. Batch desorption testing was also completed to assess the stability of the chemical attenuation mechanisms.

The MNA evaluation found that for all COCs some chemical attenuation is expected based on the results of site characterization and batch attenuation testing, but with greater chemical attenuation for lithium and molybdenum relative to boron and sulfate. The test results on these samples indicate that there is likely insufficient capacity in the downgradient aquifer system through chemical attenuation alone to attenuate groundwater concentrations of boron to below the groundwater protection standards (GWPS). Therefore, attenuation via both physical and chemical attenuation mechanisms would be required to achieve the GWPS and successfully demonstrate MNA of the COCs at the Site.

2. SITE BACKGROUND

2.1. Site Overview

This monitored natural attenuation (MNA) evaluation was completed to provide input to the corrective measures assessment (CMA) and corrective action alternatives analysis (CAAA) for potential groundwater exceedances downgradient of the North Ash Pond area (NAP; Illinois Environmental Protection Agency [IEPA] identification [ID] number [No.] W1838000002-01)/Old East Ash Pond area (OEAP; IEPA ID No. W1838000002-03) coal combustion residual (CCR) unit at the Vermilion Power Plant (VPP), which is owned by Dynegy Midwest Generation, LLC (DMG). The 37-acre NAP and 21-acre OEAP are inactive, unlined surface impoundments which overlap and have a separator berm constructed of ash for prior operational purposes. Thus, the NAP and OEAP areas have been treated as one CCR unit for the purposes of this report.

The NAP and OEAP impoundments, which are the subject of this evaluation, are located adjacent to each other in the northern portion of the VPP. The NAP is bordered to the north by fallow fields owned by the Illinois Department of Natural Resources (IDNR), to the east by the Middle Fork of the Vermilion River, to the south by the OEAP, and to the west by steep bluffs that include the Illinois Department of Conservation-designated Orchid Hill Natural Heritage Landmark. The Orchid Hill National Heritage Landmark is partially within the VPP property boundary but is administered by IDNR. The OEAP is bordered to the north and northeast by the Middle Fork, to the southeast, south, and west by steep bluffs, and to the northwest by the NAP. The NAP and OEAP are both located on terraces adjacent to the Middle Fork, which is bordered to the east and west by steep bluffs. The combined area including the NAP and OEAP will herein after be referred to as the Site.

A Hydrogeologic Site Characterization Report (HCR) detailing the Site and regional geology and hydrogeology was included in the Operating Permit submittal for the NAP/OEAP (Ramboll, 2021a). The Middle Groundwater Unit (MGU), which is continuous below the NAP/OEAP, was designated as the uppermost aquifer (UA). The Lower Groundwater Unit (LGU), which is separated from the MGU by a low-permeability confining unit, was identified as a Potential Migration Pathway (PMP).

2.2. Groundwater Monitoring

A groundwater monitoring network was proposed in accordance with Illinois Administrative Code (I.A.C) Title 35 Section 845.630 to monitor groundwater quality which passes the waste boundary as part of the Operating Permit Application to IEPA for the NAP/OEAP. The proposed groundwater monitoring network is described in the Groundwater Monitoring Plan (Ramboll, 2021b) and shown on Figure 1.

35 I.A.C § Part 845 parameters were monitored in the MGU (*i.e.,* uppermost aquifer) and LGU (*i.e.,* PMP) monitoring wells at the NAP and OEAP areas as part of the groundwater quality investigations performed between 1988 and 2018. A preliminary review of groundwater quality at wells in the groundwater monitoring network was completed using the methodology proposed in the Statistical Analysis Plan (Appendix A to the Groundwater Monitoring Plan, Ramboll 2021b), which has not been reviewed or approved by IEPA at the time of this report. The following potential exceedances above the groundwater protection standard (GWPS) were identified (Ramboll, 2021c):

- Boron;
- Lithium;
- Molybdenum;
- pH;
- Sulfate; and,
- Total dissolved solids (TDS).

The potential pH exceedance of the lower limit was not attributable to the NAP or OEAP (Ramboll, 2021d). Thus, boron, lithium, molybdenum, sulfate, and TDS were identified as constituents of concern (COCs) for the NAP/OEAP areas.

3. MNA EVALUATION

The NAP/OEAP MNA evaluation was completed following the tiered guidance established by the USEPA (USEPA, 2015) and ITRC (ITRC, 2010). In a tiered MNA evalution, multiple lines of evidence are considered to evaluate whether selection of MNA as a stand-alone groundwater remedial alternative, or a groundwater remedy component, will adequately protect human health and potential ecological receptors by reducing groundwater concentrations to below the GWPS in an appropriate time frame. The results of the tiered evaluation are summarized below.

3.1. Tier I Analysis - Initial Considerations and Source Control

Three objectives were identified for Tier I of the MNA evaluation. The first objective is to identify whether MNA should be eliminated from consideration as a groundwater remedial alternative based on the conceptual site model (CSM), as discussed in Section 3.1.1. The second objective of the Tier I analysis is to evaluate if attenuation of the COCs is likely to occur under Site conditions, as discussed in Sections 3.1.2 and 3.1.3.

The third objective of the Tier I analysis is to evaluate if the plume is stable or receding. Because source control measures have not yet been completed, the plume stability analysis could not be completed at this time. However, groundwater fate and transport modeling was completed to predict the effect of source control measures on downgradient groundwater concentrations. The fate and transport model indicates that the concentrations of COCs are expected to decline following removal of source materials (Ramboll, 2021d). The plume stability analysis would be completed as part of the long-term monitoring program following completion of source control measures (Section 3.5).

3.1.1. Tier I Analysis – Initial Considerations

The first aspect of the Tier I analysis is to develop an understanding of the CSM to evaluate whether MNA should be eliminated from further consideration.

A review of previously collected groundwater data identified potential exceedances of the site COCs. As discussed in Section 2.2, those COCs include boron, lithium, molybdenum, sulfate, and TDS. Additional wells were installed in March 2021 to delineate the extent of the groundwater COCs to the extent feasible. The location of groundwater monitoring wells which are proposed as part of the Site groundwater

monitoring network are provided in Figure 1. Key well (and soil boring) locations used in the MNA evaluation include:

- Well 03R, which is downgradient of the NAP and screened in the LGU;
- Well 07R, which is downgradient of the OEAP and is screened in the MGU;
- Well 08R, which is downgradient of the NAP and screened in the MGU:
- Well 36, which is downgradient of both the OEAP and NAP and is screened in the MGU; and,
- Well 43, which is a background monitoring location.

All source control activities being considered will largely eliminate future loading of COC mass to groundwater when completed. However, groundwater impacts from prior releases might remain following source control activities. Given that there were not any complete exposure pathways with unacceptable risk identified in Gradient (2021) and the groundwater model output (Ramboll, 2021d) predicts future concentrations are expected to be lower following source control than those currently detected, further evaluation of MNA as a potential groundwater corrective action for these impacts was deemed warranted.

3.1.2. Tier I and Tier II Analysis – Constituent Attenuation Mechanisms

For the second objective of the Tier I analysis, an initial characterization was completed to identify if attenuation might occur for each COC. Where attenuation might occur, the Tier II analysis was initiated, with the objective of characterizing the predominant attenuation mechanisms.

To support the Tier I analysis, geochemical modeling using groundwater concentration data at downgradient wells 03R, 07R, 08R, and 36 and an approximation of aquifer solids was completed to evaluate the potential for adsorption and precipitation attenuation mechanisms. Well 03R is screened in the LGU; the other three wells of interest are screened within the Middle Groundwater Unit MGU, which is also the designated UA. The average of the first six background monitoring events at wells 03R, 08R and 36 (completed March – July 2021) and the first four background monitoring events at well

07R (completed May – July 2021) were used for the groundwater composition inputs (Table 2).

The groundwater modeling to support the Tier I analysis was completed using the commercial software package Geochemist's Workbench (v12.0.4). Thermodynamic database r.8 (Lawrence Livermore) and the FeOH+ surface complexation database were used. The r.8 thermodynamic database was modified to incorporate the thermodynamic data for powellite ($CaMoO_4$) precipitation, which was available in the Visual MINTEQ database. The model calculates the percentage of each basis species adsorbed via surface complexation reactions with iron oxyhydroxides. It was conservatively assumed that 0.1 weight percent hydrous ferric oxide grain coatings were present in the aquifer solids. The model input for the available iron is lower than the total iron concentrations detected in the solid phase (Table 3). The remaining aquifer solids were conservatively assumed to be inert for this initial modeling. Therefore, additional potential attenuation mechanisms, including adsorption to clay minerals, organic matter, aluminium and magnesium oxides, were not evaluated in the model. Adsorption complexes for molybdenum and lithium were unavailable or not considered representative of site conditions (Gustafsson, 2003; Brinza et al., 2019); thus, adsorption modeling results are only available for boron and sulfate. Reaction kinetics were not included in the preliminary geochemical models. The model outputs are provided in Appendix A and discussed in Sections 3.1.2.1 through 3.1.2.4.

Following the Tier I evaluation, field investigations were completed in April 2021 to collect additional site materials for use in the Tier II MNA evaluation. These materials were analyzed to evaluate if they indicated active removal of the COCs from groundwater via chemical attenuation processes. Soil borings were advanced adjacent to the 03R/08R and 02/07R well pairs (Figure 1) to collect aquifer solids from locations downgradient of the NAP and OEAP, respectively. An additional soil boring was advanced adjacent to the 43/44 well pair to collect aquifer solids from a background location. The soil borings were logged for geologic description; the soil boring logs are provided in Appendix B. Groundwater samples were collected from existing wells 07R, 08R, and 43 for use in the MNA evaluation.

Soil samples from the interval co-located with the well screen elevation at each location were placed in double sealed bags and air was removed to the maximum extent feasible. The soil was shipped to SiREM Laboratories (Guelph, ON) for sample storage at 4˚C. A

portion of each sample was submitted to SGS Analytical (Guelph, ON) for initial characterization. The analyses included:

- Total metals via USEPA Method 200.8. Results are provided in Table 3.
- Total organic carbon (TOC) via SM 5310C. Results are provided in Table 3.
- Acid volatile sulfides (AVS) via analysis of generated hydrogen sulfide following extraction of the soil with 1 normal (N) hydrochloric acid (HCl). AVS analysis was completed by PRIMA Environmental of El Dorado Hills, CA. Results are provided in Table 3.
- X-Ray diffraction (XRD) via Rietvelt refinement. Results are provided in Table 4.

An additional sample of composited material from each boring location was submitted to Eurofins TestAmerica (Knoxville, TN) for sequential extraction procedure (SEP). SEP testing can provide insight into the attenuation mechanism, capacity, and reversibility under specific conditions. Results of the SEP analysis are provided in Table 5.

The results of the initial characterization found that the elemental composition (Table 3) and mineral composition (Table 4) was generally consistent at both locations sampled in the MGU. Further, the mineral composition of the MGU was generally comparable to the composition of the LGU. One notable difference was the detection of pyrite (FeS_2) within the LGU sample (Table 4). The preliminary assessment regarding attenuation mechanism for each COC based on the characterization data are provided below.

3.1.2.1. Boron

The total boron concentrations in the downgradient MGU aquifer solids (samples "SB-21-02/07R-12-14'" and "SB-21-03R/08R-13-15'") were both higher (12 and 17 mg/kg, respectively) than the total boron concentration detected in the background sample collected from adjacent to well 43 (6 mg/kg; Table 3). The higher total boron concentrations at the downgradient locations indicate some attenuation may be occurring. The boron concentrations in the downgradient LGU aquifer solids were comparable to background (Table 3).

The SEP results for boron were all below the detection limit for the first six extraction steps[1], precluding any insights into attenuation mechanism from this test (Table 5). Geochemical modeling predicts that boron will largely be present as the neutral $B(OH)_3$ species. Geochemical modeling also predicts that 3.8-4.5% of the boron in the groundwater system would be attenuated via surface complexation reactions with iron oxyhydroxides (Appendix A). Additionally, boron is known to be slightly attenuated via interactions with clay minerals and calcite (Goldberg, 1997); the XRD results identified the presence of a number of clay minerals and calcite at all downgradient locations (Table 4).

Thus, chemical attenuation of boron is possible at locations downgradient of the OEAP and NAP, and batch attenuation tests using Site-specific materials were completed as described in Section 3.1.3 to calculate a Site-specific boron partition coefficient.

3.1.2.2. Lithium

The total lithium concentrations in all upgradient and downgradient aquifer solids samples were similar (Table 3), indicating that lithium is not readily attenuated to a detectable degree at the site. These results are further supported by the similarity between the upgradient and downgradient SEP results, in which greater lithium concentrations were not associated with any of the exchangeable fractions (Table 5). While slightly higher lithium concentrations were associated with the sulfide fraction in the SEP results (Table 5), lithium does not readily form sulfide minerals.

The aqueous speciation results found that more than 99% of the lithium present in solution is predicted to be present as Li^+ (Appendix A). Thus, any lithium attenuation is likely to occur via interaction with cation exchange sites in the organic or clay fraction (Eckstein et. al, 1970). As noted in Section 3.2.1.1, clays were identified within the aquifer solids downgradient of the OEAP and NAP within both the MGU and LGU (Table 4). Thus, batch attenuation tests using Site-specific materials were completed as described in Section 3.1.3 to calculate a Site-specific partition coefficient for lithium.

[1] Boron is not reported for the residual fraction of the SEP analysis, as boric acid is one of the solutions used in the leaching mixture.

3.1.2.3. Molybdenum

The MGU aquifer solids sample collected downgradient of the OEAP had a total molybdenum concentration of 16 mg/kg, which is higher than the total molybdenum detected in the sample at the background location (5 mg/kg; Table 3). A similar increase was not detected in the samples collected downgradient of the NAP (SB-21-03R/08R) nor any of the samples in the LGU. These findings are reflected in the SEP results, where an order of magnitude higher amount of molybdenum was associated with both the amorphous and crystalline iron and manganese oxide phases downgradient of the OEAP when compared to the background location (Table 5).

According to the geochemical model, the molybdate oxyanion (MoO_4^-) is the predominant aqueous molybdenum species downgradient of the OEAP and NAP (Appendix A). Adsorption of the molybdate oxyanion to iron and manganese oxides, including amorphous iron oxides, is well understood and documented in literature (Smedley and Kinniburgh, 2017; Goldberg et al, 1996a). The geochemical model also predicts precipitation of iron oxides under current conditions downgradient of the OEAP and NAP; these oxides could serve as sorbing surfaces. Unfortunately, reliable modeling databases for molybdenum adsorption to iron oxides are not widely available (Gustafsson, 2003; Brinza et al., 2019) and data could not be generated to predict the precent of molybdenum attenuated via adsorption.

In addition to saturation of iron oxides, the mineral powellite ($CaMoO_4$) is predicted to precipitate at well 07R (saturation index [SI][2] = 0.19), which is downgradient of the OEAP (Appendix A). Powellite is predicted to be marginally undersaturated, and there is not predicted to precipitate as a new mineral, at the other monitoring locations of interest (SIs between -0.45 and -0.72), likely due to the slightly lower aqueous molybdenum and calcium concentrations at those locations (Table 2). Precipitation of the mineral powelllite provides an additional mechanism for attenuation of molybdenum at the site.

The geochemical conditions at the four downgradient wells selected for the evaluation are reducing. Under these conditions, interactions between molybdenum and sulfur-

[2] The calculated saturation index is the log of the ratio of the ion activity product (IAP) and solubility product constant (K_{sp}). The K_{sp} is a value which represents idealized conditions for mineral equilibrium, whereas the IAP is calculated using observed concentrations in groundwater. Saturation indices greater than -0.2 indicate potential equilibrium or supersaturation (precipitation) with respect to the mineral.

containing species, including the generation of thiomolybdates is possible (Fruend et al., 2016). Both molybdates and thiomolybdates can be adsorbed to oxides and clays. Additionally, molybdates or thiomolybdates may be adsorbed to pyrite or substituted into amorphous Fe-Mo-S structures under reducing conditions. The presence of detectable pyrite within the LGU (Table 4) indicates that either sorption onto or inclusion within pyritic minerals is a potential additional route for molybdenum attenuation at the site, even at locations where pyrite may be below the XRD detection limit (i.e., the MGU).

Thus, chemical attenuation of molybdenum via interactions with oxide minerals and various sulfur-containing species is feasible. Additional attenuation may occur via precipitation of powellite depending on aqueous molybdenum and calcium concentrations. Batch attenuation tests using Site-specific materials were completed as described in Section 3.1.3 to calculate a Site-specific molybdenum partition coefficient.

3.1.2.4. Sulfate and TDS

As illustrated in the Piper diagram provided in Figure 2, the anion composition of select wells downgradient of the OEAP and NAP is dominated by presence of sulfate. Thus, TDS concentrations are likely to be predominantly influenced by the contribution of sulfate and a reduction in sulfate concentrations will result in lower TDS concentrations as well.

The geochemical model predicts between 13.1 and 31.7% of the sulfate present in groundwater would be attenuated via surface complexation reactions with iron oxyhydroxides (Appendix A). Additional attenuation might occur via precipitation of sulfides. Samples collected from the LGU had detectable concentrations of aqueous sulfide (Table 3) and pyrite (FeS_2), a reduced iron sulfide mineral, was detected via XRD (Table 4). Similar conditions may be present but undetected in the limited samples from the MGU. Thus, batch attenuation tests using Site-specific materials were completed as described in Section 3.1.3 to calculate a Site-specific partition coefficient for sulfate.

3.1.3. Batch Attenuation Testing

Batch attenuation testing was performed to further evaluate the Tier I/II findings that each COC undergoes chemical attenuation, as predicted by the geochemical modeling and Site characterization data analysis discussed in Section 3.1.2. As part of the batch attenuation testing, Site-specific partition coefficients were developed for each COC. The Site-

specific partition coefficients represent the relative propensity for the COC to be associated with the solid versus the aqueous phase.

Four separate tests were conducted, as outlined in Table 6, to calculate the Site-specific partition coefficient for each COC under varying conditions. Each test used well 08R groundwater, which was selected to represent CCR-impacted groundwater downgradient of the NAP at the Site, and homogenized aquifer solids from background location well 43, which represent unimpacted material with the maximum amount of potential attenuation capacity. The average concentration of key constituents in groundwater at 08R over the first six background monitoring events is provided in Table 5. Given the similarities in the aquifer solids in the MGU and LGU (Table 3 and Table 4), it was assumed that the experimental design was reflective of conditions in both the MGU and LGU across the Site.

The 08R groundwater was spiked in each test to achieve the starting target concentrations on Day 0 listed in Table 6. No amendments were spiked during the fourth test to evaluate how boron and lithium, which were predicted to be poorly attenuated, interacted with the aquifer solids without interference from other amended constituents. The spiked 08R groundwater was then mixed with the aquifer solids at five different solid-to-liquid ratios provided in Table 6. Approximately 100 mL of groundwater was added to each batch reactor with the mass of aquifer solids adjusted to achieve the target ratios.

All batch attenuation tests were conducted for seven days. During that time, the microcosms were agitated once daily at room temperature (~22 °C) so the soil and groundwater remained well mixed. After 7 days of contact time, an aliquot of the free liquid was collected and filtered through a 0.45 µm filter prior to analysis for dissolved concentrations of COCs and iron. Additionally, the pH and ORP were measured at Day 0 and Day 7 for each batch reactor.

An initial sample of the stock solution for each experimental design was collected on Day 0, and a control sample (only 08R groundwater with no aquifer solids) was collected on Day 7 after tumbling in polypropylene bottleware to evaluate any loss to interactions with the bottleware or ambient conditions. Duplicates were constructed for each microcosm, including the control samples.

The pH values remained relatively constant for each amendment tested at varying soil:water ratios (Table 7). Although the attenuation isotherms were prepared under anaerobic conditions, the ORP values were variable, with lower ORP values consistently

detected in the microsms with greater soil:water ratios. These trends are attributed primarily to higher organic matter content in microcosms containing more soil, which would drive microbial reactions and shift the geochemical environment to more anaerobic conditions. The lower ORP may have affected the stability of iron oxides in the system through reductive dissolution, as greater concentrations of aqueous iron were detected at the higher soil:water ratios.

Data obtained from the tests were used to construct 5-point attenuation isotherms for the constituents of interest. Mathematical fitting was used to calculate the attenuation distribution coefficients (K_d), assuming linear adsorption. The linear adsorption equation was used:

$$q_e = K_d \times C_e \quad \text{Eq. 1}$$

where q_e is the mass of constituent adsorbed to the solid phase at equilibrium, C_e is the remaining aqueous constituent concentration at equilibrium, and K_d is the linear sorption coefficient. Linear graphs for the adsorption isotherms are provided in Figure 3. Some of the data showed a deviation from a linear trend, and so were also fitted using a non-linear isotherm. A common non-linear Freundlich equation was used:

$$q_e = K_F(C_e)^{1/n} \quad \text{Eq. 2}$$

where q_e is the mass of constituent adsorbed to the solid phase at equilibrium, C_e is the remaining aqueous constituent concentration at equilibrium, K_F is the Freundlich distribution coefficient, and $1/n$ is a non-linearity constant. The adsorption data were plotted as log-transformed values to perform the non-linear isotherm fitting using the linearized Freundlich equation:

$$log(q_e) = \log(K_F) + (1/n)\log(C_e) \quad \text{Eq. 3}$$

The log-transformed Freundlich plots are provided in Figure 4. The calculated linear and Freundlich adsorption distribution coefficients (K_d and K_{dF}, respectively) and $1/n$ values are shown in Table 8. The selected coefficient for each parameter is bolded and shaded blue.

A comparison of the Site-specific partition coefficient to literature values is discussed for each COC in Sections 3.1.3.1 through 3.1.3.4.

3.1.3.1. Boron

The K_{dF} value of 0.43 L/kg for boron derived from the sulfate-amended batch attenuation test was selected as most representative of Site conditions. The Freundlich transformation paired with the sulfate amended dataset resulted in the highest correlation coefficient (R^2=0.85), indicating a good fit to the model data. Previous studies found that boron adsorption often exhibits non-linear behavior (EPRI, 2005), further supporting the selection of the Freundlich transformation. The Freundlich coefficient (1/n) derived from the sulfate amended dataset (4.15) indicates highly non-linear behavior. A K_d or K_{dF} value was not generated for boron using the results of the unamended dataset because a slightly negative correlation was calculated, indicating no relationship between boron concentration and adsorption under those conditions.

The selected K_{dF} value is comparable to those observed at other sites with a sand, loamy sand, or sandy loam composition, which had a mean K_{dF} value of 1.149 ± 0.692 L/kg (EPRI, 2005). Additionally, the calculated K_{dF} value, which is indicative of high mobility in the groundwater system, is consistent with the geochemical modeling which predicted limited boron adsorption to iron oxide surfaces (Appendix B).

3.1.3.2. Lithium

The K_d value of 8.53 L/kg for lithium derived from the sulfate-amended batch attenuation test was selected as the most representative of Site conditions. The linear transformation paired with the sulfate-amended dataset resulted in the highest correlation coefficient (R^2=0.81), indicating a good fit to the experimental data. The selection of a linear partition coefficient is appropriate because lithium was not amended in any of the experimental designs, indicating that adsorption sites are likely not satuated at even the lowest soil:water ratio. The sulfate amended batch results were selected as the K_d value given the higher correlation coefficient and selection of the same dataset for boron.

Literature K_d values for lithium are highly variable, ranging from 0.02-0.25 L/kg in a sandy aquifer (EPRI, 2006) to 190-370 L/kg in organic rich sediments and clays (Sheppard et al, 2009). The XRD analysis of the MGU soils 03R/08R identified 68% sand, with contributions of clays and carbonates (Table 4). Thus, the selected K_d value is at the lower end of this range, as would be expected for a sandier aquifer with detectable concentrations of clays. As discussed in Section 3.1.3.2, lithium is likely associated with the clay fraction of the solid phase via cation exchange processes.

3.1.3.3. Molybdenum

The K_{dF} value of 109 L/kg for molybdenum derived from the molybdenum and sulfate-amended batch attenuation test was selected as the most representative of Site conditions. Both the linear and Freundlich transformation of the molybdenum and sulfate-amended batch attenuation test had correlation coefficients (R^2) of 0.97, indicating a good fit to the experimental data. However, the Freundlich transformation was selected given that it was more representative of reported partition coefficients for lithologies with relatively low amounts of organics, such as sands or lower-organic fraction clays (Sheppard et al, 2009; IAEA, 2004).

The higher correlation coefficients for the molybdenum and sulfate-amended dataset compared to molybdenum alone indicates a relationship between the two constituents. Freundlich behavior has been detected for molybdenum and sulfate solutions in the past, with high concentrations of sulfate reducing molybdate adsorption (Wu et al., 2002).

3.1.3.4. Sulfate

The K_d value of 9.97 L/kg for sulfate derived from the sulfate-amended batch attenuation test was selected as the most representative of Site conditions. The linear transformation paired with the molybdenum and sulfate-amended dataset resulted in the highest correlation coefficient (R^2=0.74), indicating a good fit to the experimental data. This was the same set of data selected for the molybdenum Site-specific partition coefficient, further indicating a relationship between sulfate and molybdenum attenuation behavior. The Site-specific partition coefficients were not calculated for the other three experimental designs (molybdenum amendment, sulfate amendment, no amendment) because slightly negative slopes were calculated, indicating no relationship between sulfate concentration and attenuation under those conditions.

The calculated sulfate K_d value is much lower than the K_{dF} calculated for molybdenum, which is consistent with literature that says molybdate is much more readily adsorbed to aluminum oxides than sulfate (Wu et. al, 2002). Sulfate is more readily adsorbed at lower pH values, with a detected maximum around pH 4.0 (Courchesne and Hendershot, 1988). The pH values recorded in the test microcosm were slightly acidic (pH 6.6 – 6.8) but below the observed pH values in the field, indicating the potential for diminished sulfate chemical attenuation capacity under Site conditions.

3.2. Tier II Analysis – Rate of Attenuation Assessment

Two objectives were identified for Tier II of the MNA analysis. The first objective, presented in Section 3.1.2, is to identify potential chemical attenuation mechanisms for each COC based on Site conditions. The second objective for Tier II of the MNA evaluation is to establish whether the rates for the identified attenuation mechanisms are sufficient for attaining the GWPS.

Because source control measures have not yet been completed, calculation of attenuation rates using declining groundwater concentrations could not be completed at this time. Instead, a fate and transport model was generated by Ramboll (2021d) to predict how groundwater concentrations will decline following completion of source control measures. The fate and transport modeling report prepared by Ramboll (2021d) was included in the Construction Permit application to which this MNA report is attached.

In addition to the groundwater fate and transport modeling completed by Ramboll (2021d), which predicts declines in aqueous concentrations due to physical attenuation mechanisms, the results of the batch attenuation testing described in Section 3.1.3. were used to understand short-term rates of the chemical attenuation mechanisms. USEPA guidance (2007) indicates that adsorption reaction kinetics are fast relative to typical advective groundwater flow velocities. These results were confirmed by the batch tests site-specific materials because partitioning to aquifer solids was detected during the relatively short timeframe of the test (one week).

3.3. Tier III – System Capacity and Attenuation Stability Assessment

Two objectives were identified for Tier III of the MNA analysis. The first objective is to investigate the Site-specific attenuation capacity for the COCs, as discussed in Section 3.3.1. The second objective of the Tier III analysis is evaluate the stability of the predominant attenuation mechanisms under future geochemical conditions that should return to background conditions. The batch desorption testing completed to support the attenuation stability assessment is discussed in Section 3.3.2. While variable redox conditions were evaluated, the pH conditions of the microcosms were not adjusted, as the pH at background locations is comparable to current downgradient pH conditions.

3.3.1. System Capacity

A review of the system chemical attenuation capacity was completed to understand if sufficient capacity is available in the downgradient aquifer to attenuate the constituents of concern via chemical attenuation processes (i.e., adsorption and precipitation). The Site-specific partition coefficients calculated from the batch attenuation tests (Section 3.1.3) were used to estimate the chemical attenuation capacity of the aquifer downgradient of the Site.

Based on the linearity of the batch attenuation isotherm results, the maximum chemical attenuation capacity (q_{max}) for each COC was not identified. However, because the batch attenuation tests were performed at COC concentrations which are comparable to or exceed the groundwater COC concentrations at the Site, a conservative estimate of the chemical attenuation capacity of the aquifer was calculated using the maximum COC concentrations used during the tests. The selected groundwater concentrations and calculated chemical attenuation capacity of the MGU associated with each respective groundwater concentration are provided in Table 9.

The estimated chemical attenuation capacity was compared to the estimated mass flux of each COC to evaluate whether sufficient capacity is available to reduce groundwater concentrations to below the GWPS. The potential total mass flux for boron was calculated using the estimated mass of boron migrating toward the Vermilion River predicted by the groundwater fate and transport model prepared by Ramboll (2021d). The total estimated discharged mass includes both historical and future post-closure periods, assuming a 40-year timeframe since the beginning of groundwater impacts and selection of Closure Scenario #1 (removal with on-site disposal and 10 years of operation of a groundwater collection trench) as described in the groundwater modeling report (Ramboll, 2021d). Closure Scenario #1 was selected as the most conservative approach for these calculations based on the modeled mass flux. The modeled mass flux included boron in both the MGU, upper confining unit (UCU), and LGU; thus, comparison to the capacity into the MGU alone further resulted in a conservative approach.

Modeled mass flux data was only available for boron, so the mass flux of the other COCs was based on the correlation of each COC to the concentration and flux of boron. The historical mass flux of each COC from the CCR unit to groundwater was estimated using the respective ratios of the average concentrations of lithium, molybdenum, or sulfate in leachate wells ND3 and OED1 to the average concentration of boron in those same wells.

The estimated chemical attenuation capacity is greater than the predicted total mass flux for lithium, sulfate, and molybdenum (Table 9), suggesting that sufficient capacity is available to reduce groundwater concentrations for these COCs. Further decreases in the concentration of these COCs are predicted due to physical attenuation, as described in the groundwater fate and transport model (Ramboll, 2021d). This physical attenuation is of particular importance for boron, which is not readily attenuated and where the calculated chemical attenuation capacity appears to be exhausted (Table 9).

Thus, the attenuation capacity testing and groundwater fate and transport modeling calculations found that there is sufficient combined chemical and physical attenuation capacity in the downgradient aquifer to attenuate the concentration of COCs to below the GWPS.

3.3.2. Batch Desorption Tests

Batch desorption testing was completed to evaluate the stability of the chemical attenuation mechanisms under variable redox conditions. Aquifer solids collected from background well 43 were used to construct the microcosms, which were considered representative of both the MGU and LGU. Based on the results of the attenuation tests, varying soil:water ratios and groundwater from well 08R were used to construct the reactors for each constituent. Amendments were added to produce attenuated COCs on the background aquifer solids. For the boron and sulfate tests, the groundwater was amended with sulfate only. For lithium and molybdenum, the groundwater was amended with both molybdenum and sulfate, as that experimental design provided the best correlation in the batch attenuation tests.

A summary of the experimental design is provided in Table 10. The batch reactors were allowed to tumble for seven days following construction to provide time for COC attenuation, after which the aqueous phase was decanted and replaced with unamended groundwater from location 43, which is representative of unimpacted background groundwater that will return beneath and downgradient of the CCR units in the future. While the aquifer solids were loaded with COC mass for seven days, COCs are more likely to be attenuated under site conditions where the reaction time is even longer and the material can become more tightly associated with the aquifer solids.

Following the addition of unimpacted groundwater, the batch reactors were exposed to three different redox conditions to constrain how future geochemical changes may affect attenuation reversibility following closure activities. Strongly reducing (hydrogen

sparged) and strongly oxidizing (oxygen sparged) conditions were generated by respectively amending the reactors with 5 mL of hydrogen gas and 5 mL of oxygen (O_2) gas daily. A set of unamended microcosms was also run to represent ambient conditions.

All batch desorption tests were conducted for seven days. During that time, the microcosms were agitated once daily at room temperature (~22 °C) to ensure the soil and groundwater remained well mixed. After 7 days of contact time, an aliquot of the free liquid was collected and filtered through a 0.45 µm filter prior to analysis for dissolved concentrations of COCs and iron. Additionally, the pH and ORP in each batch reactor were measured on Day 0 and Day 7.

The results of the batch desorption tests are summarized in Table 10 and Figure 5. A summary of the results and the implications for attenuation stability is discussed for each COC in Sections 3.3.2.1 through 3.3.2.4.

3.3.2.1. Boron

Of the total boron mass which sorbed to the sediments during the initial phase of the desorption tests, approximately 70% was subsequently released under all three redox conditions. These results indicate that, even if redox conditions change following closure activities at the OEAP and NAP areas, the extent of boron adsorption will remain relatively consistent but is not stable. The lack of correlation between boron desorption and dissolved iron concentrations (Table 10) indicates that boron is more likely attenuated via interaction with the clay, calcite, or organic fractions than iron oxides. Regardless of attenuation mechanism, physical attenuation is expected to contribute more to declining boron groundwater concentrations than chemical interactions.

3.3.2.2. Lithium

The mass of lithium desorbed varied between 25% and 32% for all three treatments, indicating that desorption is only slightly affected by variations in redox conditions (Table 10). This coincides with the prediction that the primary mechanism of lithium attenuation is via cation exchange with clays or the organic fraction in soils. These results indicate that, even if redox conditions change following closure activities at the OEAP and NAP areas, the desorption of lithium will be relatively limited. Instead, displacement of lithium from cation exchange sites following significant changes in the pH or ionic strength of recharge water may be a more significant driver of lithium desorption.

However, pH and ionic strength are expected to be generally stable, thus desorption is not anticipated and attenuation of lithium is more stable than boron.

3.3.2.3. Molybdenum

The extent of molybdenum desorption averaged 8.1% across the three redox treatments, with the greatest desorption under ambient conditions (8.7%) and the lowest under reducing conditions (7.7%). Molybdenum was the least readily desorbed of the constituents of concern (Table 10; Figure 5). The relatively low extent of desorption indicate high sorption affinity between molybdenum and the soil matrix, which is consistent with the relatively high Site-specific partition coefficient that was calculated for molybdenum compared to the other COCs. Further, the consistently low desorption indicate that molybdenum associated with the soil solids at the Site will remain largely immobilized, indicating that chemical attenuation represents a significant mechanism for natural molybdenum attenuation. The lack of correlation between molybdenum desorption and dissolved iron concentrations (Table 10) indicates that adsorption to iron oxides is not a primary attenuation mechanism for molybdenum. Thus, chemical attenuation via interaction with sulfur species or as precipitation of powellite is expected to be the more significant molybdenum attenuation mechanism.

3.3.2.4. Sulfate

Sulfate was readily desorbed across all three redox conditions, with the greatest desorption occurring under oxidizing conditions (94.6%; Table 10). These results indicate that the irreversible sulfate retention capacity of the soils is low regardless of redox conditions. Thus, physical attenuation is expected to contribute more to declining sulfate groundwater concentrations than chemical attenuation.

3.4. Geochemical Conceptual Site Model

The results of the Tiers I through III analyses were combined to develop a geochemical CSM for attenuation of each constituent at the site, as summarized below:

- Under Site conditions, boron is expected to be present as the neutral $B(OH)_3$ species. Because the majority of boron in groundwater is neutral, boron is only slightly attenuated via chemical interaction with the aquifer solids. This attenuation likely occurs through interactions with the clay minerals, calcite or organic materials; however, some interaction with iron oxides is also predicted.

Boron attenuation at the Site is highly reversible and while chemical attenuation will likely result in some decline in groundwater concentrations, physical attenuation is more likely to contribute to concentration reductions.

- Under Site conditions, lithium is expected to be present as the monovalent cation Li^+ species. Thus, any lithium attenuation is likely to occur via interaction with cation exchange sites in the organic or clay fraction. This attenuation is moderately reversible and likely to be dependent on pH. While chemical attenuation will likely result in some decline in groundwater concentrations, physical attenuation will also contribute to concentration reductions.

- Under Site conditions, molybdenum is expected to be more strongly attenuated via interaction with aquifer solid compared to boron and lithium. While SEP results indicate that molybdenum is attenuated via interaction with iron or manganese oxides, testing found that the dissolution of iron oxides did not result in greater desorption rates of molybdenum. Desorption tests resulted in very limited reversal of attenuation. Thus, molybdenum is likely well-attenuated via interaction with sulfur species or as precipitation of powellite. Molybendum concentrations in groundwater will decline from both physical and chemical attenuation mechanisms.

- Under Site conditions, sulfate is only slightly attenuated via chemical interaction with aquifer solids. Some sulfate may be attenuated via precipitation of sulfides, which were identified in the LGU. Additional sulfate attenuation may occur through interaction with iron oxides or clay minerals. Sulfate chemical attenuation is highly reversible; thus, physical attenuation is more likely to contribute to reductions in groundwater concentrations.

3.5. Tier IV Analysis – Long-Term Monitoring and Remedy Evaluation

If MNA is selected as a component of the groundwater corrective action, then a long-term monitoring (LTM) plan and contingency plan will be developed as part of Tier IV of the MNA evaluation. The LTM plan is required to provide data to evaluate the performance of the MNA remedy and the progress of the natural attenuation processes at the Site, particularly following completion of Site closure activities.

Tier IV of the MNA evaluation also calls for a consideration of the contingency plan if the observed declines in groundwater concentrations of COCs are not consistent with the

groundwater fate and transport model predictions. Alternatively, the contingency plan may need to be considered if Site conditions which are identified as key for MNA performance are no longer present. The contingency plan may specify a technology that is different from MNA or it may call for modifications to the selected MNA remedy depending on observed changes in Site conditions or performance.

4. SUMMARY

A tiered MNA evaluation was completed to assess if Site conditions are favorable for the implementation of MNA as a groundwater corrective measure in combination with aggressive source control measures. The evaluation found that for all COCs, some chemical attenuation is expected based on the results of site characterization and batch attenuation testing efforts. Significantly greater chemical attenuation is predicted for lithium and molybdenum relative to boron and sulfate based on the results of the desorption testing efforts. There is insufficient capacity in the aquifer system through chemical attenuation alone to attenuate the predicted future contaminant mass flux of boron, so MNA of the COCs will be achieved through a combination of both physical and chemical mechanisms. If MNA is selected as a component of the groundwater corrective action, then a LTM plan and contingency plan will be developed.

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TABLES

Table 1: Surface Water Analytical Results
Vermilion Power Plant

Analyte	SW-1-20210607	DUP-SW-1-20210607	SW-2-20210607	SW-3-20210709	SW-4-20210709	SW-5-20210709
Description	**Upstream**	**Upstream**	**Site-Adjacent**	**Site-Adjacent**	**Site-Adjacent**	**Downstream**
Boron	0.053	0.054	0.055	0.055	0.058	0.069
Calcium	76	80	76	72	71	72
Iron	0.14	0.12	0.20	0.49	0.51	0.5
Lithium	0.0047	0.0050	0.0050	0.007	0.0056	0.0056
Magnesium	34	35	34	30	30	30
Manganese	0.0098	0.0098	0.0094	0.022	0.022	0.021
Molybdenum	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01
Potassium	1.2	1.3	1.2	2.4	2.3	2.3
Sodium	8.1	8.7	8.0	7.6	7.3	7.6
Chloride	25	26	26	18	18	19
Sulfate	38	39	29	25	26	26
Dissolved Organic Carbon	2.7	2.7	2.6	3.7	3.1	3.2
Alkalinity	230	220	230	240	230	240
Total Dissolved Solids	380	280	350	340	420	270
Phosphorus as PO_4	0.36	0.20	0.19	0.4	0.43	0.4
Sulfide	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0

Notes:
All results shown in milligrams per liter (mg/L)
< - compound not detected, the associated value is the detection limit
DUP = duplicate sample

Table 2: Tier I Geochemical Model Inputs
Vermilion Power Plant

Parameter	Units	03R	07R	08R	36
Description		Downgradient LGU	Downgradient MGU	Downgradient MGU	Downgradient MGU
Alkalinity (as bicarbonate)	mg/L	312	70.3	222	198
Boron	mg/L	19.3	36.3	27.2	13.9
Calcium	mg/L	166	930	234	350
Chloride	mg/L	29.8	6.25	5.67	24.33
Iron	mg/L	4.99	1.59	0.16	5.09
Lithium	mg/L	0.0033	0.57	0.26	0.19
Magnesium	mg/L	79.2	90.3	33.8	72.1
Manganese	mg/L	0.0829	4.14	0.25	1.77
Molybdenum	mg/L	0.33	0.53	0.25	0.14
Potassium	mg/L	2.7	60.2	13.6	14.4
Sodium	mg/L	83.3	51.6	36.8	47.4
Sulfate	mg/L	498	1945	520	1003
pH	SU	7.28	7.32	7.19	7.13
ORP	mV	-138	-103	-50	-96
Eh	V	0.062	0.10	0.15	0.10
Temp	°C	12.6	13.1	11.8	11.9

Notes:

While aqueuos iron concentrations are shown, iron was input in the Spec8 system via the Fe(OH)3 sorbing surface.

Eh values were calculated by converting field ORP measurements from mV to V and adding 0.2 V to account for the difference between an Ag/AgCl electrode used in the field and the standard hydrogen electrode.

Porosity was set to 0.33

Bulk Volume was set to 1000 cm^3

Inert Volume was set to 669 cm^3

°C - degrees Celsius

mg/L - milligrams per liter

mV - millivolts

SU - standard units

V - volts

MGU - middle groundwater unit

LGU - lower groundwater uit

Table 3: Solid Phase Total Constituent Concentrations
Vermilion Power Plant

Boring ID		SB-21-02R/07R	SB-21-02R/07R	SB-21-03R/08R	SB-21-03R/08R	SB-21-43
Sample Depth (ft bgs)		12-14'	30-31'	13-15'	31-32'	62.75-63'
Description	Unit	Downgradient MGU	Downgradient LGU	Downgradient MGU	Downgradient LGU	Background
Arsenic	mg/kg	5.4	5.1	3.2	9.7	2.5
Boron	mg/kg	12	5	17	5	6
Lithium	mg/kg	5	7	4	6	8
Molybdenum	mg/kg	16	0.5	0.6	0.8	0.5
Sulfide	wt %	< 0.04	0.13	< 0.04	0.25	0.04
Sulfate	mg/kg	2063	305	111	244	93
Sulfur	wt %	0.26	0.19	0.016	0.32	0.055
AVS	mg/kg	<0.18	1.5	<0.19	0.69	2.4
Iron	mg/kg	13000	11000	5900	11000	10000
TOC	wt %	0.538	0.541	0.272	0.574	0.711

Notes:

Values represent total metals in the solid phase.

mg/kg - milligrams per kilogram

wt% - weight percent

< - compound not detected, the associated value is the detection limit

TOC - total organic carbon

AVS - acid volatile sulfide

ft bgs - feet below ground surface

MGU - middle groundwater unit

LGU - lower groundwater unit

Table 4: X-Ray Diffraction Results
Vermilion Power Plant

Site Material		SB-21-02R/07R	SB-21-02R/07R	SB-21-03R/08R	SB-21-03R/08R	SB-21-43
Sample Depth (ft bgs)		12-14'	30-31'	13-15'	31-32'	62.75-63'
Mineral	Mineral Composition	Downgradient MGU	Downgradient LGU	Downgradient MGU	Downgradient LGU	Background
Quartz	SiO_2	51.1	56	68.1	49.9	58.4
Calcite	$CaCO_3$	0.4	3.6	2.2	5.2	3
Albite	$NaAlSi_3O_8$	8.6	7.7	8.7	10.9	9.8
Muscovite	$KAl_2(AlSi_3O_{10})(OH)_2$	3.1	6.2	2.5	1.9	7.6
Dolomite	$CaMg(CO_3)_2$	15.4	10.7	3.8	14.8	6.1
Microcline	$KAlSi_3O_8$	5.5	6.8	8.4	5.9	7.3
Ankerite	$CaFe(CO_3)_2$	5.1	4.9	1.1	4.4	2.4
Biotite	$K(Mg,Fe)_3(AlSi_3O_{10})(OH)_2$	2	1.9	1.6	1.9	1.7
Chlorite	$(Fe,(Mg,Mn)_5,Al)(Si_3Al)O_{10}(OH)_8$	1.1	0.9	0.7	1	1.1
Diopside	$CaMgSi_2O_6$	1.5	1.2	1.5	1.9	1.2
Actinolite	$Ca_2(Mg,Fe)_5Si_8O_{22}(OH)_2$	1.5	-	1.4	2	1.2
Gypsum	$CaSO_4{\cdot}2H2O$	4.7	-	-	-	-
Pyrite	FeS_2	-	0.1	-	0.2	0

Notes:

All samples represented as weight percent normalized to a sum of 100%. A quantity of amorphous material has not been determined.

Zero values indicate that the mineral was included in the refinement, but the calculated concentration is below a measureable value.

-- - not detected

XRD - X-ray diffraction

Table 5: Sequential Extraction Procedure Results
Vermilion Power Plant

Analyte	SEP Fraction	SB-21-43	SB-21-08R	SB-21-07R
		Background	Downgradient NAP	Downgradient OEAP
Boron	Exchangeable	< 48	< 47	< 47
	Carbonate	< 36	< 35	< 35
	Amorphous Fe/Mn Oxides	< 12	< 12	< 12
	Crystalline Fe/Mn Oxides	< 12	< 12	< 12
	Organic-Bound	< 180	< 180	< 180
	Sulfides	< 12	< 12	< 12
Lithium	Exchangeable	< 12	< 12	< 12
	Carbonate	< 8.9	< 8.8	< 8.9
	Amorphous Fe/Mn Oxides	0.18	0.23	0.20
	Crystalline Fe/Mn Oxides	2.00	1.20	1.30
	Organic-Bound	14.00	9.90	13.00
	Sulfides	3.20	3.70	5.20
	Residual	5.30	3.20	7.70
Molybdenum	Exchangeable	< 9.5	< 9.4	0.68
	Carbonate	< 7.1	< 7.0	< 7.1
	Amorphous Fe/Mn Oxides	0.12	0.16	1.70
	Crystalline Fe/Mn Oxides	< 2.4	0.13	2.00
	Organic-Bound	< 36	< 35	< 35
	Sulfides	< 2.4	0.18	0.43
	Residual	< 2.4	< 2.3	0.26

Notes:
All results are reported in mg of constituent/kg of total sample mass
< - compound not detected, the associated value is the detection limit
SEP = sequential extraction procedure
Sulfate data is unavailable using SEP analysis.
Boron data is unavailable for the 'residual' fraction of the SEP analysis because it is the extraction reagent.
Composited sample for both the MGU and LGU at each downgradient location was analyzed.

Table 6: Batch Attenuation Test Design
Vermilion Power Plant

Isotherm	Amendment	Target Concentration (mg/L)	Soil:Water Ratio (grams soil:grams water)				
			Test #1	Test #2	Test #3	Test #4	Test #5
Mo	$Na_2MoO_4 \cdot 2H_2O$	Mo = 0.9	1:0.75	1:1.3	1:6.0	1:11.8	1:29.2
Mo + SO_4	$Na_2MoO_4 \cdot 2H_2O + Na_2SO_4$	Mo = 0.9; SO_4^{2-} = 1200	1:0.75	1:1.3	1:5.9	1:12.0	1:28.8
SO_4	Na_2SO_4	SO_4^{2-} = 1200	1:0.75	1:1.3	1:6.0	1:11.4	1:29.6
Unamended	--	--	1:0.75	1:1.4	1:6.0	1:11.8	1:28.9

Notes:
The 'unamended' dataset was prepared using groundwater from well 08R only.
The soil:water ratio was calculated assuming the groundwater had a specific gravity of 1.0.

Table 7: Batch Attenuation Test Aqueous Phase Analytical Results

Vermilion Power Plant

Amendment	Soil:Water Ratio	Molybdenum	Boron	Lithium	Iron	Sulfate	pH	ORP
		mg/L	mg/L	mg/L	mg/L	mg/L	SU	mV
Molybdenum	GW Only	0.80	39.53	0.35	0.02	847	6.76	148.0
	1:0.5	0.08	24.70	0.04	2.01	649	6.88	22.5
	1:1	0.12	31.30	0.10	2.30	728	6.83	-6.0
	1.5:1	0.41	36.95	0.24	1.21	704	6.84	56.5
	1:10	0.69	33.05	0.22	0.44	573	6.83	88.5
	1:20	0.77	33.40	0.28	0.09	576	6.87	136.0
Molybdenum and Sulfate	GW Only	0.82	41.35	0.35	0.03	1,271	6.77	127.0
	1:0.5	0.09	26.20	0.05	2.21	915	6.87	18.0
	1:1	0.16	31.00	0.09	2.00	1,099	6.76	116.5
	1.5:1	0.43	36.75	0.19	0.01	1,097	6.80	118.5
	1:10	0.55	38.30	0.27	0.01	1,193	6.76	90.0
	1:20	0.67	38.30	0.26	0.01	1,261	6.74	123.5
Sulfate	GW Only	0.46	41.20	0.34	0.02	1,023	6.62	140.5
	1:0.5	0.06	27.10	0.06	3.10	919	6.86	34.5
	1:1	0.10	31.05	0.09	2.32	1,033	6.78	63.5
	1.5:1	0.27	37.00	0.22	0.07	1,056	6.74	142.0
	1:10	0.35	38.95	0.25	0.02	955	6.70	120.5
	1:20	0.36	39.75	0.29	0.01	966	6.65	159.5
Unamended	GW Only	0.47	45.48	0.26	0.04	705	6.62	140.5
	1:0.5	0.09	42.95	0.08	1.23	624	6.83	26.5
	1:1	0.05	34.90	0.03	1.80	630	6.73	34.5
	1.5:1	0.27	49.15	0.19	1.01	692	6.70	95.5
	1:10	0.33	49.95	0.23	0.32	655	6.69	126.0
	1:20	0.38	49.20	0.24	0.21	706	6.73	159.5

Notes:
The average values of two replicates are provided.
Mo, B, Li, Fe, SO4 are filtered analytical results.
'GW Only' represents the control samples.
mg/L - milligrams per liter
SU - standard units
mV - millivolts

Table 8: Site-Specific Partition Coefficient Values

Geosyntec Consultants, Inc.

Vermilion Power Plant

Analyte		Values	Mo	Mo + SO_4	SO_4	None
Molybdenum	**Linear**	R^2	0.51	0.97	0.70	0.8
		K_d (L/kg)	1.89	6.73	8.44	13.0
	Freundlich	R^2	0.79	0.97	0.83	0.75
		1/n	0.377	0.750	0.748	0.754
		K_{dF} (L/kg)	81.7	**109**	109	126
Boron	**Linear**	R^2	0.09	0.48	0.65	--
		K_d (L/kg)	6.78	4.46	5.90	--
	Freundlich	R^2	0.22	0.69	0.85	--
		1/n	3.542	3.504	4.150	--
		K_{dF} (L/kg)	1.37	1.11	**0.43**	--
Lithium	**Linear**	R^2	0.71	0.62	0.81	0.67
		K_d (L/kg)	10.9	9.39	**8.53**	17.3
	Freundlich	R^2	0.60	0.60	0.74	0.57
		1/n	0.129	0.127	0.123	0.167
		K_{dF} (L/kg)	147	145	144	156
Sulfate	**Linear**	R^2	--	0.74	--	--
		K_d (L/kg)	--	**9.97**	--	--
	Freundlich	R^2	--	0.70	--	--
		1/n	--	6.780	--	--
		K_{dF} (L/kg)	--	1.24E-06	--	--

Notes:

1/n - slope of linearized Freundlich isotherm

K_d - linear adsorption distribution coefficient

K_{dF} - Freundlich adsorption distribution coefficient

L/kg - liters per kilogram

R^2 - linear correlation coefficient

Linearized Freundlich isotherm did not fit unamended Boron data

Sulfate K_d and K_{dF} values were not calculated for the Mo, SO_4, and unamended tests because negative trends were observed.

Blue-shaded and bolded results were selected as most representative for each constituent of concern and were used in further analyses as appropriate.

Table 9: Chemical Attenuation Capacity Calculations
Vermilion Power Plant

MGU Aquifer Parameter Assumptions	Value
Length of Aquifer [m]	30.5
Width of Aquifer [m]	756
Thickness of MGU [m]	2.99
Porosity [-]	0.27
Sediment Bulk Density [kg/m^3]	1656

	Constituent	Boron:COC Ratio	Site-Specific Partition Coefficient	Aqueous Concentration	Estimated Chemical Attenuation Capacity	Estimated Mass Release	% of Estimated Capacity
			L/kg	mg/L	kg	kg	%
Historical	Boron	1:1	0.43	44	1,576	1,527	96.9%
Post-Closure						919	58.3%
Total						**2,446**	**155.2%**
Historical	Lithium	1:0.018	8.53	0.38	270	27.5	10.2%
Post-Closure						16.6	6.1%
Total						**44.1**	**16.3%**
Historical	Molybdenum	1:0.007	109	0.9	8,170	10.1	0.12%
Post-Closure						6.1	0.07%
Total						**16.1**	**0.20%**
Historical	Sulfate	1:39.1	9.97	1200	996,382	59,726	6.0%
Post-Closure						35,931	3.6%
Total						**95,657**	**9.6%**

Assumptions:

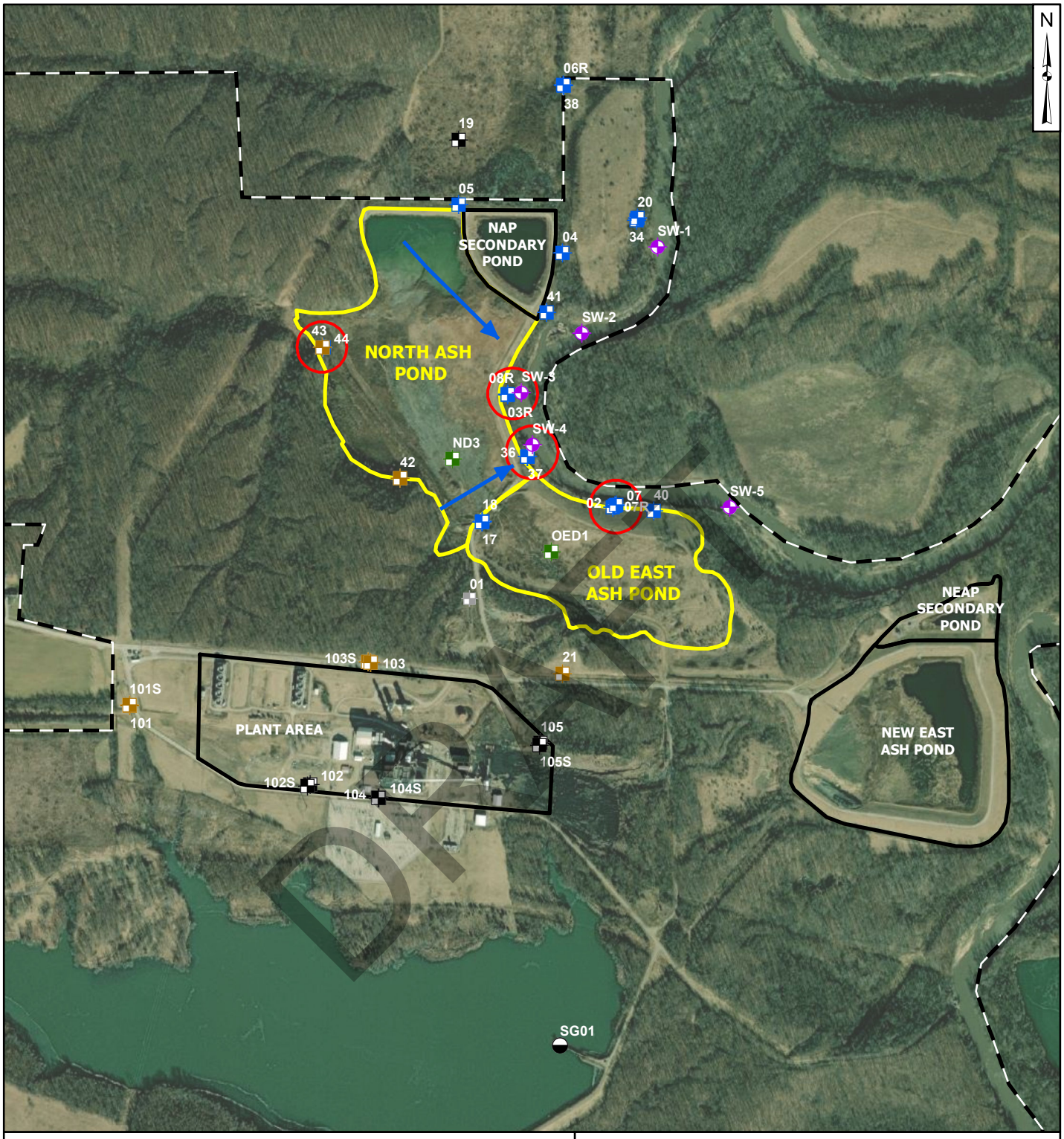
- The aqueous concentration represents the value used in the batch attenuation testing experimental design for the selected Site-specific partition coefficient (Table 8) and was used in the calculation of the estimated chemical attenuation capacity.
- Mass released for boron was generated from the groundwater fate and transport model (Ramboll, 2021d) and was corrected for the other COCs using the ratio of B:COCs in leachate wells ND3 and OED1
- Aquifer length was selected based on the 2020 *Human Health and Ecological Risk Assessment* (Gradient).
- Sediment bulk density and aquifer thickness were generated from the 2021 *Hydrogeologic Site Characterization Report* (Ramboll).
- Porosity and aquifer length were generated from the groundwater fate and transport model (Ramboll, 2021d).

Table 10: Batch Desorption Test Design and Results
Vermilion Power Plant

COC	Amendment	Target Concentration (mg/L)	Soil:Water Ratio	Redox Conditions	Initial Mass Adsorbed (mg)	Remaining Mass Adsorbed (mg)	% Mass Desorbed (%)	Dissolved Iron (mg/L)	pH (SU)	ORP (mV)
B	Na_2SO_4	SO_4^{2-} = 1200	1:6	Reducing	0.67	0.2	69.6	4.6	7.00	-60
				Ambient		0.21	68.2	3.5	7.00	-79
				Oxidizing		0.18	73.6	<0.007	7.50	183
Li	Na_2SO_4	Mo = 0.9; SO_4^{2-} = 1200	1:6	Reducing	0.016	0.011	30.6	4.6	7.00	-60
				Ambient		0.012	25.1	3.5	7.00	-79
				Oxidizing		0.011	31.9	<0.007	7.50	183
Mo	$Na_2MoO_4 \cdot 2H_2O + Na_2SO_4$	Mo = 0.9; SO_4^{2-} = 1200	1:1.3	Reducing	0.077	0.071	8.7	3.4	7.01	-55
				Ambient		0.071	8.0	4.4	7.01	-71
				Oxidizing		0.071	7.7	0.004	7.64	156
SO_4	$Na_2MoO_4 \cdot 2H_2O + Na_2SO_4$	SO_4^{2-} = 1200	1:1.3	Reducing	34.35	2.26	93.4	3.4	7.01	-55
				Ambient		1.87	94.6	4.4	7.01	-71
				Oxidizing		3.48	89.9	0.004	7.64	156

Notes:
< - compound not detected, the associated value is the detection limit
Dissolved iron concentrations reported following completion of the desorption step.
The average results for two duplicate trials are shown.
COC - Constituent of concern
mg/L - milligrams per liter
SU - standard units
mV - millivolts

FIGURES



Legend

- Compliance Well
- Background Well
- Source Sample Location
- Monitoring Well
- Monitoring Well to be Abandoned
- Staff Gauge
- Surface Water Sample Locations
- MNA Sampling Locations
- Groundwater Flow Direction
- Part 845 Regulated Unit (Subject Unit)
- Site Feature
- Property Boundary

1,000 500 0 1,000 Feet

Notes

- Figure originally from "Groundwater Monitoring Plan - North Ash Pond and Old East Ash Pond, Vermilion Power Plant." (Ramboll, 2021).
- Locations of interest for the MNA evaluation are circled in red.
- Surface water sampling locations are approximate.

Monitoring Well and Surface Water Sampling Location Map

Vermilion Power Plant
Oakwood, Illinois

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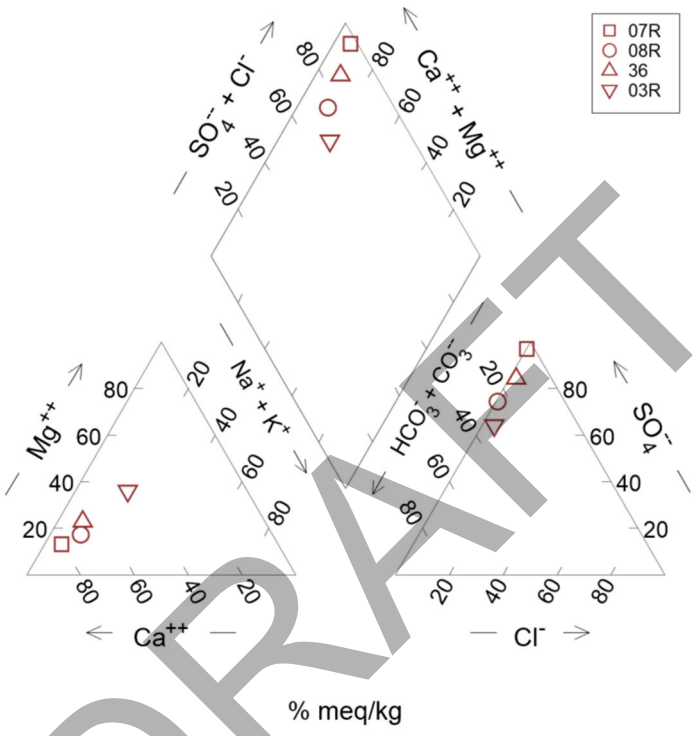
Ann Arbor, Michigan | 2021/10/27

Figure 1

Y:\Company\Projects_post_2014\CHE8404_VPS_Closure_RIA_Sprt\500 - Technical\572 - MNA and GSI Evaluation\GIS\MXDs\20211026_MW and SW Sampling Location Map.mxd. ASoltero. 10/27/2021. CHE8404B.



Notes: Results are shown in relative percentage of milliequivalents per kilogram (% meq/kg). Average results for the first six background monitoring events at wells 03R, 08R, and 36 and the first four background monitoring events at 07R were used for groundwater composition.

Piper Diagram – Downgradient Groundwater Conditions

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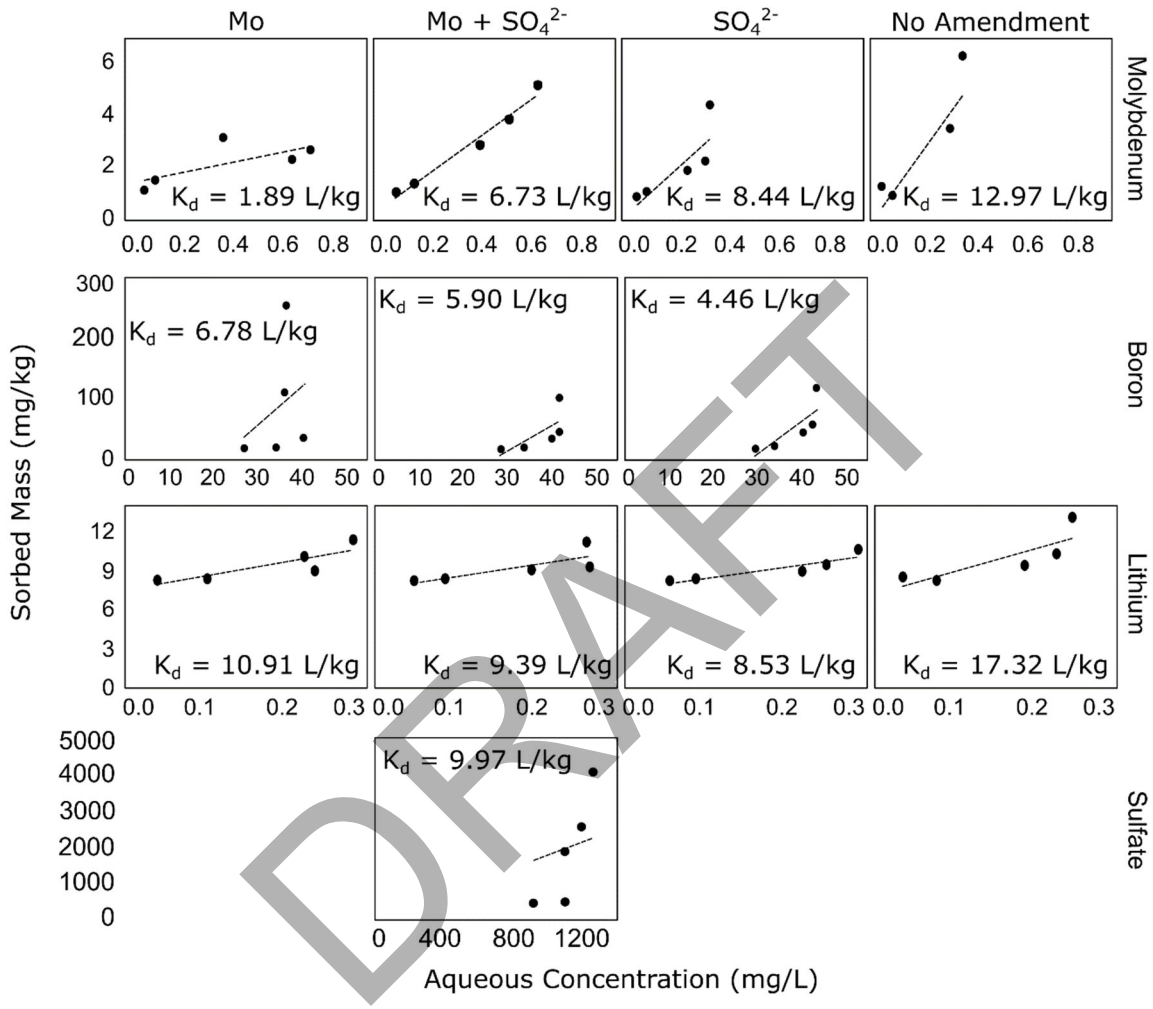
8-Sept-2021

Figure **2**



Notes: K_d values were not generated for boron in the unamended dataset or sulfate in the Mo, SO_4, or unamended datasets because negative slopes were observed. 'No Amendment' was prepared using groundwater from well 08R.

Batch Attenuation Testing – Linear Sorption Results

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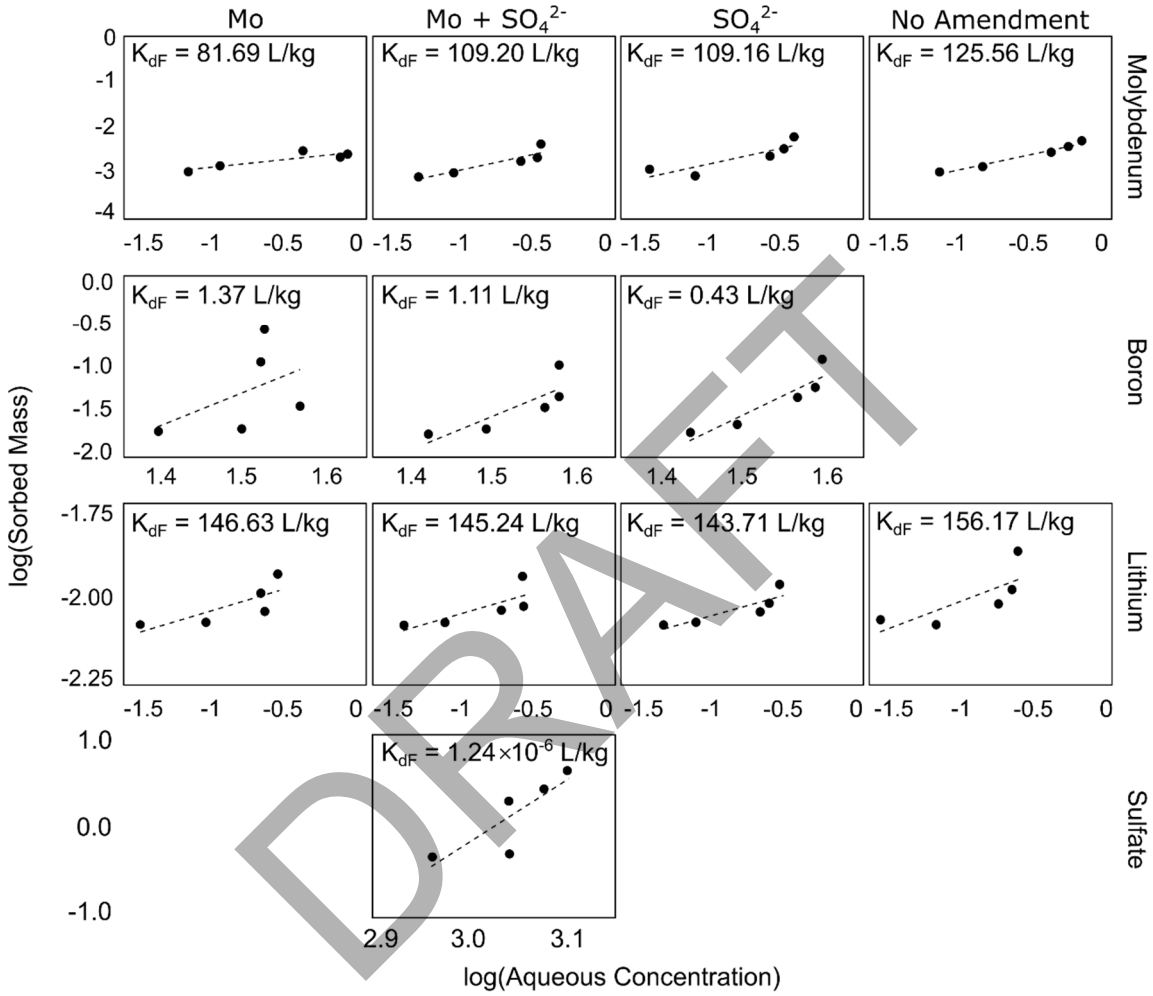
Figure 3



Notes: K_{dF} values were not generated for boron in the unamended dataset or sulfate in the Mo, SO_4, or unamended datasets because negative slopes were observed. 'No Amendment' represents groundwater from well 08R.

Batch Attenuation Testing – Freundlich Sorption Results

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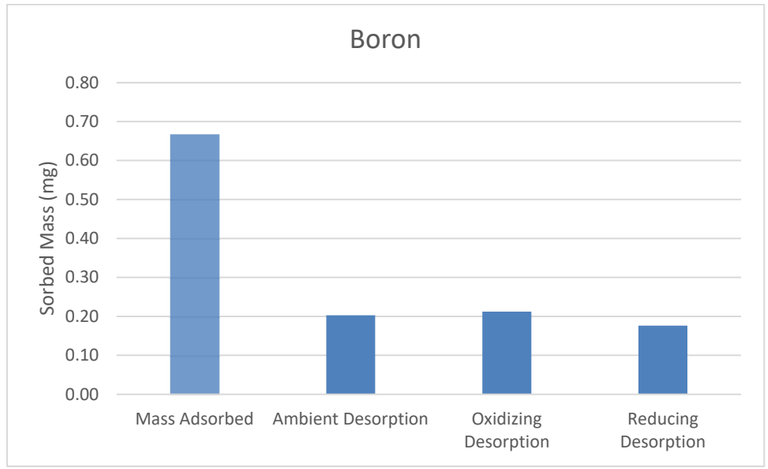
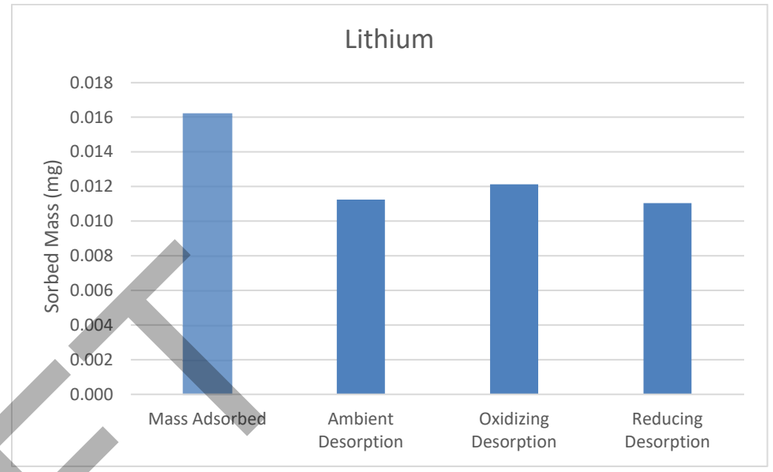
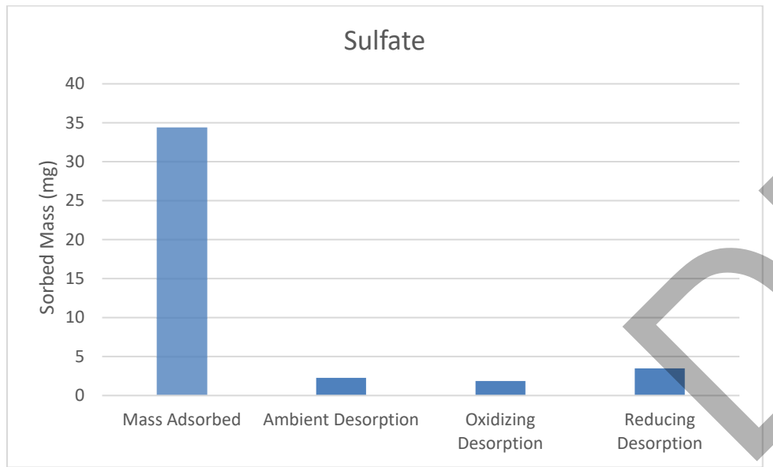
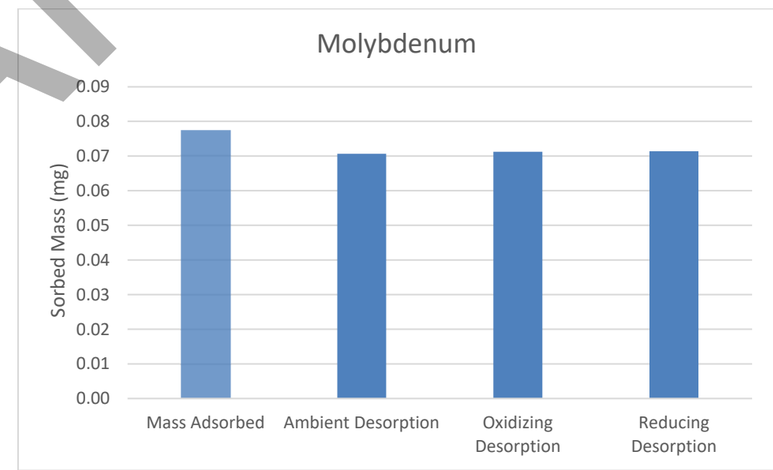
18-Oct-2021

Figure **4**









Notes:
-Mass adsorbed represents mass on the soil phase following one week of exposure to the amendment solution.
-Ambient/Oxidizing/Reducing desorption results represent the mass of the constituent adsorbed following one week of treatment under the listed experimental condition.

Desorption Testing – Remaining Mass Adsorbed

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Figure **5**

Columbus, Ohio | 13-Oct-2021

APPENDIX A
Soil Boring Logs

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

WELL LOG
Well No. MW-07R
Page: 1 of 3

Drilling Start Date:	04/27/2021	Boring Depth (ft):	40	Well Depth (ft):	21
Drilling End Date:	04/27/2021	Boring Diameter (in):		Well Diameter (in):	1
Drilling Company:	Cascade Drilling	DTW During Drilling (ft):		Screen Slot (in):	0.010
Drilling Method:	Sonic	DTW After Drilling (ft):	20	Riser Material:	Sch 40 PVC
Drilling Equipment:	Geoprobe 8140 DT	Top of Casing Elev. (ft)		Screen Material:	Sch 40 PVC Slotted
Driller:	Russ Gordon	Ground Elev. (ft):		Seal Material(s):	NA
Logged By:	Amanda Toye	Northing, Easting (NAD83):		Filter Pack:	Sand

DEPTH (ft)	LITHOLOGY	WATER LEVEL	WELL COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
0				DP	44/60			(0') No Recovery.		0
								(1.33') GRAVELLY SAND (SP); light gray, dry, fine to coarse grained.		
								(3') CLAYEY SILT (ML); burnt orange with gray and black mottling, ash throughout, trace gravel, moist.		
5				DP	19/60			(5') No Recovery.		5
								(8.4') CLAYEY SILT (ML); brown, trace gravel and sand, higher clay content at toe, moist.		
10				DP				(10') No Recovery.		10
								(11') CLAYEY SAND (SC); brown, damp.	SB-21-07R-(12-14)	
								(13') SAND WITH GRAVEL (SP); reddish brown to light gray, moist, fine to coarse grained.		
15										15

NOTES:

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

WELL LOG
Well No. MW-07R
Page: 2 of 3

Drilling Start Date:	04/27/2021	Boring Depth (ft):	40	Well Depth (ft):	21
Drilling End Date:	04/27/2021	Boring Diameter (in):		Well Diameter (in):	1
Drilling Company:	Cascade Drilling	DTW During Drilling (ft):		Screen Slot (in):	0.010
Drilling Method:	Sonic	DTW After Drilling (ft):	20	Riser Material:	Sch 40 PVC
Drilling Equipment:	Geoprobe 8140 DT	Top of Casing Elev. (ft)		Screen Material:	Sch 40 PVC Slotted
Driller:	Russ Gordon	Ground Elev. (ft):		Seal Material(s):	NA
Logged By:	Amanda Toye	Northing, Easting (NAD83):		Filter Pack:	Sand

DEPTH (ft)	LITHOLOGY	WATER LEVEL	WELL COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
15				DP	60/60			(15') CLAYEY SAND (SC); gray, wood at 19", moist, fine grained.		15
								(19.3') SAND (SP); gray, saturated, fine grained.		
20		▼		DP	60/60			(20') CLAY WITH SAND (CL); gray, trace fine gravel, saturated, medium plasticity.		20
								(24.1') SAND (SP); gray, saturated, fine grained.		
25				DP	60/60			(25') SILTY CLAY WITH SAND (CL); gray, sand seams present, trace gravel, moist.		25
30										30

NOTES:

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

WELL LOG
Well No. MW-07R
Page: 3 of 3

Drilling Start Date:	04/27/2021	Boring Depth (ft):	40	Well Depth (ft):	21
Drilling End Date:	04/27/2021	Boring Diameter (in):		Well Diameter (in):	1
Drilling Company:	Cascade Drilling	DTW During Drilling (ft):		Screen Slot (in):	0.010
Drilling Method:	Sonic	DTW After Drilling (ft):	20	Riser Material:	Sch 40 PVC
Drilling Equipment:	Geoprobe 8140 DT	Top of Casing Elev. (ft)		Screen Material:	Sch 40 PVC Slotted
Driller:	Russ Gordon	Ground Elev. (ft):		Seal Material(s):	NA
Logged By:	Amanda Toye	Northing, Easting (NAD83):		Filter Pack:	Sand

DEPTH (ft)	LITHOLOGY	WATER LEVEL	WELL COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
30				DP	60/60			(30') SAND WITH CLAY (SP); gray, moist, fine grained.	SB-21-07R-(30-31)	30
								(31') SILTY CLAY WITH SAND (CL); gray, trace fine to coarse gravel, moist.		
35				DP	60/60			(35') As above: higher sand content.		35
								(39.3') SAND (SP); gray, some clay, saturated, fine grained.		
40								(40') End of Boring.		40
45										45

NOTES:

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

BORING LOG
Boring No. SB-21-03/08R
Page: 1 of 3

Drilling Start Date:	**04/26/2021**	Boring Depth (ft):	**40**
Drilling End Date:	**04/26/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
0				DP	60/60			(0') GRAVELLY CLAY (CL); light brown, dry.		0
								(3') LEAN CLAY (CL); gray and brown mottling, dry.		
								(4') SANDY CLAY (CL); gray to brown mottling, trace gravel, dry.		
5				DP	60/60			(5') As above.		5
								(6.5') SILTY SAND (SM); gray, moist.		
								(8') SILTY CLAY (CL); gray, moist.		
10				DP	60/60			(10') SAND WITH SILT (SP); brown, moist, fine grained.		10
								(12') SAND (SP); brownish gray, moist, fine grained.		
									SB-21-08R-(13-15)	
15										15

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

BORING LOG
Boring No. SB-21-03/08R
Page: 2 of 3

Drilling Start Date:	**04/26/2021**	Boring Depth (ft):	**40**
Drilling End Date:	**04/26/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
15				DP	48/60			(15') As above.		15
								(16') SAND WITH GRAVEL (SP); gray, moist, fine to coarse grained.		
								(17.3') LEAN CLAY (CL); gray, moist, medium plasticity, till (slough).		
								(19') No Recovery.		
20				DP	60/60			(20') LEAN CLAY (CL); gray, trace gravel, moist.		20
25				DP	54/60			(25') As above.		25
								(26.5') SAND WITH CLAY AND GRAVEL (SP); gray, moist, fine to coarse grained.		
								(27.2') LEAN CLAY (CL); gray, moist, medium plasticity.		
								(28.8') SANDY SILT (ML); gray, saturated.		
30								(29.5') No Recovery.		30

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

BORING LOG
Boring No. SB-21-03/08R
Page: 3 of 3

Drilling Start Date:	**04/26/2021**	Boring Depth (ft):	**40**
Drilling End Date:	**04/26/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
30				DP	48/60			(30') SAND WITH GRAVEL AND CLAY (SP); gray, saturated.		30
								(31') SAND (SP); gray, some clay, trace gravel, moist.	SB-21-08R-(31-32)	
								(32.3') SAND, gray, some gravel, moist.		
								(33.6') No Recovery.		
35				DP	60/60			(35') SAND (SP); gray, some gravel, moist.		35
								(37.4') SAND (SP); gray, moist, fine to coarse grained.		
40								(40') End of Boring.		40
45										45

NOTES:

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

BORING LOG
Boring No. SB-21-43
Page: 1 of 5

Drilling Start Date:	**04/29/2021**	Boring Depth (ft):	**65**
Drilling End Date:	**04/29/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
0				DP	60/60			(0') CLAY (CL); grayish brown, some gray mottling, trace gravel, stiff, dry.		0
5				DP	60/60			(5') SANDY CLAY (CL); grayish brown, some orange mottling, trace gravel, dry, low plasticity.		5
10				DP	55/60			(10') As above: slightly higher clay content, dry.		10
15								(14.6') No Recovery.		15

NOTES:

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

BORING LOG
Boring No. SB-21-43
Page: 2 of 5

Drilling Start Date:	**04/29/2021**	Boring Depth (ft):	**65**
Drilling End Date:	**04/29/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
15				DP	60/60			(15') CLAY WITH SAND (CL); dark gray, trace gravel, moist, medium plasticity.		15
20				DP	60/60			(20') As above: sand lense at 15".		20
25				DP	60/60			(25') As above: some black mottling.		25
30										30

NOTES:

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

BORING LOG
Boring No. SB-21-43
Page: 3 of 5

Drilling Start Date:	**04/29/2021**	Boring Depth (ft):	**65**
Drilling End Date:	**04/29/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
30				DP	60/60			(30') CLAY WITH SAND (CL); dark gray, trace silt, moist, low plasticity.		30
								(34.3') As above: moist, medium plasticity.		
35				DP	60/60			(35') SILTY CLAY (CL); gray, few sand, trace gravel, moist, soft, medium plasticity.		35
40				DP	60/60			(40') As above.		40
45										45

NOTES:

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Client: Dynegy
Project: CHE8404B, Vermilion MNA
Address: 9878 E 2150 North Rd, Danville, IL

BORING LOG
Boring No. SB-21-43
Page: 4 of 5

Drilling Start Date:	**04/29/2021**	Boring Depth (ft):	**65**
Drilling End Date:	**04/29/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
45				DP	60/60			(45') As above.		45
50				DP	60/60			(50') As above.		50
55				DP	60/60			(55') CLAYEY SAND (SC); dark gray, saturated. (55.3') SILTY CLAY (CL); dark gray, moist, soft, medium plasticity.	SB-21-43-(54-55) SB-21-43-(55-56)	55
60								(59.5') SAND (SP); gray, saturated, fine grained.		60

NOTES:

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BORING LOG
Boring No. SB-21-43
Page: 5 of 5

Drilling Start Date:	**04/29/2021**	Boring Depth (ft):	**65**
Drilling End Date:	**04/29/2021**	Boring Diameter (in):	
Drilling Company:	**Cascade Drilling**	Sampling Method(s):	**Direct Push**
Drilling Method:	**Sonic**	DTW During Drilling (ft):	
Drilling Equipment:	**Geoprobe 8140 DT**	DTW After Drilling (ft):	
Driller:	**Russ Gordon**	Ground Surface Elev. (ft):	
Logged By:	**Amanda Toye**	Northing, Easting (NAD83):	

DEPTH (ft)	LITHOLOGY	WATER LEVEL	BORING COMPLETION	COLLECT: Sample Type	COLLECT: Recovery (in)	COLLECT: Blow Counts	COLLECT: N Value RQD (%)	SOIL/ROCK VISUAL DESCRIPTION	MEASURE: Lab Sample	DEPTH (ft)
60				DP	60/60			(60') As above.	SB-21-43-(60-61)	60
								(61') SILTY CLAY (CL); dark gray, moist, soft, medium plasticity.		
								(62') SAND (SP); gray, saturated, fine grained.	SB-21-43-(62-62.2)	
								(62.2') SILTY CLAY (CL); dark gray, moist, soft, medium plasticity.		
								(62.75') SAND (SP); gray, saturated, fine grained.	SB-21-43-(62.75-63)	
								(63.25') SILTY CLAY (CL); dark gray, moist, medium plasticity, soft.		
								(63.75') SAND (SP); gray, saturated, fine grained.	SB-21-43-(64-65)	
								(64') SILTY CLAY (CL); dark gray, moist, soft, medium plasticity.		
65								(65') End of Boring.		65
70										70

NOTES:

APPENDIX B
Tier I Geochemical Modeling Outputs

MW-03R Spec8 Output

Temperature = 12.6 C Pressure = 1.013 bars
pH = 7.275 log fO2 = -53.403
Eh = 0.0620 volts pe = 1.0943
Ionic strength = 0.025571 molal
Charge imbalance = 0.003952 eq/kg (13.19% error)
Activity of water = 0.999971
Solvent mass = 0.33679 kg
Solution mass = 0.33723 kg
Mineral mass = 1.7760 kg
Solution density = 1.022 g/cm3
Solution viscosity = 0.012 poise
Chlorinity = 0.000825 molal
Dissolved solids = 1287 mg/kg sol'n
Elect. conductivity = 1448.54 uS/cm (or umho/cm)
Hardness = 725.44 mg/kg sol'n as CaCO3
  carbonate = 222.14 mg/kg sol'n as CaCO3
  non-carbonate = 503.30 mg/kg sol'n as CaCO3
Carbonate alkalinity= 222.14 mg/kg sol'n as CaCO3
Water type = Ca-SO4
Bulk volume = 1.00e+03 cm3
Fluid volume = 330. cm3
Mineral volume = 1.15 cm3
Inert volume = 669. cm3
Porosity = 33.0 %
Permeability = 8.80e-09 cm2
HFO sorbing surface:
  Surface charge = 1.33 uC/cm2
  Surface potential = 33.9 mV
  Surface area = 2.15e+07 cm2

Minerals in system	moles	log moles	grams	volume (cm3)
Fe(OH)3	0.03351	-1.475	3.581	1.151
(total)			3.581	670.0

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.004260	259.6	0.8605	-2.4359
SO4--	0.003956	379.5	0.5444	-2.6669
Na+	0.003530	81.06	0.8605	-2.5175
Ca++	0.003446	137.9	0.5715	-2.7057
Mg++	0.002510	60.92	0.5956	-2.8254
B(OH)3(aq)	0.001735	107.1	1.0000	-2.7607
Cl-	0.0008227	29.13	0.8545	-3.1530
Fe++	0.0006503	36.27	0.5715	-3.4299
MgSO4(aq)	0.0006060	72.85	1.0000	-3.2175
CO2(aq)	0.0005423	23.84	1.0000	-3.2658
CaSO4(aq)	0.0005163	70.20	1.0000	-3.2871

CaHCO3+	9.638e-05	9.731	0.8605	-4.0813
MgHCO3+	7.106e-05	6.055	0.8605	-4.2136
K+	6.659e-05	2.600	0.8545	-4.2448
NaHCO3(aq)	2.027e-05	1.701	1.0000	-4.6932
BO2-	1.574e-05	0.6730	0.8605	-4.8683
CaCO3(aq)	7.836e-06	0.7833	1.0000	-5.1059
CO3--	4.328e-06	0.2594	0.5514	-5.6222
MgCO3(aq)	3.018e-06	0.2542	1.0000	-5.5202
MoO4--	2.019e-06	0.3224	0.5514	-5.9534
Mn++	1.186e-06	0.06510	0.5715	-6.1688
KSO4-	1.071e-06	0.1446	0.8605	-6.0355
MgCl+	9.612e-07	0.05737	0.8605	-6.0824
Li+	4.658e-07	0.003229	0.8710	-6.3918
NaCl(aq)	3.341e-07	0.01950	1.0000	-6.4761
CaCl+	3.262e-07	0.02460	0.8605	-6.5518
MnSO4(aq)	2.913e-07	0.04393	1.0000	-6.5357
FeCl+	2.079e-07	0.01896	0.8605	-6.7473
OH-	8.012e-08	0.001361	0.8576	-7.1630
H+	6.005e-08	6.044e-05	0.8841	-7.2750
NaCO3-	3.901e-08	0.003234	0.8605	-7.4740
HSO4-	9.333e-09	0.0009048	0.8605	-8.0952
KCl(aq)	1.005e-09	7.486e-05	1.0000	-8.9976
MnCl+	8.448e-10	7.626e-05	0.8605	-9.1385
CaCl2(aq)	2.638e-10	2.924e-05	1.0000	-9.5787
NaOH(aq)	3.608e-11	1.441e-06	1.0000	-10.4428
FeCO3+	1.454e-11	1.683e-06	0.8605	-10.9026
LiCl(aq)	8.294e-12	3.512e-07	1.0000	-11.0812
HCl(aq)	7.866e-12	2.864e-07	1.0000	-11.1042
FeCl2(aq)	6.210e-13	7.861e-08	1.0000	-12.2069
KHSO4(aq)	2.716e-14	3.694e-09	1.0000	-13.5661
Fe+++	9.064e-16	5.056e-11	0.3240	-15.5321
FeSO4+	4.196e-17	6.365e-12	0.8605	-16.4425
FeCl4--	1.712e-18	3.379e-13	0.5444	-18.0306
Formate	8.976e-20	4.036e-15	0.8576	-19.1136
FeCl++	3.216e-20	2.933e-15	0.5514	-19.7511
H2(aq)	7.977e-21	1.606e-17	1.0000	-20.0982
Ca(For)+	5.188e-21	4.409e-16	0.8605	-20.3503
Mg(For)+	4.630e-21	3.206e-16	0.8605	-20.3996
Fe(For)+	2.824e-21	2.845e-16	0.8605	-20.6144
Na(For)(aq)	2.753e-22	1.870e-17	1.0000	-21.5602
Formic_acid(aq)	2.388e-23	1.098e-18	1.0000	-22.6219
SO3--	1.057e-23	8.450e-19	0.5514	-23.2345
HSO3-	5.194e-24	4.205e-19	0.8605	-23.3498
K(For)(aq)	4.544e-24	3.818e-19	1.0000	-23.3425
Mn(For)+	3.549e-24	3.543e-19	0.8605	-23.5151
CO(aq)	4.108e-26	1.149e-21	1.0000	-25.3863
Oxalate	1.028e-26	9.038e-22	0.5444	-26.2521
SO2(aq)	1.340e-29	8.571e-25	1.0000	-28.8730
H-Oxalate	5.771e-30	5.132e-25	0.8605	-29.3040
Mn+++	3.157e-31	1.732e-26	0.2687	-31.0715

Oxalic_acid(aq)	4.795e-36	4.312e-31	1.0000	-35.3192
Fe(For)2(aq)	3.879e-39	5.651e-34	1.0000	-38.4113
Mg(For)2(aq)	3.174e-39	3.624e-34	1.0000	-38.4984
Ca(For)2(aq)	2.959e-39	3.845e-34	1.0000	-38.5288
Na(For)2-	1.690e-41	1.907e-36	0.8605	-40.8375
Mn(For)2(aq)	3.587e-42	5.194e-37	1.0000	-41.4452
HS-	4.087e-43	1.350e-38	0.8576	-42.4553
H2S(aq)	2.831e-43	9.638e-39	1.0000	-42.5480
K(For)2-	2.386e-43	3.078e-38	0.8605	-42.6875
Formaldehyde(aq)	7.356e-45	2.206e-40	1.0000	-44.1334
S2O6--	2.385e-46	3.815e-41	0.5444	-45.8866
ClO-	1.575e-47	8.092e-43	0.8605	-46.8680
S2O3--	5.684e-48	6.366e-43	0.5444	-47.5094
Methane(aq)	9.965e-49	1.597e-44	1.0000	-48.0015
S--	5.809e-49	1.860e-44	0.5583	-48.4890
Methanol(aq)	1.892e-49	6.056e-45	1.0000	-48.7230
HO2-	8.197e-51	2.702e-46	0.8605	-50.1516
S2O5--	5.829e-52	8.390e-47	0.5444	-51.4985
Acetate	9.134e-54	5.386e-49	0.8632	-53.1032
Glycolate	4.036e-55	3.025e-50	0.8605	-54.4593
MgCH3COO+	3.242e-55	2.699e-50	0.8605	-54.5544
CaCH3COO+	1.608e-55	1.592e-50	0.8605	-54.8590
FeCH3COO+	7.558e-56	8.673e-51	0.8605	-55.1869
Ca(Glyc)+	4.041e-56	4.646e-51	0.8605	-55.4588
Fe(Glyc)+	3.004e-56	3.927e-51	0.8605	-55.5875
Acetic_acid(aq)	2.423e-56	1.453e-51	1.0000	-55.6156
NaCH3COO(aq)	1.986e-56	1.627e-51	1.0000	-55.7020
Mg(Glyc)+	1.431e-56	1.419e-51	0.8605	-55.9098
O2(aq)	6.413e-57	2.050e-52	1.0000	-56.1929
HSO5-	4.956e-57	5.597e-52	0.8605	-56.3701
Na(Glyc)(aq)	1.264e-57	1.238e-52	1.0000	-56.8982
KCH3COO(aq)	2.335e-58	2.289e-53	1.0000	-57.6317
Glycolic_acid(aq	1.305e-58	9.914e-54	1.0000	-57.8843
MnCH3COO+	1.159e-58	1.319e-53	0.8605	-58.0012
K(Glyc)(aq)	2.087e-59	2.379e-54	1.0000	-58.6806
Mn(Glyc)+	1.227e-59	1.593e-54	0.8605	-58.9763
LiCH3COO(aq)	7.534e-60	4.965e-55	1.0000	-59.1229
S2O4--	2.798e-60	3.581e-55	0.5583	-59.8062
Malonate	4.525e-62	4.611e-57	0.5444	-61.6085
H-Malonate	7.159e-64	7.368e-59	0.8605	-63.2104
MnO4--	2.496e-67	2.965e-62	0.5444	-66.8668
Malonic_acid(aq)	2.386e-68	2.480e-63	1.0000	-67.6222
S2O8--	2.146e-72	4.118e-67	0.5444	-71.9325
MnO4-	1.660e-76	1.972e-71	0.8576	-75.8465
Acetaldehyde(aq)	1.152e-76	5.069e-72	1.0000	-75.9385
S3O6--	1.510e-78	2.899e-73	0.5444	-78.0851
S2--	1.489e-78	9.534e-74	0.5444	-78.0913
ClO2-	5.394e-84	3.634e-79	0.8605	-83.3334
Ethanol(aq)	7.000e-86	3.221e-81	1.0000	-85.1549
Ethane(aq)	1.746e-89	5.243e-85	1.0000	-88.7579

Ethylene(aq)	1.269e-90	3.555e-86	1.0000	-89.8966
Lactate	1.639e-91	1.458e-86	0.8605	-90.8507
Propanoate	2.453e-92	1.790e-87	0.8605	-91.6755
Fe(Lac)+	1.077e-92	1.559e-87	0.8605	-92.0330
Ca(Lac)+	9.653e-93	1.245e-87	0.8605	-92.0806
Mg(Lac)+	5.930e-93	6.714e-88	0.8605	-92.2922
Na(Lac)(aq)	5.226e-94	5.848e-89	1.0000	-93.2819
Fe(Prop)+	4.666e-94	6.007e-89	0.8605	-93.3964
Ca(Prop)+	2.398e-94	2.710e-89	0.8605	-93.6854
Mg(Prop)+	2.355e-94	2.290e-89	0.8605	-93.6934
S4O6--	2.207e-94	4.943e-89	0.5444	-93.9203
Propanoic_acid(a	8.738e-95	6.464e-90	1.0000	-94.0586
Na(Prop)(aq)	7.713e-95	7.400e-90	1.0000	-94.1128
Lactic_acid(aq)	5.578e-95	5.019e-90	1.0000	-94.2535
K(Lac)(aq)	8.627e-96	1.104e-90	1.0000	-95.0641
Mn(Lac)+	3.525e-96	5.069e-91	0.8605	-95.5182
K(Prop)(aq)	1.273e-96	1.426e-91	1.0000	-95.8951
Mn(Prop)+	3.625e-97	4.635e-92	0.8605	-96.5059
Ethyne(aq)	1.028e-98	2.673e-94	1.0000	-97.9881
Succinate	4.867e-99	5.641e-94	0.5444	-98.5769
H-Succinate	7.205e-101	8.424e-96	0.8605	-100.2077
Succinic_acid(aq	5.719e-104	6.745e-99	1.0000	-103.2427
ClO3-	5.263e-106	4.386e-101	0.8576	-105.3455
Ca(CH3COO)2(aq)	2.165e-107	3.420e-102	1.0000	-106.6645
Mg(CH3COO)2(aq)	1.811e-107	2.576e-102	1.0000	-106.7420
Fe(CH3COO)2(aq)	1.159e-107	2.014e-102	1.0000	-106.9358
S3--	3.308e-108	3.178e-103	0.5444	-107.7445
Fe(Glyc)2(aq)	5.931e-109	1.220e-103	1.0000	-108.2268
Ca(Glyc)2(aq)	2.540e-109	4.824e-104	1.0000	-108.5952
Na(CH3COO)2-	9.959e-110	1.403e-104	0.8605	-109.0671
Mg(Glyc)2(aq)	5.386e-110	9.381e-105	1.0000	-109.2687
Acetone(aq)	2.656e-110	1.541e-105	1.0000	-109.5758
Mn(CH3COO)2(aq)	6.904e-111	1.193e-105	1.0000	-110.1609
K(CH3COO)2-	7.832e-112	1.230e-106	0.8605	-111.1714
Na(Glyc)2-	5.452e-112	9.423e-107	0.8605	-111.3287
Li(CH3COO)2-	9.152e-113	1.143e-107	0.8605	-112.1038
Mn(Glyc)2(aq)	3.141e-113	6.432e-108	1.0000	-112.5029
K(Glyc)2-	7.869e-114	1.487e-108	0.8605	-113.1693
Propanal(aq)	1.136e-114	6.589e-110	1.0000	-113.9446
1-Propanol(aq)	2.138e-124	1.283e-119	1.0000	-123.6700
1-Propene(aq)	6.757e-127	2.840e-122	1.0000	-126.1702
Propane(aq)	2.156e-128	9.493e-124	1.0000	-127.6664
2-Hydroxybutanoa	1.815e-130	1.869e-125	0.8605	-129.8065
Butanoate	2.141e-131	1.862e-126	0.8605	-130.7346
BH4-	2.066e-131	3.063e-127	0.8605	-130.7501
ClO4-	2.064e-132	2.050e-127	0.8576	-131.7520
1-Propyne(aq)	4.366e-133	1.747e-128	1.0000	-132.3599
Fe(But)+	4.204e-133	6.002e-128	0.8605	-132.4416
Ca(But)+	1.436e-133	1.824e-128	0.8605	-132.9080
Mg(But)+	1.345e-133	1.496e-128	0.8605	-132.9367

Na(But)(aq)	6.466e-134	7.109e-129	1.0000	-133.1894
Butanoic_acid(aq	6.139e-134	5.402e-129	1.0000	-133.2119
2-Hydroxybutanoi	5.474e-134	5.691e-129	1.0000	-133.2617
K(But)(aq)	1.067e-135	1.345e-130	1.0000	-134.9716
Mn(But)+	2.696e-136	3.824e-131	0.8605	-135.6345
Glutarate	3.527e-137	4.583e-132	0.5444	-136.7166
S4--	4.343e-138	5.564e-133	0.5444	-137.6263
H-Glutarate	3.065e-139	4.013e-134	0.8605	-138.5789
S5O6--	6.799e-140	1.741e-134	0.5444	-139.4316
Glutaric_acid(aq	3.119e-142	4.115e-137	1.0000	-141.5060
Ethylacetate(aq)	5.102e-143	4.490e-138	1.0000	-142.2922
Butanal(aq)	3.531e-155	2.542e-150	1.0000	-154.4522
Mn(CH3COO)3-	2.112e-163	4.894e-158	0.8605	-162.7406
1-Butanol(aq)	3.566e-164	2.640e-159	1.0000	-163.4478
1-Butene(aq)	3.588e-166	2.010e-161	1.0000	-165.4452
n-Butane(aq)	2.326e-167	1.350e-162	1.0000	-166.6334
S5--	3.362e-168	5.384e-163	0.5444	-167.7375
2-Hydroxypentano	3.013e-169	3.525e-164	0.8605	-168.5862
Pentanoate	2.225e-170	2.248e-165	0.8605	-169.7178
Fe(Pent)+	4.082e-172	6.400e-167	0.8605	-171.4544
1-Butyne(aq)	3.600e-172	1.945e-167	1.0000	-171.4437
Ca(Pent)+	8.837e-173	1.246e-167	0.8605	-172.1189
Mg(Pent)+	8.087e-173	1.013e-167	0.8605	-172.1575
Na(Pent)(aq)	7.090e-173	8.788e-168	1.0000	-172.1494
Pentanoic_acid(a	6.943e-173	7.082e-168	1.0000	-172.1585
2-Hydroxypentano	5.371e-173	6.337e-168	1.0000	-172.2700
K(Pent)(aq)	1.170e-174	1.639e-169	1.0000	-173.9317
Mn(Pent)+	2.164e-175	3.373e-170	0.8605	-174.7299
Adipate	9.642e-178	1.388e-172	0.5444	-177.2799
H-Adipate	8.194e-180	1.188e-174	0.8605	-179.1517
Fe(Lac)2(aq)	7.754e-182	1.812e-176	1.0000	-181.1105
Ca(Lac)2(aq)	1.585e-182	3.455e-177	1.0000	-181.7999
Mg(Lac)2(aq)	9.839e-183	1.989e-177	1.0000	-182.0071
Adipic_acid(aq)	9.705e-183	1.416e-177	1.0000	-182.0130
Fe(Prop)2(aq)	1.220e-184	2.462e-179	1.0000	-183.9135
Na(Lac)2-	9.359e-185	1.880e-179	0.8605	-184.0941
Mg(Prop)2(aq)	1.148e-185	1.955e-180	1.0000	-184.9399
Ca(Prop)2(aq)	8.820e-186	1.640e-180	1.0000	-185.0545
Mn(Lac)2(aq)	6.189e-186	1.441e-180	1.0000	-185.2084
Na(Prop)2-	1.368e-186	2.311e-181	0.8605	-185.9291
K(Lac)2-	1.351e-186	2.930e-181	0.8605	-185.9347
Mn(Prop)2(aq)	4.638e-188	9.314e-183	1.0000	-187.3337
K(Prop)2-	1.971e-188	3.647e-183	0.8605	-187.7705
Phenol(aq)	4.579e-192	4.304e-187	1.0000	-191.3392
Pentanal(aq)	6.416e-194	5.520e-189	1.0000	-193.1927
Benzene(aq)	1.338e-199	1.044e-194	1.0000	-198.8735
1-Pentanol(aq)	6.766e-202	5.957e-197	1.0000	-201.1696
Benzoate	7.821e-203	9.460e-198	0.8710	-202.1668
1-Pentene(aq)	2.907e-205	2.036e-200	1.0000	-204.5366
Benzoic_acid(aq)	5.932e-206	7.235e-201	1.0000	-205.2268

n-Pentane(aq)	2.077e-206	1.497e-201	1.0000	-205.6825
2-Hydroxyhexanoa	2.075e-208	2.717e-203	0.8605	-207.7483
Hexanoate	1.846e-209	2.123e-204	0.8605	-208.7990
o-Phthalate	1.446e-209	2.370e-204	0.5444	-209.1040
1-Pentyne(aq)	3.075e-211	2.092e-206	1.0000	-210.5121
Hexanoic_acid(aq	6.026e-212	6.991e-207	1.0000	-211.2200
2-Hydroxyhexanoi	5.271e-212	6.958e-207	1.0000	-211.2781
Pimelate	1.371e-215	2.165e-210	0.5444	-215.1272
H-Pimelate	1.180e-217	1.876e-212	0.8605	-216.9933
Pimelic_acid(aq)	1.667e-220	2.666e-215	1.0000	-219.7782
Hexanal(aq)	5.097e-233	5.099e-228	1.0000	-232.2927
Toluene(aq)	9.986e-236	9.190e-231	1.0000	-235.0006
p-Toluate	1.232e-238	1.662e-233	0.8605	-237.9748
m-Toluate	6.708e-239	9.054e-234	0.8605	-238.2387
o-Toluate	6.326e-241	8.538e-236	0.8605	-240.2641
p-Toluic_acid(aq	1.354e-241	1.841e-236	1.0000	-240.8685
1-Hexanol(aq)	1.161e-241	1.185e-236	1.0000	-240.9350
m-Toluic_acid(aq	5.758e-242	7.829e-237	1.0000	-241.2398
1-Hexene(aq)	3.723e-244	3.129e-239	1.0000	-243.4291
o-Toluic_acid(aq	2.150e-244	2.923e-239	1.0000	-243.6676
n-Hexane(aq)	1.378e-245	1.186e-240	1.0000	-244.8607
2-Hydroxyheptano	2.031e-247	2.945e-242	0.8605	-246.7575
Heptanoate	2.099e-248	2.708e-243	0.8605	-247.7432
1-Hexyne(aq)	2.089e-250	1.714e-245	1.0000	-249.6800
Heptanoic_acid(a	7.434e-251	9.665e-246	1.0000	-250.1288
2-Hydroxyheptano	5.173e-251	7.552e-246	1.0000	-250.2863
Suberate	5.262e-256	9.048e-251	0.5444	-255.5430
H-Suberate	4.392e-258	7.597e-253	0.8605	-257.4226
Suberic_acid(aq)	6.514e-261	1.133e-255	1.0000	-260.1861
Fe(But)2(aq)	9.187e-263	2.111e-257	1.0000	-262.0368
Mg(But)2(aq)	3.725e-264	7.386e-259	1.0000	-263.4288
Ca(But)2(aq)	3.231e-264	6.914e-259	1.0000	-263.4907
Na(But)2-	9.177e-265	1.807e-259	0.8605	-264.1026
Mn(But)2(aq)	2.494e-266	5.707e-261	1.0000	-265.6031
K(But)2-	1.322e-266	2.816e-261	0.8605	-265.9440
Heptanal(aq)	4.978e-273	5.677e-268	1.0000	-272.3029
1-Heptanol(aq)	8.942e-282	1.038e-276	1.0000	-281.0485
1-Heptene(aq)	3.473e-283	3.405e-278	1.0000	-282.4593
n-Heptane(aq)	1.343e-284	1.344e-279	1.0000	-283.8718
2-Hydroxyoctanoa	1.988e-286	3.162e-281	0.8605	-285.7667
Octanoate	3.447e-287	4.930e-282	0.8605	-286.5279
1-Heptyne(aq)	1.294e-289	1.243e-284	1.0000	-288.8881
Octanoic_acid(aq	1.237e-289	1.782e-284	1.0000	-288.9075
2-Hydroxyoctanoi	5.076e-290	8.121e-285	1.0000	-289.2945
Azelate	3.783e-297	7.034e-292	0.5444	-296.6863
H-Azelate	3.095e-299	5.786e-294	0.8605	-298.5746
Azelaic_acid(aq)	4.798e-302	9.019e-297	1.0000	-300.0000
Octanal(aq)	2.261e-311	2.896e-306	1.0000	-300.0000
n-Propylbenzene(	1.376e-313	1.652e-308	1.0000	-300.0000
1-Octanol(aq)	1.714e-320	2.230e-315	1.0000	-300.0000

1-Octene(aq)	2.322e-322	2.602e-317	1.0000	-300.0000
n-Octane(aq)	1.482e-323	1.691e-318	1.0000	-300.0000
2-Hydroxynonanoi	0.000	0.000	1.0000	-300.0000
Nonanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Nonanoate	0.000	0.000	0.8605	-300.0000
Nonanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxynonanoa	0.000	0.000	0.8605	-300.0000
Na(Pent)2-	0.000	0.000	0.8605	-300.0000
Fe(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
Mn(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoi	0.000	0.000	1.0000	-300.0000
Mg(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoa	0.000	0.000	0.8605	-300.0000
Ethylbenzene(aq)	0.000	0.000	1.0000	-300.0000
1-Octyne(aq)	0.000	0.000	1.0000	-300.0000
Dodecanoic_acid(	0.000	0.000	1.0000	-300.0000
Dodecanoate	0.000	0.000	0.8605	-300.0000
Decanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Decanoate	0.000	0.000	0.8605	-300.0000
Decanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hexanone(aq)	0.000	0.000	1.0000	-300.0000
K(Pent)2-	0.000	0.000	0.8605	-300.0000
2-Heptanone(aq)	0.000	0.000	1.0000	-300.0000
n-Pentylbenzene(	0.000	0.000	1.0000	-300.0000
n-Octylbenzene(a	0.000	0.000	1.0000	-300.0000
2-Pentanone(aq)	0.000	0.000	1.0000	-300.0000
2-Butanone(aq)	0.000	0.000	1.0000	-300.0000
n-Hexylbenzene(a	0.000	0.000	1.0000	-300.0000
n-Heptylbenzene(	0.000	0.000	1.0000	-300.0000
n-Butylbenzene(a	0.000	0.000	1.0000	-300.0000
2-Octanone(aq)	0.000	0.000	1.0000	-300.0000
Undecanoic_acid(	0.000	0.000	1.0000	-300.0000
Undecanoate	0.000	0.000	0.8605	-300.0000
Sebacic_acid(aq)	0.000	0.000	1.0000	-300.0000
Sebacate	0.000	0.000	0.5444	-300.0000
Ca(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
H-Sebacate	0.000	0.000	0.8605	-300.0000

Surface species	molality	moles	Boltzman fct.	log molality
>(w)FeOH	0.01116	0.003760	1.0000	-1.9522
>(w)FeOH2+	0.003089	0.001040	3.7411	-2.5102
>(w)FeOMg+	0.002111	0.0007109	3.7411	-2.6756
>(w)FeOHSO4--	0.002075	0.0006987	0.071449	-2.6830
>(w)FeO-	0.0009243	0.0003113	0.26730	-3.0342
>(s)FeOHCa++	0.0004122	0.0001388	13.996	-3.3849
>(w)FeSO4-	0.0002877	9.690e-05	0.26730	-3.5410
>(w)FeOCa+	0.0001563	5.266e-05	3.7411	-3.8059
>(w)FeH2BO3	8.075e-05	2.719e-05	1.0000	-4.0929
>(s)FeOMn+	4.266e-05	1.437e-05	3.7411	-4.3700

>(s)FeOH	3.139e-05	1.057e-05	1.0000	-4.5032
>(w)FeOMn+	1.205e-05	4.059e-06	3.7411	-4.9190
>(s)FeOH2+	8.685e-06	2.925e-06	3.7411	-5.0612
>(s)FeO-	2.599e-06	8.753e-07	0.26730	-5.5852

(Boltzman factor = exp(zF PSI/RT), where PSI is surface potential)

Mineral saturation states

	log Q/K		log Q/K
Magnetite	11.6010s/sat	MgSO4	-11.0301
Hematite	11.5075s/sat	B2O3	-11.1929
Goethite	5.2885s/sat	Thermonatrite	-11.3632
Siderite	1.3663s/sat	Na2CO3	-11.6737
Dolomite-ord	1.1993s/sat	Portlandite	-11.6944
Dolomite	1.1993s/sat	MnSO4	-11.9559
Ferrite-Mg	1.1404s/sat	Borax	-12.9526
Ferrite-Ca	0.9070s/sat	Hydromagnesite	-13.3295
Calcite	0.0999s/sat	MnCl2:4H2O	-15.3112
Fe(OH)3	0.0000 sat	MgOHCl	-15.5116
Aragonite	-0.0451	MnCl2:2H2O	-16.7334
Ice	-0.0916	MgCl2:4H2O	-16.8112
Dolomite-dis	-0.4385	Pyrolusite	-18.2287
Magnesite	-0.6074	MnCl2:H2O	-18.3985
Monohydrocalcite	-0.7041	Bixbyite	-18.9938
Powellite	-0.7245	Lawrencite	-19.4506
Gypsum	-0.8768	C	-20.6566
Anhydrite	-1.1754	Hydrophilite	-21.3997
Rhodochrosite	-1.2886	Scacchite	-21.7885
Bassanite	-1.8241	Lime	-22.2096
CaSO4:0.5H2O(bet	-2.0082	Hausmannite	-22.3309
Boric_acid	-2.4456	MgCl2:2H2O	-22.5882
Wustite	-3.1708	Fe	-22.6449
FeO	-3.2184	Ferrite-Dicalciu	-24.1663
Huntite	-3.3847	MgCl2:H2O	-26.1363
Fe(OH)2	-3.5120	S	-30.7125
Melanterite	-3.6418	KMgCl3:2H2O	-31.0698
Nesquehonite	-3.6932	Chloromagnesite	-32.1771
Jarosite	-4.5695	Troilite	-34.8325
Nahcolite	-4.7067	Pyrrhotite	-34.9358
Brucite	-5.4234	KMgCl3	-38.7725
Mirabilite	-5.9841	Molysite	-39.6522
Artinite	-6.9061	Alabandite	-41.1191
Halite	-7.2158	Fe2(SO4)3	-44.0714
Thenardite	-7.3820	Mn	-50.2823
Mn(OH)2(am)	-7.6729	Mo	-50.7844
Sylvite	-8.0969	Na	-51.4711
Mg1.25SO4(OH)0.5	-8.5315	Pyrite	-54.6915
Arcanite	-9.1432	K	-56.8921
FeSO4	-9.2784	Na2O	-60.5968
Natron	-9.4347	Li	-61.0223

Mg1.5SO4(OH)	-9.8136	B	-75.0214
Na2CO3:7H2O	-9.9590	K2O	-81.2349
NaFeO2	-10.0804	Mg	-88.3959
Manganosite	-10.4668	Ca	-106.1760
Periclase	-10.7546	o-Phthalic_acid	-213.6992

Gases	partial press. (bar)	fugacity	fug. coef.	log fug.
H2O(g)	0.01274	0.01193	0.9364	-1.9235
CO2(g)	0.01082	0.01076	0.9942	-1.9682
H2(g)	9.234e-18	9.241e-18	1.001	-17.0343
HCl(g)	5.087e-18	5.087e-18	1.000*	-17.2936
CO(g)	3.286e-23	3.286e-23	1.000*	-22.4834
SO2(g)	5.610e-30	5.508e-30	0.9819	-29.2590
H2S(g)	1.966e-42	1.949e-42	0.9913	-41.7103
CH4(g)	5.379e-46	5.368e-46	0.9980	-45.2702
Cl2(g)	4.512e-53	4.512e-53	1.000*	-52.3456
O2(g)	3.957e-54	3.954e-54	0.9992	-53.4030
Na(g)	1.718e-66	1.718e-66	1.000*	-65.7650
K(g)	6.945e-69	6.945e-69	1.000*	-68.1583
S2(g)	5.048e-77	5.048e-77	1.000*	-76.2969
Li(g)	3.957e-85	3.957e-85	1.000*	-84.4026
C2H4(g)	1.922e-88	1.922e-88	1.000*	-87.7163
Mg(g)	6.163e-110	6.163e-110	1.000*	-109.2102
Ca(g)	1.826e-133	1.826e-133	1.000*	-132.7384
C(g)	1.977e-144	1.977e-144	1.000*	-143.7039
B(g)	2.619e-171	2.619e-171	1.000*	-170.5819

*no data, gas taken to be ideal

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
H2O	18.8	18.7	9.99e+05	-0.000124		-6.63
B(OH)3(aq)	0.000617	0.000590	108.	2.72e-05		4.99
Ca++	0.00156	0.00137	163.	0.000191		22.8
Cl-	0.000278	0.000278	29.2			
Fe++	0.0337	0.000219	36.3			
H+	-0.0668	0.000172	0.515	4.60e-05		0.138
HCO3-	0.00169	0.00169	305.			
K+	2.28e-05	2.28e-05	2.64			
Li+	1.57e-07	1.57e-07	0.00323			
Mg++	0.00179	0.00107	77.5	0.000711		51.2
Mn++	1.89e-05	4.98e-07	0.0811	1.84e-05		3.00
MoO4--	6.80e-07	6.80e-07	0.322			
Na+	0.00120	0.00120	81.5			
O2(aq)	0.00838	1.22e-12	1.16e-07			
SO4--	0.00251	0.00171	487.	0.000796		227.
>(s)FeOH	0.000168					
>(w)FeOH	0.00670					

Sorbed	fraction	log fraction
B(OH)3(aq)	0.04409	-1.356
Ca++	0.1227	-0.911
Mg++	0.3981	-0.400
Mn++	0.9737	-0.012
SO4--	0.3174	-0.498

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Boron	0.0006168	0.0005896	18.90	2.719e-05	0.8718
Calcium	0.001561	0.001370	162.8	0.0001915	22.75
Carbon	0.001686	0.001686	60.03		
Chlorine	0.0002777	0.0002777	29.19		
Hydrogen	37.49	37.39	1.118e+05	-0.0001206	-0.3604
Iron	0.03373	0.0002191	36.28		
Lithium	1.569e-07	1.569e-07	0.003229		
Magnesium	0.001786	0.001075	77.45	0.0007109	51.24
Manganese	1.892e-05	4.980e-07	0.08112	1.843e-05	3.002
Molybdenum	6.799e-07	6.799e-07	0.1934		
Oxygen	18.81	18.71	8.876e+05	0.003140	149.0
Potassium	2.279e-05	2.279e-05	2.642		
Sodium	0.001196	0.001196	81.53		
Sulfur	0.002506	0.001711	162.7	0.0007956	75.66

MW-07R Spec8 Output

Temperature = 13.1 C Pressure = 1.013 bars
pH = 7.320 log fO2 = -50.638
Eh = 0.0969 volts pe = 1.7068
Ionic strength = 0.069287 molal
Charge imbalance = 0.015968 eq/kg (22.31% error)
Activity of water = 0.999994
Solvent mass = 0.33632 kg
Solution mass = 0.33743 kg
Mineral mass = 1.7760 kg
Solution density = 1.023 g/cm3
Solution viscosity = 0.012 poise
Chlorinity = 0.000173 molal
Dissolved solids = 3303 mg/kg sol'n
Elect. conductivity = 3301.01 uS/cm (or umho/cm)
Hardness = 2633.64 mg/kg sol'n as CaCO3
  carbonate = 51.02 mg/kg sol'n as CaCO3
  non-carbonate = 2582.62 mg/kg sol'n as CaCO3
Carbonate alkalinity= 51.02 mg/kg sol'n as CaCO3
Water type = Ca-SO4
Bulk volume = 1.00e+03 cm3
Fluid volume = 330. cm3
Mineral volume = 1.15 cm3
Inert volume = 669. cm3
Porosity = 33.0 %
Permeability = 8.80e-09 cm2
HFO sorbing surface:
  Surface charge = 1.68 uC/cm2
  Surface potential = 26.7 mV
  Surface area = 2.15e+07 cm2

Minerals in system	moles	log moles	grams	volume (cm3)
Fe(OH)3	0.03351	-1.475	3.581	1.151
(total)			3.581	670.0

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Ca++	0.01744	696.8	0.4514	-2.1037
SO4--	0.01334	1277.	0.4074	-2.2648
CaSO4(aq)	0.005221	708.5	1.0000	-2.2822
B(OH)3(aq)	0.003261	201.0	1.0000	-2.4866
Mg++	0.002410	58.37	0.4899	-2.9280
Na+	0.002198	50.36	0.8027	-2.7535
K+	0.001451	56.55	0.7904	-2.9405
MgSO4(aq)	0.001221	146.5	1.0000	-2.9133
HCO3-	0.0009245	56.22	0.8027	-3.1296
Cl-	0.0001725	6.095	0.7904	-3.8654
Fe++	0.0001375	7.655	0.4514	-4.2070

CO2(aq)	9.814e-05	4.305	1.0000	-4.0082
CaHCO3+	8.355e-05	8.419	0.8027	-4.1735
Li+	8.114e-05	0.5614	0.8236	-4.1750
KSO4-	5.841e-05	7.869	0.8027	-4.3289
Mn++	4.959e-05	2.715	0.4514	-4.6500
BO2-	3.558e-05	1.518	0.8027	-4.5442
MnSO4(aq)	2.438e-05	3.669	1.0000	-4.6130
MgHCO3+	1.217e-05	1.035	0.8027	-5.0103
CaCO3(aq)	7.176e-06	0.7159	1.0000	-5.1441
MoO4--	5.466e-06	0.8714	0.4190	-5.6401
NaHCO3(aq)	2.363e-06	0.1979	1.0000	-5.6265
CO3--	1.294e-06	0.07737	0.4190	-6.2660
MgCO3(aq)	5.434e-07	0.04566	1.0000	-6.2649
CaCl+	2.710e-07	0.02040	0.8027	-6.6624
MgCl+	1.574e-07	0.009372	0.8027	-6.8985
OH-	9.923e-08	0.001682	0.7967	-7.1020
H+	5.645e-08	5.670e-05	0.8480	-7.3200
NaCl(aq)	3.771e-08	0.002197	1.0000	-7.4235
HSO4-	2.301e-08	0.002227	0.8027	-7.7334
FeCl+	7.222e-09	0.0006572	0.8027	-8.2368
MnCl+	5.854e-09	0.0005274	0.8027	-8.3280
NaCO3-	5.451e-09	0.0004509	0.8027	-8.3590
KCl(aq)	3.963e-09	0.0002945	1.0000	-8.4019
LiCl(aq)	2.654e-10	1.121e-05	1.0000	-9.5761
CaCl2(aq)	3.941e-11	4.360e-06	1.0000	-10.4044
NaOH(aq)	2.403e-11	9.580e-07	1.0000	-10.6192
FeCO3+	2.351e-12	2.715e-07	0.8027	-11.7241
HCl(aq)	1.373e-12	4.991e-08	1.0000	-11.8622
KHSO4(aq)	1.265e-12	1.717e-07	1.0000	-11.8978
FeCl2(aq)	3.905e-15	4.934e-10	1.0000	-14.4083
Fe+++	9.472e-16	5.273e-11	0.2155	-15.6901
FeSO4+	7.996e-17	1.211e-11	0.8027	-16.1925
FeCl++	5.828e-21	5.303e-16	0.4190	-20.6123
Formate	9.574e-22	4.296e-17	0.7967	-21.1176
FeCl4--	5.417e-22	1.067e-16	0.4074	-21.6562
H2(aq)	3.944e-22	7.924e-19	1.0000	-21.4041
Ca(For)+	2.197e-22	1.863e-17	0.8027	-21.7536
Mg(For)+	3.850e-23	2.660e-18	0.8027	-22.5100
Fe(For)+	4.970e-24	4.997e-19	0.8027	-23.3990
SO3--	1.729e-24	1.380e-19	0.4190	-24.1401
Na(For)(aq)	1.582e-24	1.072e-19	1.0000	-23.8008
Mn(For)+	1.238e-24	1.233e-19	0.8027	-24.0027
K(For)(aq)	9.088e-25	7.619e-20	1.0000	-24.0415
HSO3-	6.261e-25	5.059e-20	0.8027	-24.2988
Formic_acid(aq)	2.131e-25	9.776e-21	1.0000	-24.6714
CO(aq)	3.701e-28	1.033e-23	1.0000	-27.4317
Mn+++	7.987e-29	4.373e-24	0.1487	-28.9253
Oxalate	2.767e-29	2.427e-24	0.4074	-28.9480
SO2(aq)	1.370e-30	8.747e-26	1.0000	-29.8633
H-Oxalate	1.126e-32	9.993e-28	0.8027	-32.0438

Oxalic_acid(aq)	7.874e-39	7.066e-34	1.0000	-38.1038
Ca(For)2(aq)	1.152e-42	1.495e-37	1.0000	-41.9384
Mg(For)2(aq)	2.411e-43	2.747e-38	1.0000	-42.6178
Fe(For)2(aq)	6.245e-44	9.081e-39	1.0000	-43.2044
Mn(For)2(aq)	1.148e-44	1.659e-39	1.0000	-43.9400
Na(For)2-	1.022e-45	1.151e-40	0.8027	-45.0860
K(For)2-	5.042e-46	6.490e-41	0.8027	-45.3928
S2O6--	8.566e-47	1.367e-41	0.4074	-46.4572
ClO-	8.210e-47	4.210e-42	0.8027	-46.1811
HS-	5.168e-48	1.703e-43	0.7967	-47.3854
Formaldehyde(aq)	3.245e-48	9.710e-44	1.0000	-47.4888
H2S(aq)	2.950e-48	1.002e-43	1.0000	-47.5302
HO2-	2.550e-49	8.389e-45	0.8027	-48.6889
S2O3--	2.011e-52	2.248e-47	0.4074	-52.0865
S--	1.013e-53	3.236e-49	0.4302	-53.3610
S2O5--	9.835e-54	1.413e-48	0.4074	-53.3972
Methanol(aq)	3.885e-54	1.241e-49	1.0000	-53.4106
O2(aq)	3.703e-54	1.181e-49	1.0000	-53.4314
Methane(aq)	9.353e-55	1.496e-50	1.0000	-54.0290
HSO5-	3.167e-55	3.569e-50	0.8027	-54.5949
Acetate	1.862e-60	1.096e-55	0.8084	-59.8224
Glycolate	1.802e-60	1.347e-55	0.8027	-59.8398
Ca(Glyc)+	7.180e-61	8.238e-56	0.8027	-60.2393
CaCH3COO+	1.314e-61	1.298e-56	0.8027	-60.9769
MgCH3COO+	5.199e-62	4.319e-57	0.8027	-61.3795
Mg(Glyc)+	5.023e-62	4.974e-57	0.8027	-61.3944
Fe(Glyc)+	2.217e-62	2.893e-57	0.8027	-61.7496
MnO4--	1.063e-62	1.260e-57	0.4074	-62.3635
Acetic_acid(aq)	4.168e-63	2.494e-58	1.0000	-62.3801
Na(Glyc)(aq)	3.050e-63	2.980e-58	1.0000	-62.5157
FeCH3COO+	2.572e-63	2.945e-58	0.8027	-62.6852
NaCH3COO(aq)	2.198e-63	1.797e-58	1.0000	-62.6579
S2O4--	2.179e-63	2.782e-58	0.4302	-63.0282
Mn(Glyc)+	1.799e-63	2.330e-58	0.8027	-62.8405
K(Glyc)(aq)	1.752e-63	1.993e-58	1.0000	-62.7564
KCH3COO(aq)	8.999e-64	8.803e-59	1.0000	-63.0458
MnCH3COO+	7.796e-64	8.857e-59	0.8027	-63.2035
Glycolic_acid(aq	4.891e-64	3.708e-59	1.0000	-63.3106
LiCH3COO(aq)	2.355e-64	1.549e-59	1.0000	-63.6280
Malonate	2.363e-69	2.404e-64	0.4074	-69.0165
S2O8--	4.022e-70	7.701e-65	0.4074	-69.7856
H-Malonate	2.708e-71	2.781e-66	0.8027	-70.6629
MnO4-	2.470e-71	2.928e-66	0.7967	-70.7060
Malonic_acid(aq)	7.581e-76	7.863e-71	1.0000	-75.1203
ClO2-	6.962e-82	4.681e-77	0.8027	-81.2527
S3O6--	1.170e-82	2.242e-77	0.4074	-82.3217
Acetaldehyde(aq)	9.760e-85	4.286e-80	1.0000	-84.0105
S2--	5.755e-87	3.679e-82	0.4074	-86.6299
Ethanol(aq)	2.802e-95	1.287e-90	1.0000	-94.5525
Ethylene(aq)	5.197e-100	1.453e-95	1.0000	-99.2843

Ethane(aq)	3.249e-100	9.737e-96	1.0000	-99.4883
Lactate	1.429e-101	1.268e-96	0.8027	-100.9406
S4O6--	3.553e-102	7.941e-97	0.4074	-101.8394
Ca(Lac)+	3.350e-102	4.312e-97	0.8027	-101.5704
ClO3-	1.607e-102	1.337e-97	0.7967	-101.8926
Mg(Lac)+	4.078e-103	4.608e-98	0.8027	-102.4850
Fe(Lac)+	1.552e-103	2.242e-98	0.8027	-102.9046
Propanoate	9.879e-104	7.195e-99	0.8027	-103.1007
Na(Lac)(aq)	2.461e-104	2.749e-99	1.0000	-103.6089
K(Lac)(aq)	1.414e-104	1.806e-99	1.0000	-103.8495
Mn(Lac)+	1.009e-104	1.448e-99	0.8027	-104.0917
Lactic_acid(aq)	4.085e-105	3.668e-100	1.0000	-104.3888
Ca(Prop)+	3.856e-105	4.348e-100	0.8027	-104.5093
Mg(Prop)+	7.430e-106	7.212e-101	0.8027	-105.2244
Fe(Prop)+	3.111e-106	3.998e-101	0.8027	-105.6025
Propanoic_acid(a	2.958e-106	2.184e-101	1.0000	-105.5291
Na(Prop)(aq)	1.678e-106	1.607e-101	1.0000	-105.7752
K(Prop)(aq)	9.641e-107	1.078e-101	1.0000	-106.0159
Ethyne(aq)	9.483e-107	2.461e-102	1.0000	-106.0231
Mn(Prop)+	4.795e-107	6.118e-102	0.8027	-106.4146
Succinate	4.978e-111	5.760e-106	0.4074	-110.6929
H-Succinate	5.320e-113	6.209e-108	0.8027	-112.3695
Succinic_acid(aq	3.542e-116	4.168e-111	1.0000	-115.4508
Ca(Glyc)2(aq)	1.741e-119	3.300e-114	1.0000	-118.7592
Ca(CH3COO)2(aq)	3.126e-120	4.928e-115	1.0000	-119.5050
S3--	2.748e-120	2.634e-115	0.4074	-119.9510
Fe(Glyc)2(aq)	1.680e-120	3.447e-115	1.0000	-119.7748
Mg(Glyc)2(aq)	7.269e-121	1.263e-115	1.0000	-120.1385
Mg(CH3COO)2(aq)	5.108e-121	7.250e-116	1.0000	-120.2917
Fe(CH3COO)2(aq)	6.934e-122	1.202e-116	1.0000	-121.1590
Mn(Glyc)2(aq)	1.776e-122	3.629e-117	1.0000	-121.7506
Mn(CH3COO)2(aq)	8.204e-123	1.415e-117	1.0000	-122.0860
Na(Glyc)2-	5.815e-123	1.003e-117	0.8027	-122.3309
Acetone(aq)	4.371e-123	2.531e-118	1.0000	-122.3594
K(Glyc)2-	2.930e-123	5.525e-118	0.8027	-122.6285
Na(CH3COO)2-	2.234e-123	3.142e-118	0.8027	-122.7463
K(CH3COO)2-	6.140e-124	9.620e-119	0.8027	-123.3073
Li(CH3COO)2-	5.772e-124	7.193e-119	0.8027	-123.3341
Propanal(aq)	1.891e-127	1.095e-122	1.0000	-126.7232
ClO4-	1.498e-127	1.484e-122	0.7967	-126.9233
BH4-	3.307e-136	4.892e-132	0.8027	-135.5760
1-Propanol(aq)	1.683e-138	1.008e-133	1.0000	-137.7739
1-Propene(aq)	5.412e-141	2.270e-136	1.0000	-140.2666
Propane(aq)	7.906e-144	3.475e-139	1.0000	-143.1020
2-Hydroxybutanoa	3.119e-145	3.205e-140	0.8027	-144.6015
1-Propyne(aq)	7.818e-146	3.122e-141	1.0000	-145.1069
Butanoate	1.699e-147	1.475e-142	0.8027	-146.8652
2-Hydroxybutanoi	7.905e-149	8.202e-144	1.0000	-148.1021
Ca(But)+	4.552e-149	5.770e-144	0.8027	-148.4373
Mg(But)+	8.365e-150	9.288e-145	0.8027	-149.1730

Fe(But)+	5.523e-150	7.869e-145	0.8027	-149.3533
Butanoic_acid(aq	4.100e-150	3.601e-145	1.0000	-149.3872
Na(But)(aq)	2.772e-150	3.041e-145	1.0000	-149.5573
K(But)(aq)	1.592e-150	2.003e-145	1.0000	-149.7979
Mn(But)+	7.027e-151	9.949e-146	0.8027	-150.2486
S5O6--	2.429e-151	6.206e-146	0.4074	-151.0046
S4--	7.756e-154	9.915e-149	0.4074	-153.5004
Glutarate	7.097e-154	9.203e-149	0.4074	-153.5389
H-Glutarate	4.458e-156	5.826e-151	0.8027	-155.4463
Glutaric_acid(aq	3.812e-159	5.019e-154	1.0000	-158.4189
Ethylacetate(aq)	3.508e-159	3.080e-154	1.0000	-158.4550
Butanal(aq)	1.165e-172	8.374e-168	1.0000	-171.9336
Mn(CH3COO)3-	5.058e-182	1.170e-176	0.8027	-181.3914
1-Butanol(aq)	5.546e-183	4.098e-178	1.0000	-182.2560
1-Butene(aq)	5.672e-185	3.172e-180	1.0000	-184.2463
n-Butane(aq)	1.682e-187	9.743e-183	1.0000	-186.7742
S5--	1.292e-187	2.064e-182	0.4074	-187.2788
2-Hydroxypentano	1.020e-188	1.191e-183	0.8027	-188.0867
1-Butyne(aq)	1.272e-189	6.856e-185	1.0000	-188.8956
Pentanoate	3.482e-191	3.509e-186	0.8027	-190.5537
2-Hydroxypentano	1.530e-192	1.801e-187	1.0000	-191.8154
Ca(Pent)+	5.520e-193	7.768e-188	0.8027	-192.3535
Fe(Pent)+	1.056e-193	1.653e-188	0.8027	-193.0717
Mg(Pent)+	9.916e-194	1.240e-188	0.8027	-193.0991
Pentanoic_acid(a	9.142e-194	9.306e-189	1.0000	-193.0390
Na(Pent)(aq)	5.984e-194	7.403e-189	1.0000	-193.2230
K(Pent)(aq)	3.438e-194	4.805e-189	1.0000	-193.4637
Mn(Pent)+	1.111e-194	1.729e-189	0.8027	-194.0496
Adipate	3.847e-199	5.526e-194	0.4074	-198.8049
H-Adipate	2.364e-201	3.420e-196	0.8027	-200.7218
Ca(Lac)2(aq)	4.150e-202	9.026e-197	1.0000	-201.3819
Fe(Lac)2(aq)	8.377e-203	1.954e-197	1.0000	-202.0769
Mg(Lac)2(aq)	5.085e-203	1.026e-197	1.0000	-202.2937
Adipic_acid(aq)	2.354e-204	3.429e-199	1.0000	-203.6282
Mn(Lac)2(aq)	1.334e-204	3.099e-199	1.0000	-203.8749
Na(Lac)2-	3.806e-205	7.629e-200	0.8027	-204.5150
K(Lac)2-	1.917e-205	4.152e-200	0.8027	-204.8127
Ca(Prop)2(aq)	4.948e-208	9.185e-203	1.0000	-207.3055
Fe(Prop)2(aq)	2.821e-208	5.679e-203	1.0000	-207.5496
Mg(Prop)2(aq)	1.256e-208	2.134e-203	1.0000	-207.9009
Mn(Prop)2(aq)	2.134e-209	4.276e-204	1.0000	-208.6709
Na(Prop)2-	1.187e-209	2.001e-204	0.8027	-209.0211
K(Prop)2-	5.970e-210	1.102e-204	0.8027	-209.3195
Phenol(aq)	5.292e-215	4.964e-210	1.0000	-214.2763
Pentanal(aq)	4.172e-216	3.582e-211	1.0000	-215.3796
Benzene(aq)	7.284e-224	5.671e-219	1.0000	-223.1376
1-Pentanol(aq)	2.066e-225	1.815e-220	1.0000	-224.6849
Benzoate	9.102e-228	1.099e-222	0.8236	-227.1251
1-Pentene(aq)	9.065e-229	6.337e-224	1.0000	-228.0426
Benzoic_acid(aq)	5.878e-231	7.154e-226	1.0000	-230.2308

n-Pentane(aq)	2.964e-231	2.132e-226	1.0000	-230.5281
2-Hydroxyhexanoa	1.386e-232	1.812e-227	0.8027	-231.9536
1-Pentyne(aq)	2.143e-233	1.455e-228	1.0000	-232.6691
Hexanoate	5.698e-235	6.540e-230	0.8027	-234.3397
o-Phthalate	4.319e-235	7.064e-230	0.4074	-234.7546
2-Hydroxyhexanoi	2.961e-236	3.900e-231	1.0000	-235.5286
Hexanoic_acid(aq	1.565e-237	1.812e-232	1.0000	-236.8055
Pimelate	1.074e-241	1.693e-236	0.4074	-241.3590
H-Pimelate	6.692e-244	1.062e-238	0.8027	-243.2699
Pimelic_acid(aq)	7.946e-247	1.268e-241	1.0000	-246.0999
Hexanal(aq)	6.538e-260	6.527e-255	1.0000	-259.1845
Toluene(aq)	1.063e-264	9.761e-260	1.0000	-263.9735
p-Toluate	2.825e-268	3.805e-263	0.8027	-267.6445
m-Toluate	1.541e-268	2.076e-263	0.8027	-267.9076
1-Hexanol(aq)	7.036e-270	7.165e-265	1.0000	-269.1527
o-Toluate	1.458e-270	1.964e-265	0.8027	-269.9317
p-Toluic_acid(aq	2.608e-271	3.539e-266	1.0000	-270.5837
m-Toluic_acid(aq	1.111e-271	1.508e-266	1.0000	-270.9543
1-Hexene(aq)	2.289e-272	1.920e-267	1.0000	-271.6404
o-Toluic_acid(aq	4.179e-274	5.671e-269	1.0000	-273.3790
n-Hexane(aq)	3.877e-275	3.330e-270	1.0000	-274.4115
2-Hydroxyheptano	2.677e-276	3.873e-271	0.8027	-275.6679
1-Hexyne(aq)	2.872e-277	2.351e-272	1.0000	-276.5418
Heptanoate	1.278e-278	1.645e-273	0.8027	-277.9891
2-Hydroxyheptano	5.729e-280	8.348e-275	1.0000	-279.2419
Heptanoic_acid(a	3.806e-281	4.939e-276	1.0000	-280.4195
Suberate	8.170e-287	1.402e-281	0.4074	-286.4777
H-Suberate	4.932e-289	8.513e-284	0.8027	-288.4025
Suberic_acid(aq)	6.150e-292	1.068e-286	1.0000	-291.2111
Fe(But)2(aq)	8.250e-296	1.892e-290	1.0000	-295.0836
Ca(But)2(aq)	7.050e-296	1.506e-290	1.0000	-295.1518
Mg(But)2(aq)	1.585e-296	3.136e-291	1.0000	-295.7999
Mn(But)2(aq)	4.460e-297	1.019e-291	1.0000	-296.3507
Na(But)2-	3.092e-297	6.077e-292	0.8027	-296.6052
K(But)2-	1.555e-297	3.306e-292	0.8027	-296.9037
Heptanal(aq)	1.264e-304	1.438e-299	1.0000	-300.0000
1-Heptanol(aq)	1.073e-314	1.242e-309	1.0000	-300.0000
1-Heptene(aq)	4.210e-316	4.120e-311	1.0000	-300.0000
n-Heptane(aq)	7.455e-319	7.445e-314	1.0000	-300.0000
2-Hydroxyoctanoa	5.167e-320	8.199e-315	0.8027	-300.0000
1-Heptyne(aq)	3.513e-321	3.367e-316	1.0000	-300.0000
Octanoate	4.101e-322	5.853e-317	0.8027	-300.0000
2-Hydroxyoctanoi	9.881e-324	1.578e-318	1.0000	-300.0000
H-Azelate	0.000	0.000	0.8027	-300.0000
Octanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Octanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxynonanoi	0.000	0.000	1.0000	-300.0000
Nonanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Nonanoate	0.000	0.000	0.8027	-300.0000
Nonanal(aq)	0.000	0.000	1.0000	-300.0000

2-Hydroxynonanoa	0.000	0.000	0.8027	-300.0000
Na(Pent)2-	0.000	0.000	0.8027	-300.0000
Fe(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
Mn(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoi	0.000	0.000	1.0000	-300.0000
Mg(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoa	0.000	0.000	0.8027	-300.0000
Ethylbenzene(aq)	0.000	0.000	1.0000	-300.0000
Azelate	0.000	0.000	0.4074	-300.0000
1-Octyne(aq)	0.000	0.000	1.0000	-300.0000
Dodecanoic_acid(	0.000	0.000	1.0000	-300.0000
Azelaic_acid(aq)	0.000	0.000	1.0000	-300.0000
Dodecanoate	0.000	0.000	0.8027	-300.0000
Decanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Decanoate	0.000	0.000	0.8027	-300.0000
Decanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hexanone(aq)	0.000	0.000	1.0000	-300.0000
1-Octene(aq)	0.000	0.000	1.0000	-300.0000
K(Pent)2-	0.000	0.000	0.8027	-300.0000
2-Heptanone(aq)	0.000	0.000	1.0000	-300.0000
n-Propylbenzene(	0.000	0.000	1.0000	-300.0000
n-Pentylbenzene(	0.000	0.000	1.0000	-300.0000
n-Octylbenzene(a	0.000	0.000	1.0000	-300.0000
n-Octane(aq)	0.000	0.000	1.0000	-300.0000
2-Pentanone(aq)	0.000	0.000	1.0000	-300.0000
2-Butanone(aq)	0.000	0.000	1.0000	-300.0000
1-Octanol(aq)	0.000	0.000	1.0000	-300.0000
n-Hexylbenzene(a	0.000	0.000	1.0000	-300.0000
n-Heptylbenzene(	0.000	0.000	1.0000	-300.0000
n-Butylbenzene(a	0.000	0.000	1.0000	-300.0000
2-Octanone(aq)	0.000	0.000	1.0000	-300.0000
Undecanoic_acid(	0.000	0.000	1.0000	-300.0000
Undecanoate	0.000	0.000	0.8027	-300.0000
Sebacic_acid(aq)	0.000	0.000	1.0000	-300.0000
Sebacate	0.000	0.000	0.4074	-300.0000
Ca(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
H-Sebacate	0.000	0.000	0.8027	-300.0000

Surface species	molality	moles	Boltzman fct.	log molality
>(w)FeOH	0.009586	0.003224	1.0000	-2.0184
>(w)FeOH2+	0.003164	0.001064	2.8270	-2.4997
>(w)FeOHSO4--	0.002567	0.0008635	0.12512	-2.5905
>(w)FeOMg+	0.002100	0.0007064	2.8270	-2.6777
>(w)FeOCa+	0.0007880	0.0002650	2.8270	-3.1035
>(w)FeO-	0.0006652	0.0002237	0.35373	-3.1771
>(w)FeOMn+	0.0005015	0.0001687	2.8270	-3.2997
>(w)FeSO4-	0.0004248	0.0001429	0.35373	-3.3718
>(s)FeOHCa++	0.0002877	9.677e-05	7.9921	-3.5410
>(s)FeOMn+	0.0002061	6.931e-05	2.8270	-3.6860

>(w)FeH2BO3	0.0001303	4.383e-05	1.0000	-3.8850
>(s)FeOH	3.129e-06	1.052e-06	1.0000	-5.5046
>(s)FeOH2+	1.033e-06	3.474e-07	2.8270	-5.9859
>(s)FeO-	2.171e-07	7.302e-08	0.35373	-6.6633

(Boltzman factor = exp(zF PSI/RT), where PSI is surface potential)

Mineral saturation states

	log Q/K		log Q/K
Hematite	11.4965s/sat	MgSO4	-10.7071
Magnetite	10.9266s/sat	Periclase	-10.7260
Goethite	5.2825s/sat	Portlandite	-10.9671
Ferrite-Ca	1.6250s/sat	Na2CO3:7H2O	-11.0853
Ferrite-Mg	1.1579s/sat	Borax	-12.2600
Dolomite-ord	0.4169s/sat	Thermonatrite	-12.4764
Dolomite	0.4169s/sat	Na2CO3	-12.7837
Powellite	0.1914s/sat	Bixbyite	-14.3787
Gypsum	0.1267s/sat	MnCl2:4H2O	-15.2141
Calcite	0.0597s/sat	Pyrolusite	-15.2409
Fe(OH)3	0.0000 sat	Hausmannite	-16.0857
Siderite	-0.0511	MgOHCl	-16.2494
Aragonite	-0.0852	Hydromagnesite	-16.2660
Ice	-0.0932	MnCl2:2H2O	-16.6303
Anhydrite	-0.1676	MnCl2:H2O	-18.2912
Rhodochrosite	-0.4131	MgCl2:4H2O	-18.3269
Monohydrocalcite	-0.7451	Lime	-21.4646
Bassanite	-0.8161	Lawrencite	-21.6304
CaSO4:0.5H2O(bet	-0.9996	Scacchite	-21.6754
Dolomite-dis	-1.2176	Hydrophilite	-22.2012
Magnesite	-1.3469	Ferrite-Dicalciu	-22.6988
Boric_acid	-2.1771	C	-24.0507
Jarosite	-2.6145	MgCl2:2H2O	-24.0911
Wustite	-3.7231	Fe	-24.6113
FeO	-3.8766	MgCl2:H2O	-27.6319
Melanterite	-4.0205	KMgCl3:2H2O	-31.9848
Fe(OH)2	-4.1729	Chloromagnesite	-33.6620
Nesquehonite	-4.4275	S	-34.3793
Brucite	-5.4054	KMgCl3	-39.6727
Huntite	-5.6402	Troilite	-40.4933
Nahcolite	-5.6414	Pyrrhotite	-40.5965
Mn(OH)2(am)	-6.0370	Molysite	-41.9078
Mirabilite	-6.0740	Fe2(SO4)3	-43.1170
Arcanite	-6.1401	Alabandite	-44.4796
Thenardite	-7.4523	Mn	-49.9177
Sylvite	-7.5102	Na	-52.2485
Artinite	-7.6343	Mo	-54.5156
Halite	-8.1657	K	-56.1258
Mg1.25SO4(OH)0.5	-8.2097	Li	-59.3365
Manganosite	-8.8248	Na2O	-60.8824
Mg1.5SO4(OH)	-9.4871	Pyrite	-64.0383

FeSO4	-9.6348	B	-76.6450
MnSO4	-10.0186	K2O	-78.4193
NaFeO2	-10.2495	Mg	-89.5856
Natron	-10.5683	Ca	-106.6400
B2O3	-10.6403	o-Phthalic_acid	-239.4482

Gases	partial press. (bar)	fugacity	fug. coef.	log fug.
H2O(g)	0.01309	0.01226	0.9369	-1.9114
CO2(g)	0.001987	0.001975	0.9942	-2.7044
HCl(g)	9.316e-19	9.316e-19	1.000*	-18.0308
H2(g)	4.581e-19	4.585e-19	1.001	-18.3387
CO(g)	2.986e-25	2.986e-25	1.000*	-24.5249
SO2(g)	5.840e-31	5.735e-31	0.9820	-30.2415
H2S(g)	2.074e-47	2.056e-47	0.9913	-46.6870
O2(g)	2.306e-51	2.304e-51	0.9992	-50.6376
CH4(g)	5.099e-52	5.088e-52	0.9980	-51.2934
Cl2(g)	3.428e-53	3.428e-53	1.000*	-52.4650
Na(g)	3.073e-67	3.073e-67	1.000*	-66.5124
K(g)	4.293e-68	4.293e-68	1.000*	-67.3673
Li(g)	2.126e-83	2.126e-83	1.000*	-82.6725
S2(g)	2.539e-84	2.539e-84	1.000*	-83.5953
C2H4(g)	7.966e-98	7.966e-98	1.000*	-97.0987
Mg(g)	4.379e-111	4.379e-111	1.000*	-110.3586
Ca(g)	7.037e-134	7.037e-134	1.000*	-133.1526
C(g)	1.256e-147	1.256e-147	1.000*	-146.9011
B(g)	8.915e-173	8.915e-173	1.000*	-172.0499

*no data, gas taken to be ideal

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
H2O	18.8	18.7	9.97e+05	-0.000187	-9.97	
B(OH)3(aq)	0.00115	0.00111	203.	4.38e-05	8.03	
Ca++	0.00802	0.00765	909.	0.000362	43.0	
Cl-	5.82e-05	5.82e-05	6.11			
Fe++	0.0336	4.63e-05	7.66			
H+	-0.0672	1.80e-05	0.0538	-0.000226	-0.674	
HCO3-	0.000380	0.000380	68.7			
K+	0.000508	0.000508	58.8			
Li+	2.73e-05	2.73e-05	0.561			
Mg++	0.00193	0.00123	88.3	0.000706	50.9	
Mn++	0.000263	2.49e-05	4.05	0.000238	38.7	
MoO4--	1.84e-06	1.84e-06	0.871			
Na+	0.000740	0.000740	50.4			
O2(aq)	0.00838	1.98e-13	1.88e-08			
SO4--	0.00769	0.00668	1.90e+03	0.00101	286.	
>(s)FeOH	0.000168					
>(w)FeOH	0.00670					

Sorbed	fraction	log fraction
B(OH)3(aq)	0.03803	-1.420
Ca++	0.04514	-1.345
Mg++	0.3657	-0.437
Mn++	0.9054	-0.043
SO4--	0.1309	-0.883

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Boron	0.001153	0.001109	35.53	4.383e-05	1.404
Calcium	0.008015	0.007653	909.0	0.0003618	42.97
Carbon	0.0003799	0.0003799	13.52		
Chlorine	5.818e-05	5.818e-05	6.112		
Hydrogen	37.44	37.34	1.115e+05	-0.0004677	-1.397
Iron	0.03356	4.625e-05	7.655		
Lithium	2.729e-05	2.729e-05	0.5614		
Magnesium	0.001932	0.001225	88.26	0.0007064	50.88
Manganese	0.0002629	2.488e-05	4.051	0.0002380	38.75
Molybdenum	1.838e-06	1.838e-06	0.5227		
Oxygen	18.80	18.70	8.866e+05	0.003970	188.2
Potassium	0.0005077	0.0005077	58.83		
Sodium	0.0007400	0.0007400	50.41		
Sulfur	0.007688	0.006682	634.9	0.001006	95.63

MW-08R Spec8 Output

Temperature =	11.8 C	Pressure =	1.013 bars
pH =	7.193	log fO2 =	-47.727
Eh =	0.1505 volts	pe =	2.6622
Ionic strength	=	0.022848 molal	
Charge imbalance	=	0.002308 eq/kg (9.083% error)	
Activity of water	=	0.999994	
Solvent mass	=	0.33700 kg	
Solution mass	=	0.33740 kg	
Mineral mass	=	1.7760 kg	
Solution density	=	1.022 g/cm3	
Solution viscosity	=	0.013 poise	
Chlorinity	=	0.000156 molal	
Dissolved solids	=	1195 mg/kg sol'n	
Elect. conductivity	=	1279.51 uS/cm (or umho/cm)	
Hardness	=	708.44 mg/kg sol'n as CaCO3	
carbonate	=	154.00 mg/kg sol'n as CaCO3	
non-carbonate	=	554.44 mg/kg sol'n as CaCO3	
Carbonate alkalinity	=	154.00 mg/kg sol'n as CaCO3	
Water type	=	Ca-SO4	
Bulk volume	=	1.00e+03 cm3	
Fluid volume	=	330. cm3	
Mineral volume	=	1.15 cm3	
Inert volume	=	669. cm3	
Porosity	=	33.0 %	
Permeability	=	8.80e-09 cm2	
HFO sorbing surface:			
Surface charge	=	1.19 uC/cm2	
Surface potential	=	32.3 mV	
Surface area	=	2.15e+07 cm2	

Minerals in system	moles	log moles	grams	volume (cm3)
Fe(OH)3	0.03351	-1.475	3.581	1.151
(total)			3.581	670.0

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Ca++	0.004817	192.8	0.5854	-2.5498
SO4--	0.004207	403.6	0.5600	-2.6279
HCO3-	0.002963	180.6	0.8664	-2.5906
B(OH)3(aq)	0.002447	151.1	1.0000	-2.6113
Na+	0.001560	35.81	0.8664	-2.8693
Mg++	0.001059	25.72	0.6081	-3.1910
CaSO4(aq)	0.0008058	109.6	1.0000	-3.0938
CO2(aq)	0.0004664	20.50	1.0000	-3.3312
K+	0.0003339	13.04	0.8610	-3.5414
MgSO4(aq)	0.0002795	33.61	1.0000	-3.5536
Cl-	0.0001561	5.529	0.8610	-3.8715

CaHCO3+	9.626e-05	9.720	0.8664	-4.0788
Li+	3.686e-05	0.2555	0.8761	-4.4910
Fe++	3.457e-05	1.928	0.5854	-4.6939
MgHCO3+	2.134e-05	1.819	0.8664	-4.7330
BO2-	1.786e-05	0.7636	0.8664	-4.8105
NaHCO3(aq)	6.422e-06	0.5389	1.0000	-5.1923
CaCO3(aq)	6.265e-06	0.6263	1.0000	-5.2031
KSO4-	5.874e-06	0.7931	0.8664	-5.2933
Mn++	3.531e-06	0.1937	0.5854	-5.6847
MoO4--	2.573e-06	0.4111	0.5666	-5.8362
CO3--	2.391e-06	0.1433	0.5666	-5.8681
MnSO4(aq)	9.633e-07	0.1453	1.0000	-6.0162
MgCO3(aq)	7.323e-07	0.06167	1.0000	-6.1353
CaCl+	8.880e-08	0.006699	0.8664	-7.1139
MgCl+	7.909e-08	0.004721	0.8664	-7.1642
H+	7.214e-08	7.262e-05	0.8882	-7.1933
OH-	6.128e-08	0.001041	0.8637	-7.2763
NaCl(aq)	2.829e-08	0.001652	1.0000	-7.5483
HSO4-	1.198e-08	0.001162	0.8664	-7.9838
NaCO3-	1.001e-08	0.0008299	0.8664	-8.0618
FeCl+	2.150e-09	0.0001960	0.8664	-8.7299
KCl(aq)	9.551e-10	7.112e-05	1.0000	-9.0200
MnCl+	4.800e-10	4.333e-05	0.8664	-9.3811
LiCl(aq)	1.258e-10	5.325e-06	1.0000	-9.9005
FeCO3+	1.752e-11	2.027e-06	0.8664	-10.8188
CaCl2(aq)	1.400e-11	1.552e-06	1.0000	-10.8538
NaOH(aq)	1.244e-11	4.970e-07	1.0000	-10.9051
HCl(aq)	1.821e-12	6.631e-08	1.0000	-11.7397
KHSO4(aq)	1.756e-13	2.389e-08	1.0000	-12.7554
Fe+++	1.694e-15	9.452e-11	0.3384	-15.2415
FeCl2(aq)	1.234e-15	1.562e-10	1.0000	-14.9087
FeSO4+	8.668e-17	1.315e-11	0.8664	-16.1244
FeCl++	1.121e-20	1.022e-15	0.5666	-20.1971
FeCl4--	1.207e-22	2.382e-17	0.5600	-22.1703
Formate	6.512e-23	2.928e-18	0.8637	-22.2499
H2(aq)	8.160e-24	1.643e-20	1.0000	-23.0883
Ca(For)+	5.426e-24	4.611e-19	0.8664	-23.3278
Mg(For)+	1.474e-24	1.020e-19	0.8664	-23.8939
Fe(For)+	1.134e-25	1.143e-20	0.8664	-25.0075
Na(For)(aq)	8.975e-26	6.096e-21	1.0000	-25.0470
Formic_acid(aq)	2.112e-26	9.711e-22	1.0000	-25.6752
K(For)(aq)	1.673e-26	1.406e-21	1.0000	-25.7765
SO3--	1.160e-26	9.273e-22	0.5666	-26.1824
Mn(For)+	7.937e-27	7.924e-22	0.8664	-26.1626
HSO3-	6.971e-27	5.645e-22	0.8664	-26.2190
CO(aq)	3.565e-29	9.974e-25	1.0000	-28.4479
Mn+++	3.135e-29	1.720e-24	0.2849	-29.0491
Oxalate	5.077e-30	4.463e-25	0.5600	-29.5463
SO2(aq)	2.148e-32	1.375e-27	1.0000	-31.6679
H-Oxalate	3.497e-33	3.109e-28	0.8664	-32.5186

Oxalic_acid(aq)	3.528e-39	3.173e-34	1.0000	-38.4525
Ca(For)2(aq)	2.301e-45	2.990e-40	1.0000	-44.6381
ClO-	1.910e-45	9.817e-41	0.8664	-44.7812
Mg(For)2(aq)	7.609e-46	8.690e-41	1.0000	-45.1187
Fe(For)2(aq)	1.170e-46	1.705e-41	1.0000	-45.9318
Mn(For)2(aq)	5.993e-48	8.677e-43	1.0000	-47.2224
Na(For)2-	4.073e-48	4.598e-43	0.8664	-47.4524
HO2-	3.960e-48	1.306e-43	0.8664	-47.4646
K(For)2-	6.445e-49	8.313e-44	0.8664	-48.2531
S2O6--	3.756e-49	6.006e-44	0.5600	-48.6772
Formaldehyde(aq)	6.653e-51	1.995e-46	1.0000	-50.1770
O2(aq)	3.099e-51	9.905e-47	1.0000	-50.5088
HSO5-	3.808e-54	4.301e-49	0.8664	-53.4815
HS-	7.832e-55	2.587e-50	0.8637	-54.1698
H2S(aq)	6.813e-55	2.319e-50	1.0000	-54.1666
S2O5--	1.038e-57	1.494e-52	0.5600	-57.2357
Methanol(aq)	1.974e-58	6.317e-54	1.0000	-57.7047
S2O3--	1.434e-59	1.606e-54	0.5600	-59.0952
Methane(aq)	1.241e-60	1.989e-56	1.0000	-59.9062
S--	8.523e-61	2.730e-56	0.5730	-60.3112
MnO4--	1.384e-61	1.644e-56	0.5600	-61.1108
Glycolate	2.917e-64	2.187e-59	0.8664	-63.5973
Ca(Glyc)+	4.222e-65	4.855e-60	0.8664	-64.4367
Acetate	7.841e-66	4.624e-61	0.8689	-65.1667
Mg(Glyc)+	4.488e-66	4.454e-61	0.8664	-65.4102
Fe(Glyc)+	1.207e-66	1.578e-61	0.8664	-65.9807
Na(Glyc)(aq)	4.111e-67	4.025e-62	1.0000	-66.3861
CaCH3COO+	1.982e-67	1.963e-62	0.8664	-66.7651
MgCH3COO+	1.218e-67	1.014e-62	0.8664	-66.9767
Glycolic_acid(aq	1.151e-67	8.740e-63	1.0000	-66.9391
K(Glyc)(aq)	7.663e-68	8.737e-63	1.0000	-67.1156
Mn(Glyc)+	2.736e-68	3.552e-63	0.8664	-67.6252
Acetic_acid(aq)	2.532e-68	1.518e-63	1.0000	-67.5966
NaCH3COO(aq)	7.660e-69	6.277e-64	1.0000	-68.1158
S2O4--	5.529e-69	7.076e-64	0.5730	-68.4992
FeCH3COO+	3.564e-69	4.090e-64	0.8664	-68.5103
MnO4-	3.105e-69	3.689e-64	0.8637	-68.5715
S2O8--	1.994e-69	3.827e-64	0.5600	-68.9520
KCH3COO(aq)	1.016e-69	9.959e-65	1.0000	-68.9931
LiCH3COO(aq)	5.244e-70	3.456e-65	1.0000	-69.2803
MnCH3COO+	3.059e-70	3.482e-65	0.8664	-69.5767
Malonate	2.603e-74	2.653e-69	0.5600	-73.8363
H-Malonate	5.068e-76	5.216e-71	0.8664	-75.3575
ClO2-	4.286e-79	2.887e-74	0.8664	-78.4303
Malonic_acid(aq)	2.059e-80	2.140e-75	1.0000	-79.6863
S3O6--	5.338e-90	1.025e-84	0.5600	-89.5245
Acetaldehyde(aq)	1.240e-91	5.455e-87	1.0000	-90.9066
ClO3-	3.020e-98	2.517e-93	0.8637	-97.5836
S2--	4.905e-99	3.142e-94	0.5600	-98.5612
Ethanol(aq)	8.429e-104	3.878e-99	1.0000	-103.0742

Ethylene(aq)	1.460e-108	4.090e-104	1.0000	-107.8357
Lactate	1.364e-109	1.213e-104	0.8664	-108.9276
Ethane(aq)	2.429e-110	7.297e-106	1.0000	-109.6145
Ca(Lac)+	1.161e-110	1.497e-105	0.8664	-109.9976
Mg(Lac)+	2.130e-111	2.412e-106	0.8664	-110.7339
Fe(Lac)+	4.983e-112	7.212e-107	0.8664	-111.3648
Na(Lac)(aq)	1.958e-112	2.192e-107	1.0000	-111.7081
Lactic_acid(aq)	5.653e-113	5.086e-108	1.0000	-112.2477
K(Lac)(aq)	3.651e-113	4.674e-108	1.0000	-112.4376
Propanoate	2.388e-113	1.743e-108	0.8664	-112.6843
Ethyne(aq)	9.342e-114	2.430e-109	1.0000	-113.0296
Mn(Lac)+	9.043e-114	1.301e-108	0.8664	-113.1060
S4O6--	1.887e-114	4.226e-109	0.5600	-113.9761
Ca(Prop)+	3.355e-115	3.792e-110	0.8664	-114.5366
Propanoic_acid(a	1.035e-115	7.656e-111	1.0000	-114.9852
Mg(Prop)+	1.003e-115	9.751e-111	0.8664	-115.0612
Na(Prop)(aq)	3.382e-116	3.244e-111	1.0000	-115.4709
Fe(Prop)+	2.516e-116	3.240e-111	0.8664	-115.6616
K(Prop)(aq)	6.304e-117	7.063e-112	1.0000	-116.2004
Mn(Prop)+	1.087e-117	1.390e-112	0.8664	-117.0261
Succinate	3.205e-120	3.715e-115	0.5600	-119.7460
ClO4-	8.423e-122	8.367e-117	0.8637	-121.1381
H-Succinate	5.873e-122	6.868e-117	0.8664	-121.2934
Succinic_acid(aq	5.701e-125	6.724e-120	1.0000	-124.2440
Ca(Glyc)2(aq)	1.971e-127	3.744e-122	1.0000	-126.7053
Fe(Glyc)2(aq)	1.789e-128	3.680e-123	1.0000	-127.7474
Mg(Glyc)2(aq)	1.265e-128	2.203e-123	1.0000	-127.8979
Na(Glyc)2-	1.306e-130	2.258e-125	0.8664	-129.9462
Mn(Glyc)2(aq)	5.203e-131	1.065e-125	1.0000	-130.2838
Ca(CH3COO)2(aq)	2.360e-131	3.728e-126	1.0000	-130.6271
K(Glyc)2-	2.116e-131	3.999e-126	0.8664	-130.7367
Mg(CH3COO)2(aq)	6.070e-132	8.634e-127	1.0000	-131.2168
Fe(CH3COO)2(aq)	4.883e-133	8.483e-128	1.0000	-132.3113
Na(CH3COO)2-	3.361e-134	4.736e-129	0.8664	-133.5358
Acetone(aq)	3.325e-134	1.929e-129	1.0000	-133.4782
Mn(CH3COO)2(aq)	1.612e-134	2.786e-129	1.0000	-133.7926
Li(CH3COO)2-	5.623e-135	7.022e-130	0.8664	-134.3123
K(CH3COO)2-	2.961e-135	4.649e-130	0.8664	-134.5908
S3--	2.468e-137	2.372e-132	0.5600	-136.8594
Propanal(aq)	1.390e-138	8.062e-134	1.0000	-137.8570
BH4-	1.832e-143	2.715e-139	0.8664	-142.7994
1-Propanol(aq)	2.922e-151	1.754e-146	1.0000	-150.5343
1-Propene(aq)	8.927e-154	3.752e-149	1.0000	-153.0493
1-Propyne(aq)	4.625e-157	1.851e-152	1.0000	-156.3349
2-Hydroxybutanoa	1.705e-157	1.756e-152	0.8664	-156.8304
Propane(aq)	3.390e-158	1.493e-153	1.0000	-157.4698
2-Hydroxybutanoi	6.263e-161	6.513e-156	1.0000	-160.2032
Butanoate	2.356e-161	2.050e-156	0.8664	-160.6901
Ca(But)+	2.271e-163	2.884e-158	0.8664	-162.7061
Butanoic_acid(aq	8.200e-164	7.216e-159	1.0000	-163.0862

Mg(But)+	6.469e-164	7.198e-159	0.8664	-163.2514
Na(But)(aq)	3.207e-164	3.526e-159	1.0000	-163.4939
Fe(But)+	2.565e-164	3.663e-159	0.8664	-163.6531
K(But)(aq)	5.979e-165	7.536e-160	1.0000	-164.2234
Mn(But)+	9.141e-166	1.297e-160	0.8664	-165.1013
Glutarate	2.637e-167	3.427e-162	0.5600	-166.8307
S5O6--	1.235e-168	3.161e-163	0.5600	-168.1603
H-Glutarate	2.828e-169	3.703e-164	0.8664	-168.6109
Glutaric_acid(aq	3.504e-172	4.624e-167	1.0000	-171.4554
Ethylacetate(aq)	6.437e-173	5.664e-168	1.0000	-172.1913
S4--	7.329e-176	9.389e-171	0.5600	-175.3868
Butanal(aq)	4.828e-188	3.477e-183	1.0000	-187.3163
Mn(CH3COO)3-	4.362e-199	1.011e-193	0.8664	-198.4226
1-Butanol(aq)	5.484e-200	4.060e-195	1.0000	-199.2609
1-Butene(aq)	5.342e-202	2.994e-197	1.0000	-201.2723
1-Butyne(aq)	4.304e-205	2.325e-200	1.0000	-204.3661
2-Hydroxypentano	3.203e-205	3.747e-200	0.8664	-204.5568
n-Butane(aq)	4.132e-206	2.399e-201	1.0000	-205.3838
2-Hydroxypentano	6.940e-209	8.188e-204	1.0000	-208.1587
Pentanoate	2.767e-209	2.795e-204	0.8664	-208.6202
Ca(Pent)+	1.580e-211	2.228e-206	0.8664	-210.8637
Pentanoic_acid(a	1.048e-211	1.069e-206	1.0000	-210.9798
Mg(Pent)+	4.399e-212	5.511e-207	0.8664	-211.4189
Na(Pent)(aq)	3.982e-212	4.937e-207	1.0000	-211.3999
Fe(Pent)+	2.820e-212	4.422e-207	0.8664	-211.6120
K(Pent)(aq)	7.424e-213	1.040e-207	1.0000	-212.1294
Mn(Pent)+	8.303e-214	1.294e-208	0.8664	-213.1430
S5--	1.281e-214	2.051e-209	0.5600	-214.1444
Adipate	8.051e-217	1.159e-211	0.5600	-216.3460
Ca(Lac)2(aq)	1.627e-218	3.546e-213	1.0000	-217.7887
H-Adipate	8.441e-219	1.224e-213	0.8664	-218.1359
Fe(Lac)2(aq)	3.098e-219	7.240e-214	1.0000	-218.5090
Mg(Lac)2(aq)	3.038e-219	6.143e-214	1.0000	-218.5174
Na(Lac)2-	2.974e-221	5.974e-216	0.8664	-220.5890
Mn(Lac)2(aq)	1.359e-221	3.164e-216	1.0000	-220.8667
Adipic_acid(aq)	1.216e-221	1.775e-216	1.0000	-220.9152
K(Lac)2-	4.817e-222	1.045e-216	0.8664	-221.3795
Ca(Prop)2(aq)	1.228e-227	2.284e-222	1.0000	-226.9107
Fe(Prop)2(aq)	6.639e-228	1.339e-222	1.0000	-227.1779
Mg(Prop)2(aq)	4.933e-228	8.398e-223	1.0000	-227.3069
Na(Prop)2-	5.958e-229	1.006e-223	0.8664	-228.2872
Mn(Prop)2(aq)	1.393e-229	2.799e-224	1.0000	-228.8559
K(Prop)2-	9.633e-230	1.782e-224	0.8664	-229.0785
Phenol(aq)	6.311e-234	5.932e-229	1.0000	-233.1999
Pentanal(aq)	9.925e-236	8.538e-231	1.0000	-235.0033
Benzene(aq)	2.077e-244	1.620e-239	1.0000	-243.6826
1-Pentanol(aq)	1.186e-246	1.044e-241	1.0000	-245.9260
Benzoate	8.474e-248	1.025e-242	0.8761	-247.1294
1-Pentene(aq)	4.884e-250	3.422e-245	1.0000	-249.3112
Benzoic_acid(aq)	7.827e-251	9.547e-246	1.0000	-250.1064

1-Pentyne(aq)	4.150e-253	2.823e-248	1.0000	-252.3820
2-Hydroxyhexanoa	2.487e-253	3.258e-248	0.8664	-252.6666
n-Pentane(aq)	4.160e-254	2.998e-249	1.0000	-253.3809
o-Phthalate	1.066e-254	1.747e-249	0.5600	-254.2242
2-Hydroxyhexanoi	7.690e-257	1.015e-251	1.0000	-256.1140
Hexanoate	2.589e-257	2.978e-252	0.8664	-256.6491
Hexanoic_acid(aq	1.026e-259	1.191e-254	1.0000	-258.9887
Pimelate	1.302e-263	2.057e-258	0.5600	-263.1372
H-Pimelate	1.381e-265	2.196e-260	0.8664	-264.9220
Pimelic_acid(aq)	2.373e-268	3.797e-263	1.0000	-267.6247
Hexanal(aq)	8.897e-284	8.901e-279	1.0000	-283.0508
Toluene(aq)	1.780e-289	1.638e-284	1.0000	-288.7497
p-Toluate	1.549e-292	2.090e-287	0.8664	-291.8724
m-Toluate	8.406e-293	1.135e-287	0.8664	-292.1377
o-Toluate	7.878e-295	1.063e-289	0.8664	-294.1659
1-Hexanol(aq)	2.270e-295	2.317e-290	1.0000	-294.6440
p-Toluic_acid(aq	2.074e-295	2.820e-290	1.0000	-294.6833
m-Toluic_acid(aq	8.793e-296	1.196e-290	1.0000	-295.0559
1-Hexene(aq)	7.069e-298	5.943e-293	1.0000	-297.1506
o-Toluic_acid(aq	3.235e-298	4.399e-293	1.0000	-297.4901
1-Hexyne(aq)	3.180e-301	2.609e-296	1.0000	-300.0000
2-Hydroxyheptano	2.750e-301	3.988e-296	0.8664	-300.0000
n-Hexane(aq)	3.119e-302	2.685e-297	1.0000	-300.0000
2-Hydroxyheptano	8.521e-305	1.244e-299	1.0000	-300.0000
Heptanoate	3.326e-305	4.292e-300	0.8664	-300.0000
Heptanoic_acid(a	1.431e-307	1.860e-302	1.0000	-300.0000
Suberate	5.592e-313	9.617e-308	0.5600	-300.0000
H-Suberate	5.758e-315	9.961e-310	0.8664	-300.0000
Suberic_acid(aq)	1.039e-317	1.807e-312	1.0000	-300.0000
Ca(But)2(aq)	4.941e-324	1.057e-318	1.0000	-300.0000
Fe(But)2(aq)	4.941e-324	1.135e-318	1.0000	-300.0000
H-Azelate	0.000	0.000	0.8664	-300.0000
2-Hydroxyoctanoa	0.000	0.000	0.8664	-300.0000
Octanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Octanoate	0.000	0.000	0.8664	-300.0000
Octanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxynonanoi	0.000	0.000	1.0000	-300.0000
Nonanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Nonanoate	0.000	0.000	0.8664	-300.0000
Nonanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxynonanoa	0.000	0.000	0.8664	-300.0000
Na(Pent)2-	0.000	0.000	0.8664	-300.0000
Na(But)2-	0.000	0.000	0.8664	-300.0000
Fe(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
Mn(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
Mn(But)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoi	0.000	0.000	1.0000	-300.0000
1-Heptanol(aq)	0.000	0.000	1.0000	-300.0000
Mg(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoa	0.000	0.000	0.8664	-300.0000

Ethylbenzene(aq)	0.000	0.000	1.0000	-300.0000
Mg(But)2(aq)	0.000	0.000	1.0000	-300.0000
Azelate	0.000	0.000	0.5600	-300.0000
1-Octyne(aq)	0.000	0.000	1.0000	-300.0000
Dodecanoic_acid(	0.000	0.000	1.0000	-300.0000
Azelaic_acid(aq)	0.000	0.000	1.0000	-300.0000
Dodecanoate	0.000	0.000	0.8664	-300.0000
Decanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Decanoate	0.000	0.000	0.8664	-300.0000
Decanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hexanone(aq)	0.000	0.000	1.0000	-300.0000
1-Octene(aq)	0.000	0.000	1.0000	-300.0000
1-Heptyne(aq)	0.000	0.000	1.0000	-300.0000
K(Pent)2-	0.000	0.000	0.8664	-300.0000
2-Heptanone(aq)	0.000	0.000	1.0000	-300.0000
K(But)2-	0.000	0.000	0.8664	-300.0000
n-Propylbenzene(	0.000	0.000	1.0000	-300.0000
n-Pentylbenzene(	0.000	0.000	1.0000	-300.0000
n-Octylbenzene(a	0.000	0.000	1.0000	-300.0000
n-Octane(aq)	0.000	0.000	1.0000	-300.0000
2-Pentanone(aq)	0.000	0.000	1.0000	-300.0000
2-Butanone(aq)	0.000	0.000	1.0000	-300.0000
1-Octanol(aq)	0.000	0.000	1.0000	-300.0000
n-Hexylbenzene(a	0.000	0.000	1.0000	-300.0000
n-Heptylbenzene(	0.000	0.000	1.0000	-300.0000
n-Heptane(aq)	0.000	0.000	1.0000	-300.0000
n-Butylbenzene(a	0.000	0.000	1.0000	-300.0000
Heptanal(aq)	0.000	0.000	1.0000	-300.0000
2-Octanone(aq)	0.000	0.000	1.0000	-300.0000
Undecanoic_acid(	0.000	0.000	1.0000	-300.0000
Undecanoate	0.000	0.000	0.8664	-300.0000
Sebacic_acid(aq)	0.000	0.000	1.0000	-300.0000
Sebacate	0.000	0.000	0.5600	-300.0000
Ca(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
H-Sebacate	0.000	0.000	0.8664	-300.0000
2-Hydroxyoctanoi	0.000	0.000	1.0000	-300.0000
1-Heptene(aq)	0.000	0.000	1.0000	-300.0000

Surface species	molality	moles	Boltzman fct.	log molality
>(w)FeOH	0.01147	0.003865	1.0000	-1.9405
>(w)FeOH2+	0.004075	0.001373	3.5162	-2.3898
>(w)FeOHSO4--	0.002060	0.0006941	0.080881	-2.6862
>(w)FeOMg+	0.0008237	0.0002776	3.5162	-3.0842
>(w)FeO-	0.0007395	0.0002492	0.28440	-3.1311
>(s)FeOHCa++	0.0004015	0.0001353	12.364	-3.3963
>(w)FeSO4-	0.0003668	0.0001236	0.28440	-3.4356
>(w)FeOCa+	0.0002028	6.833e-05	3.5162	-3.6930
>(w)FeH2BO3	0.0001170	3.943e-05	1.0000	-3.9318
>(s)FeOMn+	6.889e-05	2.322e-05	3.5162	-4.1618

>(w)FeOMn+	3.327e-05	1.121e-05	3.5162	-4.4779
>(s)FeOH	1.886e-05	6.357e-06	1.0000	-4.7244
>(s)FeOH2+	6.703e-06	2.259e-06	3.5162	-5.1737
>(s)FeO-	1.216e-06	4.099e-07	0.28440	-5.9150

(Boltzman factor = exp(zF PSI/RT), where PSI is surface potential)

Mineral saturation states

	log Q/K		log Q/K
Hematite	11.5294s/sat	Periclase	-11.3650
Magnetite	10.1482s/sat	MgSO4	-11.4034
Goethite	5.3004s/sat	MnSO4	-11.4655
Ferrite-Ca	0.8481s/sat	Portlandite	-11.7718
Ferrite-Mg	0.5517s/sat	Thermonatrite	-12.3180
Dolomite-ord	0.4864s/sat	Na2CO3	-12.6349
Dolomite	0.4864s/sat	Borax	-13.1789
Calcite	0.0065s/sat	Pyrolusite	-15.0626
Fe(OH)3	0.0000 sat	Bixbyite	-15.5436
Ice	-0.0885	MnCl2:4H2O	-16.2700
Aragonite	-0.1385	Hydromagnesite	-16.4266
Siderite	-0.1506	MgOHCl	-16.7408
Powellite	-0.4525	MnCl2:2H2O	-17.7041
Gypsum	-0.6806	Hausmannite	-18.6022
Monohydrocalcite	-0.7958	MgCl2:4H2O	-18.6365
Anhydrite	-0.9879	MnCl2:H2O	-19.3776
Rhodochrosite	-1.0515	Lawrencite	-22.1952
Dolomite-dis	-1.1581	Lime	-22.3220
Magnesite	-1.2326	Hydrophilite	-22.7225
Bassanite	-1.6369	Scacchite	-22.7789
CaSO4:0.5H2O(bet	-1.8221	Ferrite-Dicalciu	-24.3468
Boric_acid	-2.2851	MgCl2:2H2O	-24.4388
Jarosite	-3.5063	C	-26.6238
Nesquehonite	-4.3289	Fe	-27.1153
Wustite	-4.4218	MgCl2:H2O	-28.0014
FeO	-4.7033	KMgCl3:2H2O	-32.9274
Melanterite	-4.8595	Chloromagnesite	-34.0635
Fe(OH)2	-4.9912	S	-39.3599
Nahcolite	-5.2032	KMgCl3	-40.6595
Huntite	-5.3600	Molysite	-41.5951
Brucite	-6.0130	Fe2(SO4)3	-43.5001
Mirabilite	-6.6093	Troilite	-47.8956
Mn(OH)2(am)	-7.4061	Pyrrhotite	-47.9992
Arcanite	-7.6820	Alabandite	-52.4427
Thenardite	-8.0459	Mn	-53.0743
Sylvite	-8.1013	Na	-53.5318
Artinite	-8.1076	K	-57.9039
Halite	-8.2832	Mo	-59.4019
Mg1.25SO4(OH)0.5	-9.0408	Li	-60.8511
Manganosite	-10.2119	Na2O	-61.6549
Natron	-10.3490	Pyrite	-76.3637

Mg1.5SO4(OH)	-10.4706	B	-79.4785
FeSO4	-10.5405	K2O	-80.2227
NaFeO2	-10.5575	Mg	-92.1705
Na2CO3:7H2O	-10.8878	Ca	-109.4708
B2O3	-10.9028	o-Phthalic_acid	-258.6393

Gases	partial press. (bar)	fugacity	fug. coef.	log fug.
H2O(g)	0.01206	0.01128	0.9352	-1.9476
CO2(g)	0.009050	0.008997	0.9941	-2.0459
HCl(g)	1.071e-18	1.071e-18	1.000*	-17.9702
H2(g)	9.379e-21	9.386e-21	1.001	-20.0275
CO(g)	2.802e-26	2.802e-26	1.000*	-25.5525
SO2(g)	8.684e-33	8.525e-33	0.9817	-32.0693
O2(g)	1.878e-48	1.876e-48	0.9992	-47.7267
Cl2(g)	1.564e-51	1.564e-51	1.000*	-50.8059
H2S(g)	4.614e-54	4.574e-54	0.9912	-53.3397
CH4(g)	6.568e-58	6.554e-58	0.9979	-57.1835
Na(g)	1.303e-68	1.303e-68	1.000*	-67.8850
K(g)	6.035e-70	6.035e-70	1.000*	-69.2193
Li(g)	4.796e-85	4.796e-85	1.000*	-84.3192
S2(g)	2.182e-94	2.182e-94	1.000*	-93.6612
C2H4(g)	2.159e-106	2.159e-106	1.000*	-105.6658
Mg(g)	8.581e-114	8.581e-114	1.000*	-113.0665
Ca(g)	7.381e-137	7.381e-137	1.000*	-136.1319
C(g)	8.685e-151	8.685e-151	1.000*	-150.0612
B(g)	4.491e-176	4.491e-176	1.000*	-175.3477

*no data, gas taken to be ideal

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
H2O	18.8	18.7	9.99e+05	-0.000163		-8.71
B(OH)3(aq)	0.000870	0.000831	152.	3.94e-05		7.23
Ca++	0.00213	0.00193	229.	0.000204		24.2
Cl-	5.27e-05	5.27e-05	5.54			
Fe++	0.0335	1.17e-05	1.93			
H+	-0.0660	0.000148	0.442	0.000869		2.60
HCO3-	0.00120	0.00120	217.			
K+	0.000114	0.000114	13.3			
Li+	1.24e-05	1.24e-05	0.256			
Mg++	0.000736	0.000459	33.0	0.000278		20.0
Mn++	3.59e-05	1.51e-06	0.247	3.44e-05		5.61
MoO4--	8.67e-07	8.67e-07	0.411			
Na+	0.000528	0.000528	36.0			
O2(aq)	0.00838	1.48e-12	1.40e-07			
SO4--	0.00260	0.00179	508.	0.000818		233.
>(s)FeOH	0.000168					
>(w)FeOH	0.00670					

Sorbed	fraction	log fraction
B(OH)3(aq)	0.04532	-1.344
Ca++	0.09546	-1.020
Mg++	0.3770	-0.424
Mn++	0.9579	-0.019
SO4--	0.3141	-0.503

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Boron	0.0008702	0.0008307	26.62	3.943e-05	1.263
Calcium	0.002133	0.001929	229.2	0.0002036	24.19
Carbon	0.001201	0.001201	42.74		
Chlorine	5.268e-05	5.268e-05	5.536		
Hydrogen	37.52	37.42	1.118e+05	0.0006615	1.976
Iron	0.03352	1.165e-05	1.928		
Lithium	1.242e-05	1.242e-05	0.2555		
Magnesium	0.0007363	0.0004587	33.04	0.0002776	20.00
Manganese	3.594e-05	1.515e-06	0.2466	3.443e-05	5.606
Molybdenum	8.672e-07	8.672e-07	0.2466		
Oxygen	18.82	18.72	8.877e+05	0.003226	153.0
Potassium	0.0001145	0.0001145	13.27		
Sodium	0.0005277	0.0005277	35.96		
Sulfur	0.002603	0.001786	169.7	0.0008177	77.71

MW-36 Spec8 Output

Temperature = 11.9 C Pressure = 1.013 bars
pH = 7.133 log fO2 = -51.228
Eh = 0.1041 volts pe = 1.8406
Ionic strength = 0.036872 molal
Charge imbalance = 0.002285 eq/kg (5.755% error)
Activity of water = 0.999976
Solvent mass = 0.33687 kg
Solution mass = 0.33747 kg
Mineral mass = 1.7760 kg
Solution density = 1.023 g/cm3
Solution viscosity = 0.013 poise
Chlorinity = 0.000672 molal
Dissolved solids = 1770 mg/kg sol'n
Elect. conductivity = 1952.70 uS/cm (or umho/cm)
Hardness = 1145.27 mg/kg sol'n as CaCO3
  carbonate = 135.36 mg/kg sol'n as CaCO3
  non-carbonate = 1009.91 mg/kg sol'n as CaCO3
Carbonate alkalinity= 135.36 mg/kg sol'n as CaCO3
Water type = Ca-SO4
Bulk volume = 1.00e+03 cm3
Fluid volume = 330. cm3
Mineral volume = 1.15 cm3
Inert volume = 669. cm3
Porosity = 33.0 %
Permeability = 8.80e-09 cm2
HFO sorbing surface:
  Surface charge = 1.39 uC/cm2
  Surface potential = 30.0 mV
  Surface area = 2.15e+07 cm2

Minerals in system	moles	log moles	grams	volume (cm3)
Fe(OH)3	0.03351	-1.475	3.581	1.151
(total)			3.581	670.0

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
SO4--	0.007734	741.7	0.4944	-2.4175
Ca++	0.006786	271.5	0.5273	-2.4463
HCO3-	0.002576	156.9	0.8406	-2.6645
Mg++	0.002060	49.98	0.5565	-2.9406
Na+	0.002011	46.14	0.8406	-2.7721
CaSO4(aq)	0.001661	225.7	1.0000	-2.7797
B(OH)3(aq)	0.001250	77.14	1.0000	-2.9032
MgSO4(aq)	0.0008091	97.22	1.0000	-3.0920
Cl-	0.0006709	23.74	0.8328	-3.2528
CO2(aq)	0.0004512	19.82	1.0000	-3.3456
Fe++	0.0003810	21.24	0.5273	-3.6970

K+	0.0003507	13.69	0.8328	-3.5345
CaHCO3+	0.0001062	10.71	0.8406	-4.0494
MgHCO3+	3.301e-05	2.812	0.8406	-4.5567
Li+	2.745e-05	0.1902	0.8543	-4.6298
Mn++	2.260e-05	1.240	0.5273	-4.9238
KSO4-	9.987e-06	1.347	0.8406	-5.0760
MnSO4(aq)	9.024e-06	1.360	1.0000	-5.0446
BO2-	8.199e-06	0.3504	0.8406	-5.1616
NaHCO3(aq)	6.765e-06	0.5673	1.0000	-5.1698
CaCO3(aq)	5.858e-06	0.5853	1.0000	-5.2322
CO3--	1.981e-06	0.1187	0.5030	-6.0015
MoO4--	1.467e-06	0.2342	0.5030	-6.1320
MgCO3(aq)	9.594e-07	0.08075	1.0000	-6.0180
MgCl+	6.027e-07	0.03595	0.8406	-6.2953
CaCl+	4.827e-07	0.03639	0.8406	-6.3917
NaCl(aq)	1.472e-07	0.008586	1.0000	-6.8322
FeCl+	9.143e-08	0.008333	0.8406	-7.1143
H+	8.452e-08	8.504e-05	0.8710	-7.1330
OH-	5.544e-08	0.0009411	0.8368	-7.3336
HSO4-	2.308e-08	0.002236	0.8406	-7.7122
MnCl+	1.188e-08	0.001072	0.8406	-8.0006
NaCO3-	9.473e-09	0.0007849	0.8406	-8.0989
KCl(aq)	4.041e-09	0.0003007	1.0000	-8.3936
LiCl(aq)	3.798e-10	1.607e-05	1.0000	-9.4205
CaCl2(aq)	3.066e-10	3.397e-05	1.0000	-9.5134
FeCO3+	1.977e-11	2.286e-06	0.8406	-10.7794
NaOH(aq)	1.363e-11	5.443e-07	1.0000	-10.8654
HCl(aq)	8.693e-12	3.164e-07	1.0000	-11.0608
KHSO4(aq)	3.338e-13	4.537e-08	1.0000	-12.4765
FeCl2(aq)	2.117e-13	2.679e-08	1.0000	-12.6743
Fe+++	3.066e-15	1.709e-10	0.2809	-15.0650
FeSO4+	2.183e-16	3.310e-11	0.8406	-15.7364
FeCl4--	4.051e-19	7.994e-14	0.4944	-18.6983
FeCl++	7.913e-20	7.212e-15	0.5030	-19.4001
Formate	3.298e-21	1.482e-16	0.8368	-20.5592
H2(aq)	4.755e-22	9.569e-19	1.0000	-21.3228
Ca(For)+	3.479e-22	2.956e-17	0.8406	-21.5339
Mg(For)+	1.324e-22	9.161e-18	0.8406	-21.9536
Fe(For)+	5.686e-23	5.725e-18	0.8406	-22.3206
Na(For)(aq)	5.506e-24	3.738e-19	1.0000	-23.2591
Mn(For)+	2.312e-24	2.307e-19	0.8406	-23.7114
SO3--	1.235e-24	9.868e-20	0.5030	-24.2069
Formic_acid(aq)	1.190e-24	5.469e-20	1.0000	-23.9243
K(For)(aq)	8.343e-25	7.006e-20	1.0000	-24.0787
HSO3-	7.808e-25	6.319e-20	0.8406	-24.1829
CO(aq)	2.013e-27	5.628e-23	1.0000	-26.6962
Oxalate	2.381e-28	2.092e-23	0.4944	-27.9292
Mn+++	3.550e-29	1.947e-24	0.2202	-29.1069
SO2(aq)	2.687e-30	1.718e-25	1.0000	-29.5707
H-Oxalate	1.715e-31	1.524e-26	0.8406	-30.8410

Oxalic_acid(aq)	1.929e-37	1.734e-32	1.0000	-36.7146
Ca(For)2(aq)	7.017e-42	9.114e-37	1.0000	-41.1539
Mg(For)2(aq)	3.246e-42	3.705e-37	1.0000	-41.4886
Fe(For)2(aq)	2.786e-42	4.057e-37	1.0000	-41.5550
Mn(For)2(aq)	8.297e-44	1.201e-38	1.0000	-43.0811
Na(For)2-	1.261e-44	1.423e-39	0.8406	-43.9746
K(For)2-	1.623e-45	2.093e-40	0.8406	-44.8650
ClO-	1.463e-46	7.514e-42	0.8406	-45.9102
S2O6--	8.702e-47	1.391e-41	0.4944	-46.3663
Formaldehyde(aq)	2.185e-47	6.549e-43	1.0000	-46.6605
HS-	1.691e-47	5.584e-43	0.8368	-46.8491
H2S(aq)	1.633e-47	5.555e-43	1.0000	-46.7871
HO2-	6.402e-50	2.109e-45	0.8406	-49.2691
S2O3--	6.328e-52	7.083e-47	0.4944	-51.5047
Methanol(aq)	3.734e-53	1.194e-48	1.0000	-52.4278
S--	1.749e-53	5.599e-49	0.5114	-53.0484
S2O5--	1.388e-53	1.997e-48	0.4944	-53.1635
Methane(aq)	1.348e-53	2.159e-49	1.0000	-52.8702
O2(aq)	9.743e-55	3.112e-50	1.0000	-54.0113
HSO5-	1.319e-55	1.489e-50	0.8406	-54.9550
Acetate	7.400e-59	4.362e-54	0.8443	-58.2043
Glycolate	4.799e-59	3.595e-54	0.8406	-58.3942
Ca(Glyc)+	8.807e-60	1.012e-54	0.8406	-59.1305
CaCH3COO+	2.377e-60	2.352e-55	0.8406	-59.6993
MgCH3COO+	2.045e-60	1.702e-55	0.8406	-59.7647
Fe(Glyc)+	1.967e-60	2.570e-55	0.8406	-59.7816
Mg(Glyc)+	1.313e-60	1.302e-55	0.8406	-59.9571
FeCH3COO+	3.342e-61	3.832e-56	0.8406	-60.5514
Acetic_acid(aq)	2.667e-61	1.599e-56	1.0000	-60.5740
NaCH3COO(aq)	8.784e-62	7.193e-57	1.0000	-61.0563
Na(Glyc)(aq)	8.204e-62	8.029e-57	1.0000	-61.0860
Mn(Glyc)+	2.593e-62	3.364e-57	0.8406	-61.6617
Glycolic_acid(aq	2.110e-62	1.601e-57	1.0000	-61.6758
MnCH3COO+	1.666e-62	1.895e-57	0.8406	-61.8538
K(Glyc)(aq)	1.243e-62	1.416e-57	1.0000	-61.9055
KCH3COO(aq)	9.470e-63	9.278e-58	1.0000	-62.0236
S2O4--	4.231e-63	5.412e-58	0.5114	-62.6648
LiCH3COO(aq)	3.489e-63	2.298e-58	1.0000	-62.4573
MnO4--	1.662e-64	1.973e-59	0.4944	-64.0854
Malonate	2.285e-67	2.328e-62	0.4944	-66.9470
H-Malonate	4.652e-69	4.786e-64	0.8406	-68.4077
S2O8--	1.425e-70	2.734e-65	0.4944	-70.1520
MnO4-	5.181e-73	6.151e-68	0.8368	-72.3630
Malonic_acid(aq)	2.107e-73	2.188e-68	1.0000	-72.6764
ClO2-	5.853e-82	3.941e-77	0.8406	-81.3080
S3O6--	5.109e-82	9.802e-77	0.4944	-81.5976
Acetaldehyde(aq)	7.607e-83	3.345e-78	1.0000	-82.1188
S2--	4.202e-86	2.690e-81	0.4944	-85.6824
Ethanol(aq)	2.988e-93	1.374e-88	1.0000	-92.5247
Ethylene(aq)	5.197e-98	1.455e-93	1.0000	-97.2842

Ethane(aq)	4.960e-98	1.489e-93	1.0000	-97.3045
Lactate	4.204e-99	3.738e-94	0.8406	-98.4517
Ca(Lac)+	4.537e-100	5.850e-95	0.8406	-99.4186
Fe(Lac)+	1.522e-100	2.202e-95	0.8406	-99.8929
Mg(Lac)+	1.169e-100	1.322e-95	0.8406	-100.0078
S4O6--	7.407e-101	1.658e-95	0.4944	-100.4363
Propanoate	4.236e-101	3.090e-96	0.8406	-100.4485
Na(Lac)(aq)	7.324e-102	8.193e-97	1.0000	-101.1353
Lactic_acid(aq)	1.943e-102	1.747e-97	1.0000	-101.7116
Mn(Lac)+	1.606e-102	2.309e-97	0.8406	-101.8697
K(Lac)(aq)	1.110e-102	1.420e-97	1.0000	-101.9547
Ca(Prop)+	7.550e-103	8.528e-98	0.8406	-102.1974
ClO3-	7.297e-103	6.079e-98	0.8368	-102.2142
Fe(Prop)+	4.423e-103	5.692e-98	0.8406	-102.4296
Mg(Prop)+	3.160e-103	3.072e-98	0.8406	-102.5757
Propanoic_acid(a	2.046e-103	1.513e-98	1.0000	-102.6891
Na(Prop)(aq)	7.276e-104	6.977e-99	1.0000	-103.1381
Mn(Prop)+	1.111e-104	1.419e-99	0.8406	-104.0298
K(Prop)(aq)	1.103e-104	1.235e-99	1.0000	-103.9576
Ethyne(aq)	5.826e-105	1.514e-100	1.0000	-104.2347
Succinate	5.276e-108	6.113e-103	0.4944	-107.5837
H-Succinate	1.010e-109	1.181e-104	0.8406	-109.0709
Succinic_acid(aq	1.093e-112	1.288e-107	1.0000	-111.9615
Ca(Glyc)2(aq)	6.360e-117	1.207e-111	1.0000	-116.1965
Fe(Glyc)2(aq)	4.506e-117	9.264e-112	1.0000	-116.3462
Ca(CH3COO)2(aq)	2.514e-117	3.969e-112	1.0000	-116.5997
Mg(CH3COO)2(aq)	9.049e-118	1.286e-112	1.0000	-117.0434
Mg(Glyc)2(aq)	5.720e-118	9.958e-113	1.0000	-117.2426
Fe(CH3COO)2(aq)	4.063e-118	7.054e-113	1.0000	-117.3912
S3--	8.728e-119	8.381e-114	0.4944	-118.3650
Mn(CH3COO)2(aq)	7.799e-120	1.347e-114	1.0000	-119.1080
Mn(Glyc)2(aq)	7.626e-120	1.561e-114	1.0000	-119.1177
Na(Glyc)2-	4.282e-120	7.397e-115	0.8406	-119.4438
Acetone(aq)	3.819e-120	2.214e-115	1.0000	-119.4180
Na(CH3COO)2-	3.636e-120	5.120e-115	0.8406	-119.5148
K(Glyc)2-	5.641e-121	1.065e-115	0.8406	-120.3240
Li(CH3COO)2-	3.526e-121	4.401e-116	0.8406	-120.5281
K(CH3COO)2-	2.606e-121	4.089e-116	0.8406	-120.6595
Propanal(aq)	1.600e-124	9.276e-120	1.0000	-123.7959
ClO4-	3.601e-128	3.575e-123	0.8368	-127.5210
1-Propanol(aq)	1.944e-135	1.166e-130	1.0000	-134.7114
BH4-	1.002e-136	1.485e-132	0.8406	-136.0745
1-Propene(aq)	5.958e-138	2.503e-133	1.0000	-137.2249
Propane(aq)	1.299e-140	5.720e-136	1.0000	-139.8862
2-Hydroxybutanoa	9.873e-142	1.016e-136	0.8406	-141.0810
1-Propyne(aq)	5.399e-143	2.159e-138	1.0000	-142.2677
Butanoate	7.846e-144	6.821e-139	0.8406	-143.1808
2-Hydroxybutanoi	4.041e-145	4.200e-140	1.0000	-144.3935
Ca(But)+	9.593e-146	1.218e-140	0.8406	-145.0934
Fe(But)+	8.466e-146	1.208e-140	0.8406	-145.1477

Mg(But)+	3.828e-146	4.258e-141	0.8406	-145.4924
Butanoic_acid(aq	3.044e-146	2.677e-141	1.0000	-145.5165
Na(But)(aq)	1.295e-146	1.423e-141	1.0000	-145.8876
K(But)(aq)	1.963e-147	2.473e-142	1.0000	-146.7071
Mn(But)+	1.754e-147	2.486e-142	0.8406	-146.8315
S5O6--	2.013e-149	5.150e-144	0.4944	-149.0022
Glutarate	8.146e-150	1.058e-144	0.4944	-149.3950
S4--	1.070e-151	1.370e-146	0.4944	-151.2767
H-Glutarate	9.132e-152	1.195e-146	0.8406	-151.1148
Glutaric_acid(aq	1.261e-154	1.663e-149	1.0000	-153.8992
Ethylacetate(aq)	2.403e-155	2.113e-150	1.0000	-154.6193
Butanal(aq)	1.044e-168	7.518e-164	1.0000	-167.9811
Mn(CH3COO)3-	1.989e-177	4.607e-172	0.8406	-176.7769
1-Butanol(aq)	6.852e-179	5.070e-174	1.0000	-178.1642
1-Butene(aq)	6.695e-181	3.750e-176	1.0000	-180.1742
n-Butane(aq)	2.974e-183	1.725e-178	1.0000	-182.5267
2-Hydroxypentano	3.480e-184	4.069e-179	0.8406	-183.5338
S5--	7.717e-185	1.235e-179	0.4944	-184.4185
1-Butyne(aq)	9.434e-186	5.094e-181	1.0000	-185.0253
Pentanoate	1.730e-186	1.746e-181	0.8406	-185.8373
2-Hydroxypentano	8.407e-188	9.914e-183	1.0000	-187.0754
Fe(Pent)+	1.747e-188	2.738e-183	0.8406	-187.8331
Ca(Pent)+	1.253e-188	1.766e-183	0.8406	-187.9775
Pentanoic_acid(a	7.302e-189	7.445e-184	1.0000	-188.1365
Mg(Pent)+	4.887e-189	6.119e-184	0.8406	-188.3863
Na(Pent)(aq)	3.019e-189	3.741e-184	1.0000	-188.5201
K(Pent)(aq)	4.575e-190	6.404e-185	1.0000	-189.3396
Mn(Pent)+	2.990e-190	4.658e-185	0.8406	-189.5997
Adipate	4.675e-194	6.726e-189	0.4944	-193.6362
H-Adipate	5.124e-196	7.423e-191	0.8406	-195.3658
Fe(Lac)2(aq)	2.740e-197	6.401e-192	1.0000	-196.5622
Ca(Lac)2(aq)	1.844e-197	4.017e-192	1.0000	-196.7343
Mg(Lac)2(aq)	4.829e-198	9.758e-193	1.0000	-197.3162
Adipic_acid(aq)	8.226e-199	1.200e-193	1.0000	-198.0848
Mn(Lac)2(aq)	6.997e-200	1.628e-194	1.0000	-199.1551
Na(Lac)2-	3.423e-200	6.873e-195	0.8406	-199.5410
K(Lac)2-	4.509e-201	9.778e-196	0.8406	-200.4213
Fe(Prop)2(aq)	1.945e-202	3.921e-197	1.0000	-201.7111
Ca(Prop)2(aq)	4.611e-203	8.572e-198	1.0000	-202.3362
Mg(Prop)2(aq)	2.591e-203	4.409e-198	1.0000	-202.5865
Mn(Prop)2(aq)	2.374e-204	4.766e-199	1.0000	-203.6245
Na(Prop)2-	2.269e-204	3.832e-199	0.8406	-203.7195
K(Prop)2-	2.984e-205	5.519e-200	0.8406	-204.6005
Phenol(aq)	2.471e-209	2.322e-204	1.0000	-208.6071
Pentanal(aq)	4.031e-211	3.466e-206	1.0000	-210.3946
Benzene(aq)	4.696e-218	3.661e-213	1.0000	-217.3283
1-Pentanol(aq)	2.779e-220	2.445e-215	1.0000	-219.5561
Benzoate	1.657e-221	2.003e-216	0.8543	-220.8491
1-Pentene(aq)	1.149e-223	8.047e-219	1.0000	-222.9395
Benzoic_acid(aq)	1.714e-224	2.090e-219	1.0000	-223.7660

n-Pentane(aq)	5.622e-226	4.049e-221	1.0000	-225.2501
2-Hydroxyhexanoa	5.076e-227	6.645e-222	0.8406	-226.3699
o-Phthalate	1.942e-228	3.182e-223	0.4944	-228.0176
1-Pentyne(aq)	1.708e-228	1.161e-223	1.0000	-227.7676
Hexanoate	3.040e-229	3.494e-224	0.8406	-228.5926
2-Hydroxyhexanoi	1.749e-230	2.308e-225	1.0000	-229.7571
Hexanoic_acid(aq	1.343e-231	1.558e-226	1.0000	-230.8718
Pimelate	1.419e-235	2.240e-230	0.4944	-235.1541
H-Pimelate	1.573e-237	2.500e-232	0.8406	-236.8786
Pimelic_acid(aq)	3.013e-240	4.818e-235	1.0000	-239.5210
Hexanal(aq)	6.785e-254	6.784e-249	1.0000	-253.1684
Toluene(aq)	7.543e-258	6.938e-253	1.0000	-257.1224
p-Toluate	5.698e-261	7.686e-256	0.8406	-260.3197
m-Toluate	3.094e-261	4.174e-256	0.8406	-260.5849
o-Toluate	2.901e-263	3.914e-258	0.8406	-262.6128
1-Hexanol(aq)	1.000e-263	1.020e-258	1.0000	-263.0000
p-Toluic_acid(aq	8.504e-264	1.156e-258	1.0000	-263.0704
m-Toluic_acid(aq	3.607e-264	4.902e-259	1.0000	-263.4429
1-Hexene(aq)	3.123e-266	2.624e-261	1.0000	-265.5054
o-Toluic_acid(aq	1.329e-266	1.806e-261	1.0000	-265.8765
n-Hexane(aq)	7.914e-269	6.808e-264	1.0000	-268.1016
2-Hydroxyheptano	1.054e-269	1.527e-264	0.8406	-269.0527
1-Hexyne(aq)	2.457e-271	2.015e-266	1.0000	-270.6095
Heptanoate	7.332e-272	9.454e-267	0.8406	-271.2102
2-Hydroxyheptano	3.639e-273	5.311e-268	1.0000	-272.4390
Heptanoic_acid(a	3.515e-274	4.568e-269	1.0000	-273.4540
Suberate	1.145e-279	1.968e-274	0.4944	-279.2472
H-Suberate	1.232e-281	2.131e-276	0.8406	-280.9846
Suberic_acid(aq)	2.478e-284	4.309e-279	1.0000	-283.6059
Fe(But)2(aq)	6.592e-288	1.514e-282	1.0000	-287.1810
Ca(But)2(aq)	7.591e-289	1.624e-283	1.0000	-288.1197
Mg(But)2(aq)	3.776e-289	7.482e-284	1.0000	-288.4230
Na(But)2-	6.854e-290	1.349e-284	0.8406	-289.2395
Mn(But)2(aq)	5.744e-290	1.314e-284	1.0000	-289.2408
K(But)2-	9.012e-291	1.919e-285	0.8406	-290.1206
Heptanal(aq)	1.396e-297	1.591e-292	1.0000	-296.8551
1-Heptanol(aq)	1.621e-307	1.880e-302	1.0000	-300.0000
1-Heptene(aq)	6.176e-309	6.053e-304	1.0000	-300.0000
n-Heptane(aq)	1.635e-311	1.635e-306	1.0000	-300.0000
2-Hydroxyoctanoa	2.187e-312	3.475e-307	0.8406	-300.0000
1-Heptyne(aq)	3.222e-314	3.093e-309	1.0000	-300.0000
Octanoate	2.555e-314	3.652e-309	0.8406	-300.0000
2-Hydroxyoctanoi	7.570e-316	1.211e-310	1.0000	-300.0000
Octanoic_acid(aq	1.242e-316	1.788e-311	1.0000	-300.0000
H-Azelate	0.000	0.000	0.8406	-300.0000
Octanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxynonanoi	0.000	0.000	1.0000	-300.0000
Nonanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Nonanoate	0.000	0.000	0.8406	-300.0000
Nonanal(aq)	0.000	0.000	1.0000	-300.0000

2-Hydroxynonanoa	0.000	0.000	0.8406	-300.0000
Na(Pent)2-	0.000	0.000	0.8406	-300.0000
Fe(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
Mn(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoi	0.000	0.000	1.0000	-300.0000
Mg(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
2-Hydroxydecanoa	0.000	0.000	0.8406	-300.0000
Ethylbenzene(aq)	0.000	0.000	1.0000	-300.0000
Azelate	0.000	0.000	0.4944	-300.0000
1-Octyne(aq)	0.000	0.000	1.0000	-300.0000
Dodecanoic_acid(	0.000	0.000	1.0000	-300.0000
Azelaic_acid(aq)	0.000	0.000	1.0000	-300.0000
Dodecanoate	0.000	0.000	0.8406	-300.0000
Decanoic_acid(aq	0.000	0.000	1.0000	-300.0000
Decanoate	0.000	0.000	0.8406	-300.0000
Decanal(aq)	0.000	0.000	1.0000	-300.0000
2-Hexanone(aq)	0.000	0.000	1.0000	-300.0000
1-Octene(aq)	0.000	0.000	1.0000	-300.0000
K(Pent)2-	0.000	0.000	0.8406	-300.0000
2-Heptanone(aq)	0.000	0.000	1.0000	-300.0000
n-Propylbenzene(	0.000	0.000	1.0000	-300.0000
n-Pentylbenzene(	0.000	0.000	1.0000	-300.0000
n-Octylbenzene(a	0.000	0.000	1.0000	-300.0000
n-Octane(aq)	0.000	0.000	1.0000	-300.0000
2-Pentanone(aq)	0.000	0.000	1.0000	-300.0000
2-Butanone(aq)	0.000	0.000	1.0000	-300.0000
1-Octanol(aq)	0.000	0.000	1.0000	-300.0000
n-Hexylbenzene(a	0.000	0.000	1.0000	-300.0000
n-Heptylbenzene(	0.000	0.000	1.0000	-300.0000
n-Butylbenzene(a	0.000	0.000	1.0000	-300.0000
2-Octanone(aq)	0.000	0.000	1.0000	-300.0000
Undecanoic_acid(	0.000	0.000	1.0000	-300.0000
Undecanoate	0.000	0.000	0.8406	-300.0000
Sebacic_acid(aq)	0.000	0.000	1.0000	-300.0000
Sebacate	0.000	0.000	0.4944	-300.0000
Ca(Pent)2(aq)	0.000	0.000	1.0000	-300.0000
H-Sebacate	0.000	0.000	0.8406	-300.0000

Surface species	molality	moles	Boltzman fct.	log molality
>(w)FeOH	0.01015	0.003419	1.0000	-1.9936
>(w)FeOH2+	0.004534	0.001528	3.2130	-2.3435
>(w)FeOHSO4--	0.002470	0.0008322	0.096865	-2.6073
>(w)FeOMg+	0.001236	0.0004162	3.2130	-2.9081
>(w)FeSO4-	0.0005532	0.0001863	0.31123	-3.2572
>(w)FeO-	0.0005204	0.0001753	0.31123	-3.2836
>(s)FeOHCa++	0.0002985	0.0001005	10.324	-3.5251
>(w)FeOCa+	0.0002169	7.306e-05	3.2130	-3.6638
>(s)FeOMn+	0.0001851	6.235e-05	3.2130	-3.7326
>(w)FeOMn+	0.0001617	5.448e-05	3.2130	-3.7912

>(w)FeH2BO3	5.288e-05	1.781e-05	1.0000	-4.2767
>(s)FeOH	9.226e-06	3.108e-06	1.0000	-5.0350
>(s)FeOH2+	4.122e-06	1.389e-06	3.2130	-5.3849
>(s)FeO-	4.731e-07	1.594e-07	0.31123	-6.3250

(Boltzman factor = exp(zF PSI/RT), where PSI is surface potential)

Mineral saturation states

	log Q/K		log Q/K
Hematite	11.5273s/sat	MgSO4	-10.9382
Magnetite	11.0269s/sat	Periclase	-11.2274
Goethite	5.2993s/sat	B2O3	-11.4856
Ferrite-Ca	0.8360s/sat	Portlandite	-11.7822
Siderite	0.7136s/sat	Thermonatrite	-12.2564
Ferrite-Mg	0.6872s/sat	Na2CO3	-12.5727
Dolomite-ord	0.5746s/sat	MnCl2:4H2O	-14.2711
Dolomite	0.5746s/sat	Borax	-14.2766
Fe(OH)3	0.0000 sat	MnCl2:2H2O	-15.7040
Calcite	-0.0230	Hydromagnesite	-15.8173
Ice	-0.0888	MgOHCl	-15.9260
Aragonite	-0.1680	Bixbyite	-16.0110
Gypsum	-0.3669	Pyrolusite	-16.1739
Rhodochrosite	-0.4239	MgCl2:4H2O	-17.1465
Powellite	-0.6446	MnCl2:H2O	-17.3767
Anhydrite	-0.6733	Hausmannite	-18.4252
Monohydrocalcite	-0.8255	Lawrencite	-19.9567
Dolomite-dis	-1.0692	Scacchite	-20.7769
Magnesite	-1.1143	Hydrophilite	-21.3775
Bassanite	-1.3223	Lime	-22.3290
CaSO4:0.5H2O(bet	-1.5074	MgCl2:2H2O	-22.9464
Boric_acid	-2.5780	C	-23.1148
Jarosite	-2.9012	Ferrite-Dicalciu	-24.3650
Melanterite	-3.6530	Fe	-24.4685
Wustite	-3.6800	MgCl2:H2O	-26.5076
FeO	-3.8215	KMgCl3:2H2O	-30.8101
Fe(OH)2	-4.1100	Chloromagnesite	-32.5676
Nesquehonite	-4.2096	S	-33.7440
Huntite	-5.0340	KMgCl3	-38.5393
Nahcolite	-5.1809	Molysite	-39.5549
Brucite	-5.8775	Troilite	-39.6381
Mirabilite	-6.2083	Pyrrhotite	-39.7417
Mn(OH)2(am)	-6.7606	Fe2(SO4)3	-42.5037
Arcanite	-7.4592	Alabandite	-44.4204
Sylvite	-7.4766	Mn	-50.6566
Halite	-7.5675	Na	-52.5994
Thenardite	-7.6411	Mo	-54.2875
Artinite	-7.8550	K	-57.0612
Mg1.25SO4(OH)0.5	-8.5428	Li	-60.1528
FeSO4	-9.3297	Na2O	-61.5626
Manganosite	-9.5652	Pyrite	-62.4940

Mg1.5SO4(OH)	-9.9387	B	-77.1104
Natron	-10.2913	K2O	-80.3071
MnSO4	-10.4911	Mg	-90.2507
NaFeO2	-10.5164	Ca	-107.6938
Na2CO3:7H2O	-10.8287	o-Phthalic_acid	-232.3138

Gases	partial press. (bar)	fugacity	fug. coef.	log fug.
H2O(g)	0.01213	0.01134	0.9353	-1.9453
CO2(g)	0.008779	0.008728	0.9941	-2.0591
HCl(g)	5.161e-18	5.161e-18	1.000*	-17.2873
H2(g)	5.469e-19	5.474e-19	1.001	-18.2617
CO(g)	1.585e-24	1.585e-24	1.000*	-23.8001
SO2(g)	1.090e-30	1.070e-30	0.9817	-29.9706
H2S(g)	1.108e-46	1.099e-46	0.9912	-45.9591
CH4(g)	7.148e-51	7.133e-51	0.9979	-50.1467
Cl2(g)	6.364e-52	6.364e-52	1.000*	-51.1963
O2(g)	5.914e-52	5.909e-52	0.9992	-51.2285
Na(g)	1.130e-67	1.130e-67	1.000*	-66.9469
K(g)	4.248e-69	4.248e-69	1.000*	-68.3718
S2(g)	3.778e-83	3.778e-83	1.000*	-82.4227
Li(g)	2.441e-84	2.441e-84	1.000*	-83.6124
C2H4(g)	7.704e-96	7.704e-96	1.000*	-95.1133
Mg(g)	7.265e-112	7.265e-112	1.000*	-111.1388
Ca(g)	4.514e-135	4.514e-135	1.000*	-134.3454
C(g)	3.058e-147	3.058e-147	1.000*	-146.5146
B(g)	1.122e-173	1.122e-173	1.000*	-172.9498

*no data, gas taken to be ideal

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
H2O	18.8	18.7	9.98e+05	-0.000204		-10.9
B(OH)3(aq)	0.000442	0.000424	77.6	1.78e-05		3.26
Ca++	0.00306	0.00288	342.	0.000174		20.6
Cl-	0.000226	0.000226	23.8			
Fe++	0.0336	0.000128	21.2			
H+	-0.0659	0.000146	0.437	0.000934		2.79
HCO3-	0.00107	0.00107	194.			
K+	0.000122	0.000122	14.1			
Li+	9.25e-06	9.25e-06	0.190			
Mg++	0.00139	0.000978	70.5	0.000416		30.0
Mn++	0.000127	1.07e-05	1.74	0.000117		19.0
MoO4--	4.94e-07	4.94e-07	0.234			
Na+	0.000680	0.000680	46.3			
O2(aq)	0.00838	1.67e-12	1.58e-07			
SO4--	0.00446	0.00344	980.	0.00102		290.
>(s)FeOH	0.000168					
>(w)FeOH	0.00670					

Sorbed	fraction	log fraction
B(OH)3(aq)	0.04034	-1.394
Ca++	0.05679	-1.246
Mg++	0.2985	-0.525
Mn++	0.9164	-0.038
SO4--	0.2282	-0.642

Elemental composition		In fluid		Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Boron	0.0004416	0.0004238	13.58	1.781e-05	0.5707
Calcium	0.003057	0.002883	342.4	0.0001736	20.62
Carbon	0.001072	0.001072	38.14		
Chlorine	0.0002265	0.0002265	23.79		
Hydrogen	37.50	37.40	1.117e+05	0.0005788	1.729
Iron	0.03364	0.0001284	21.24		
Lithium	9.247e-06	9.247e-06	0.1902		
Magnesium	0.001394	0.0009783	70.46	0.0004162	29.98
Manganese	0.0001275	1.066e-05	1.735	0.0001168	19.02
Molybdenum	4.942e-07	4.942e-07	0.1405		
Oxygen	18.82	18.72	8.874e+05	0.003923	186.0
Potassium	0.0001215	0.0001215	14.08		
Sodium	0.0006797	0.0006797	46.30		
Sulfur	0.004462	0.003444	327.2	0.001019	96.78