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ER-0956 Updating equilibrium calculation to derive reference porewater composition of Boom Clay using ThermoChimie v.10a

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Updating equilibrium calculation to derive reference porewater composition of Boom Clay using ThermoChimie v.10a

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Glossary of abbreviations

| | |
|-----|----------------------------|
| BC | Boom Clay |
| O/N | Ondraf/Niras |
| CEC | Cation Exchange Capacity |
| GWB | The Geochemist's Workbench |

Abstract

Ondraf/Niras considers ThermoChimie as the new reference thermodynamic database to perform geochemical calculations supporting the assessment of radionuclide behavior in different scenarios and under different environmental conditions. At SCK CEN some geochemical calculations in the past were however carried out using the in-house developed thermodynamic database 'MOLDATA'. For a purpose of knowledge transfer some important geochemical calculations done in the past should be updated using the new reference database. This report updates the calculation of the reference porewater composition of Boom Clay carried out in the year of 2004 by applying the newly assigned thermodynamic database ThermoChimie v.10a. Results illustrated that replacing MOLDATA by ThermoChimie does not change the calculated reference water composition except the concentration of iron. The dissolved concentration of iron increased about an order of magnitude due to a different solubility constant of siderite selected in ThermoChimie.

Keywords

Boom Clay, porewater, solubility, geochemistry, cation exchange

1 Introduction

This report aims at updating the calculated reference porewater composition of Boom Clay (BC) using the newly assigned thermodynamic database ThermoChimie v.10a.

The porewater composition of BC is important because it is used for the description and prediction of the behavior and mobility of the waste relevant radionuclides in and through the natural barrier of the deep waste disposal facility. The last reference porewater composition of BC was determined in the year of 2004 by geochemical equilibrium calculations based on the understanding of the BC geochemistry observed at the formation level of the underground laboratory at SCK CEN site in Mol, Belgium (De Craen et al., 2004). The geochemical calculation was performed using an early version of in-house compiled thermodynamic database MOLDATA and the computer code *The Geochemist's Workbench* (GWB) v3. For the current phenomenological studies of nuclear waste geological disposal in Belgium Ondraf/Niras (O/N) decided to use the thermodynamic database ThermoChimie (Giffaut et al., 2014) as the standard database so the reference porewater composition determined in 2004 has to be updated. Also there has been new cation exchange data concerning BC published recently (Frederickx et al., 2018) which will also be considered.

Two technical objectives will be tackled in this report. Firstly, the input of the 2004 model was used with the new ThermoChimie database and the calculations were updated. This objective focuses on comparing two databases and reveals the differences in calculating results. This means that the calculations are aimed at comparing databases, so the old input will be used unless modifications are needed for running it with the new version computer code. The second objective is to include the new cation exchange data into consideration. Based on the results, the need of updating the 2004 reference model will be discussed.

1.1 Background about the 2004 reference model

Based on detailed experimental and modeling studies performed on the BC geochemistry (De Craen et al., 2004), it was concluded that the water composition varies and no single porewater composition can be derived from water samples collected at the underground laboratory at the Mol site. It was proposed that a better approach would be to develop a reference porewater model according to the understanding of the controlling mechanisms with respect to the BC mineralogy and geochemistry and to derive a porewater composition via an equilibrium calculation. An equilibrium model was run with a computer code and a thermodynamic database. The model covers the range of observed geochemical conditions and takes into account the controlling mechanisms such as solubility of minerals and cation exchange. A model calculation will be then compared to the measured water composition. A successful model is that the model output explains well the observed change in water compositions used for model testing. For the 2004 reference model compositions of water samples from piezometer MORPHEUS were used for testing the model.

The computer input to calculate the reference porewater composition of BC at 16°C as used in De Craen et al., (2004) is given in Appendix 1. This input considered geochemical processes such as solubility of minerals, cation exchange of clays, CO₂ gas solubility and equilibrium with BC minerals etc.:

- Dissolved concentrations of Ca, Si, Al, Fe are controlled by solubility of the minerals calcite, chalcedony (a proxy for SiO₂ or quartz), kaolinite, and siderite;
- Dissolved concentrations of Na, K, Mg are regulated by cation exchange assuming known selectivity coefficients and cation exchange capacity (CEC) of 18.5 meq/100 g clay;
- The redox potential is controlled by the solubility of pyrite with a known initial concentration of dissolved sulphate observed in the collected water samples;
- The pH was regulated by charge balance and the partial pressure of CO₂ (log atm) varied from 10^{-2.8} to 10^{-2.2}. The range of pCO₂ (g) was derived based on assumption of calcite equilibrium with observed Ca concentration, alkalinity, and pH;
- The system temperature was set to 16°C as measured *in situ* in the underground laboratory;
- Natural organic matters (NOM) such as humic and fulvic acids as metal complexing agents are not considered in this report. It can be however reasonably anticipate that impact of NOM on compositions of major ions will be negligible because that NOM form complexes mainly with trace metals.

1.2 Thermodynamic database

In the input of the 2004 reference model 'MOLDATA.dat' was used as the thermodynamic database. 'MOLDATA.dat' is one of the very early versions of MOLDATA used in studies of BC as a geological barrier for radioactive waste disposal in Belgium. As explained in De Craen et al., (2004) 'MOLDATA.dat' was largely identical to the LLNL database (Delany and Lundeen, 1990), but modified with solubility and speciation data of radionuclides reviewed and selected by NEA (Guillaumont et al., 2003;

Ragoussi and Brassinnes, 2015). This 'MOLDATA.dat' is quite different from the MOLDATA version(s) compiled later on/more recently (Wang et al., 2011, 2014) in-house with the purpose to develop a self-consistent and up-to-date database.

In the past years O/N decided to abandon the strategy of the in-house development of MOLDATA in favor of using ThermoChimie. The version of ThermoChimie appointed to be used in this report is the 'v.10a' for GWB downloadable from the website <https://www.thermochimie-tdb.com>. This version 'v.10a' adopted the convention 'B-dot' as the solute activity correction method which is the same as what MOLDATA used.

1.3 Computer code

The computer code used in previous studies and also in the current report is GWB, e.g., (Bethke et al., 2018). The 2004 reference model calculation(s) used one of the very early versions of GWB, i.e., v.3 while in this report the most recent version v.15, i.e., GWB 2021 is used.

2 Calculations using the ThermoChimie database

2.1 Running the 2004 input with the new version of GWB (T = 16°C)

The first step is to see if the old input of the 2004 reference model can be run by the new version 15 of GWB. It turned out that running of the old input with the new version of GWB is possible with a minor change of input with respect to the 'alter logK' command. An 'alter logK' command was used in the 2004 input (see Appendix 1) to change the default selectivity coefficients for 25°C to calculate cation exchange at 16°C. This is because a cation exchange database normally only contains data for 25°C so if an input is run for 16°C then cation exchange data will not be considered as if data does not exist. A way around was to set the same value for the different selectivity coefficients for all temperatures, and consequently the code will "consider" the selectivity coefficients at the different temperatures the same as the value at 25°C. Due to a difference in treating the database format between the old GWB versions and the recent version 15, the latter does not recognize the 'alter logK' command. This is because the older version alters the logK value(s) while the new version alters directly the K-value(s). By modifying an 'alter logK' command to an 'alter K' command the 2004 input runs well in the new GWB 15 and produce identical results.

2.2 Running the 2004 input with the new version GWB using ThermoChimie v.10a

Running the 2004 input with the new version GWB 15 using ThermoChimie v.10a is also successful with some minor changes of the input.

The first change is that the controlling mineral for silica, i.e. chalcedony in the 2004 input is replaced by quartz. This is because ThermoChimie does not contain the mineral chalcedony. The use of chalcedony as a proxy for quartz in De Craen et al. (2004) was to fit the observed concentration of Si in the porewater of BC. The solubility of quartz has since then been studied more and was updated and the solubility constant in ThermoChimie is the most up-to-date value.

Another minor modification done in order to run the 2004 input using ThermoChimie is the removal of all cation exchange reactions except those of Na, K, and Mg. This was needed because a lot of cation exchange reactions in the MOLDATA are not recognized by ThermoChimie due to different ways of writing reactions. Such removal does not impact the calculation since only cation exchange reactions concerning Na, K, and Mg are relevant in the current context.

The input file and part of the output file of the run are given in Appendix 2 and 3. The water composition chosen to be outputted as the reference is the step 30 of the calculation. This was decided by De Craen et al., (2004) that the reference water composition is the one under a $p\text{CO}_2$ of $10^{-2.6}$ (atm) which is the middle value of the observed $p\text{CO}_2$ among sampled MORPHEUS waters.

2.3 Running the 2004 input with the new version of GWB using ThermoChimie v.10a with the new cation exchange data

A run was also carried out to consider the new cation exchange data published recently (Frederickx et al., 2018). This run was aiming at testing the new cation exchange data without going too deep into cation exchange mechanisms due to the limit of resources allocated to this report. Only one site cation exchange model with median values of selectivity coefficients and CEC were used while it was illustrated by Frederickx et al., (2018) that cation selectivity and CEC of BC varies depending on sampling locations and the mineralogical composition of the clay. No cation exchange heterogeneity is considered in this report. The input and a part of the output are given in Appendix 4 and 5.

3 Results and discussions

Results of new runs are given in Table 1 together with the output of the 2004 model.

Table 1 reveals that concentrations of most of elements/species resulted from different runs are identical regardless which database was used. Obvious difference is only observed in the concentrations of iron. The concentration of aluminum also changed slightly. These changes are apparently due to differences in solubility constants of siderite and kaolinite selected in the two different databases. In Table 2 the solubility constants included in the two databases are compared.

The concentrations of iron increased by a factor of ~3 when using ThermoChimie as compared to the result based on MOLDATA. Both results are within the range of observed iron concentrations (i.e., 0.002 – 0.012 mM) according to measurements on sampled waters from MORPHEUS piezometers (De Craen et al., 2004). The result calculated by ThermoChimie is at the high end of the range. In terms thermodynamic data use, one should adopt the value of ThermoChimie to calculate the solubility of siderite. With respect to the controlling mechanism on iron concentration in BC porewater more studies are needed to demonstrate the validity of siderite as a solubility controlling mineral.

Table 1. Calculated reference porewater of BC at 16°C using different thermodynamic databases and cation exchange parameters

| Composition | 2004 ref model | 2004 ref model with TC v.10a | 2004 ref model with TC v.10a and new CE data |
|-------------------------------|---------------------|------------------------------|--|
| [conc], mM | | | |
| Na | 15.6 | 15.6 | 15.6 |
| K | 0.2 | 0.2 | 0.2 |
| Ca | 0.05 | 0.05 | 0.05 |
| Mg | 0.06 | 0.06 | 0.06 |
| Fe | <u>0.003</u> | <u>0.01</u> | <u>0.01</u> |
| Si | 0.1 | 0.1 | 0.1 |
| Al | <u>2.4e-5</u> | <u>1.8e-5</u> | <u>1.8e-5</u> |
| HCO ₃ ⁻ | 14.4 | 14.5 | 14.5 |
| TIC (mg C/l) | 15.1 | 15.1 | 15.1 |
| Cl ⁻ | 0.7 | 0.7 | 0.7 |
| SO ₄ ²⁻ | 0.02 | 0.02 | 0.02 |
| pH | 8.5 | 8.5 | 8.5 |
| pCO ₂ (atm) | 10 ^{-2.62} | 10 ^{-2.62} | 10 ^{-2.62} |
| Eh (mV) | -274 | -278 | -278 |
| T (°C) | 16 | 16 | 16 |
| Ionic strength | 0.016 | 0.016 | 0.016 |

Table 2. Comparison of solubility constants of minerals from two thermodynamic database

| Minerals | Solubility constant (logK, 25°C) | |
|-------------------|----------------------------------|--------------------|
| | MOLDATA.dat (LLNL) | ThermoChimie v.10a |
| Siderite | -0.192 | -0.47 |
| Kaolinite | 6.81 | 6.50 |
| Quartz/chalcedony | -3.72 | -3.74 |
| Pyrite | 217.40 | 217.79 |
| Calcite | 1.84 | 1.85 |

Concentrations of Na, K, and Mg are calculated to be identical using two different sets of cation exchange parameters suggesting that cation exchange parameters do not affect dissolved concentration of these cations. This seems logic since the input defines initial concentrations of these cations and the Ca concentration is controlled by the solubility of calcite. When a system parameter changes, in this case pCO₂, the solubility of calcite changes and also the other exchangeable cations, i.e. Na, K, and Mg. Cation exchange operates in the way that the concentrations of Na, K, and Mg will change in order to maintain the cation ratios in water. This mechanism means that if the calculated solubility of calcite is identical by using two different databases, then the dissolved concentrations of Na, K, and Mg will remain the same regardless the values

of the cation exchange parameters. It is on the other hand also logic that cation exchange complexes on the clay surface will change as response to the change of cation exchange parameters (see Appendixes). Discussion on how cation exchange parameters will impact cation occupancies on BC is out of scope for this report and seems less relevant in the current context to derive a reference porewater composition.

4 Updated porewater composition of BC

Based on the results illustrated in Table 1, it is clear that changing the thermodynamic database from MOLDATA.dat (LLNL) to ThermoChimie v.10a does not affect the basic characteristics and concentrations of most elements/species defining the reference porewater composition of BC at 16°C. To the author's opinion there is no need at this stage to update the reference porewater composition of BC determined by the work of De Craen et al., (2004).

The iron concentration calculated using ThermoChimie v.10a increased about an order of magnitude as compared to the calculation based on MOLDATA.dat. Putting aside the fact that ThermoChimie v.10a is considered as the state-of-the-art TDB in selection of solubility constants, the real mechanism controlling the dissolved concentration of iron in BC is not known and the assumption used in the reference model that the solubility of siderite is controlling the Fe concentration is yet to be validated. Recent studies on BC mineralogy suggest that structural iron incorporated in BC montmorillonite seems more reactive in participating in redox reactions ($\text{Fe}^{2+}/\text{Fe}^{3+}$) and/or in controlling the iron concentration than siderite (Honty, personal communication). It is thus the author's advice that in case the iron concentration is needed/relevant in a study of BC, one should consider a range of Fe-concentrations and different possible mechanisms.

5 References

- Bethke, C.M., Brian, F. and Sharon, Y. (2018) The Geochemist's Workbench, Release 12: Reaction Modeling Guide, Aqueous Solutions, LLC Champaign Illinois, Printed April 11, 2018.
- De Craen, M., Wang, L., Van Geet, M. and Moors, H. (2004) Geochemistry of Boom Clay pore water at the Mol site, SCK•CEN Report, BLG-990, 04/MDC/P-48, Mol, Belgium.
- Delany, J.M. and Lundeen, S.R. (1990) The LLNL thermochemical database, Lawrence Livermore National Laboratory Report, UCRL-21658.
- Frederickx, L., Honty, M., de Craen, M., Dohrmann, R. and Elsen, J. (2018) RELATING THE CATION EXCHANGE PROPERTIES OF THE BOOM CLAY (BELGIUM) TO MINERALOGY AND PORE-WATER CHEMISTRY. *Clays and Clay Minerals* 66, 449-465.
- Giffaut, E., Grive, M., Blanc, P., Vieillard, P., Colas, E., Gailhanou, H., Gaboreau, S., Marty, N., Made, B. and Duro, L. (2014) Andra thermodynamic database for performance assessment: ThermoChimie. *Applied Geochemistry* 49, 225-236.
- Guillaumont, R., Fanghanel, T., Neck, V., Fuger, J., Palmer, D., Grenthe, I. and Rand, M.H. (2003) Update on the chemical thermodynamics of uranium, neptunium, plutonium, americium and technetium. Elsevier, OECD, Issy-lès-Moulineaux, France.
- Ragoussi, M.E. and Brassinnes, S. (2015) The NEA Thermochemical Database Project: 30 years of accomplishments. *Radiochimica Acta* 103, 679-685.
- Wang, L., Salah, S. and De Soete, H. (2011) MOLDATA: A thermochemical data base for phenomenological and safety assessment studies for disposal of radioactive waste in Belgium – Data compilation strategy, EXTERNAL REPORT, SCK•CEN-ER-121.
- Wang, L., Salah, S. and De Soete, H. (2014) MOLDATA: A thermodynamic data base for phenomenological and safety assessment studies for disposal of radioactive waste in Belgium - Selected data and argumentations, SCK CEN report, ER-257.

Appendix 1

Input file of GWB v3 of 2004 reference model (Annex 7 in De Craen et al., 2004)

```
# React script, saved Tue Dec 09 2003 by lwang
data = "C:\Program Files\Gwb\Gtdata\MOLDATA.dat" verify
surface_data = "C:\Program Files\Gwb\Gtdata\MOLDATA ION EX.dat"
exchange_capacity IonEx = 0.925 eq
work_dir = "N:\USERS\Lwang\Projects\Topical reports\Pore water chemistry\GWB"
temperature = 16
swap Calcite for Ca++
swap Pyrite for O2(aq)
swap Siderite for Fe++
swap CO2(g) for HCO3-
swap Chalcedony for SiO2(aq)
swap Kaolinite for Al+++
1 kg free H2O
free kg Calcite = .15
free gram Pyrite = 100
free gram Siderite = 5
fugacity CO2(g) = .00158489319
free gram Chalcedony = 2000
free gram Kaolinite = 1000
total mol Na+ = .01417
total mol Mg++ = 5.41e-5
total mol K+ = .000168
total mg/kg SO4-- = 2.31
balance on H+
total mg/kg Cl- = 26
slide log fugacity of CO2(g) to -2.2

suppress >X2:Fe >X3:Al
alter >X:K -1.328 -1.328 -1.328 -1.328 -1.328 -1.328 -1.328 -1.328
alter >X2:Ca -.843 -.843 -.843 -.843 -.843 -.843 -.843 -.843
alter >X2:Mg -.678 -.678 -.678 -.678 -.678 -.678 -.678 -.678
extrapolate
precip = off
```

Appendix 2

Input file of GWB 15 of 2004 reference model using ThermoChimie v.10a

```
# React script, saved Thu May 13 2021 by Iwang
data = ThermoChimie_GWB_oxygen_v10a.tdat verify
surface_data = "MOLDATA ION EX 2021.dat"
exchange_capacity IonEx = .925 eq
conductivity = conductivity-USGS.dat
temperature = 16 C
H2O      = 1 free kg
swap Calcite for Ca++
Calcite   = .15 free kg
swap Pyrite for O2(aq)
Pyrite    = 100 free g
swap Siderite for Fe++
Siderite  = 5 free g
swap Kaolinite for Al+++
Kaolinite = 1000 free g
Na+       = .01417 total mol
Mg++      = 5.41e-5 total mol
K+        = .000168 total mol
SO4--     = 2.31 total mg/kg
balance on H+
Cl-       = 26 total mg/kg
swap CO2(g) for CO3--
CO2(g)    = .00158489319 fugacity
swap Quartz for H4(SiO4)
Quartz    = 2000 free g
slide log fugacity of CO2(g) to -2.2
alter >X:K beta = .04698941
alter >X2:Ca beta = .143548943
alter >X2:Mg beta = .209893988
extrapolate
precip = off
```

Appendix 3

A part of output running the Input file of GWB 15 of 2004 reference model using ThermoChimie v.10a (Appendix 2)

Step # 30 Xi = 0.3000

Temperature = 16.0 C Pressure = 1.013 bar
 pH = 8.489 log fO2 = -71.231
 Eh = -0.2776 volts pe = -4.8387
 Ionic strength = 0.016207 molal
 Activity of water = 0.999974
 Solvent mass = 0.99999 kg
 Solution mass = 1.0013 kg
 Mineral mass = 3.2549 kg
 Fluid density = 0.999 g/cm3
 compressibility = 4.556e-05 /bar
 expansivity = 0.0001844 /C
 viscosity = 0.011 poise
 Chlorinity = 0.000000 molal
 Dissolved solids = 1305 mg/kg sol'n
 Elect. conductivity = 1372.27 uS/cm (or umho/cm)
 Hardness = 11.60 mg/kg sol'n as CaCO3
 carbonate = 11.60 mg/kg sol'n as CaCO3
 non-carbonate = 0.00 mg/kg sol'n as CaCO3
 Carbonate alkalinity = 759.70 mg/kg sol'n as CaCO3
 Water type = Na-HCO3
 Bulk volume = 2.22e+03 cm3
 Fluid volume = 1.00e+03 cm3
 Mineral volume = 1.22e+03 cm3
 Inert volume = 0.00 cm3
 Porosity = 45.2 %
 Permeability = 5.90e-07 cm2
 Mass reacted = 0.0366 g
 IonEx sorbing surface:
 Exchange capacity = 0.925 eq

| Reactants | moles remaining | moles reacted | grams reacted | cm3 reacted | rxn rate (mol/kg sec) |
|-----------------------|-----------------|---------------|---------------|-------------|-----------------------|
| CO2(g) (sliding fug.) | | 0.0008324 | 0.03663 | -- | -- |

| Minerals in system | moles | log moles | grams | volume (cm3) |
|--------------------|---------|-----------|-------|--------------|
| Calcite | 1.498 | 0.176 | 149.9 | 55.32 |
| Kaolinite | 3.874 | 0.588 | 1000. | 384.8 |
| Pyrite | 0.8335 | -0.079 | 100.0 | 19.95 |
| Quartz | 33.29 | 1.522 | 2000. | 755.3 |
| Siderite | 0.04316 | -1.365 | 5.000 | 1.268 |
| (total) | | 3255. | 1217. | |

| Aqueous species | molality | mg/kg sol'n | act. coef. | log act. |
|-----------------|-----------|-------------|------------|----------|
| Na+ | 0.01545 | 354.8 | 0.8829 | -1.8651 |
| HCO3- | 0.01453 | 885.2 | 0.8809 | -1.8929 |
| Cl- | 0.0007314 | 25.90 | 0.8809 | -3.1909 |
| CO3-- | 0.0002503 | 15.00 | 0.6114 | -3.8153 |
| K+ | 0.0001854 | 7.239 | 0.8829 | -3.7860 |
| H4(SiO4) | 0.0001391 | 13.35 | 1.0000 | -3.8568 |
| Na(HCO3) | 0.0001135 | 9.522 | 1.0000 | -3.9450 |
| CO2 | 0.0001044 | 4.591 | 1.0000 | -3.9811 |

| | | | | |
|-------------|-----------|-----------|--------|---------|
| Mg++ | 5.579e-05 | 1.354 | 0.6216 | -4.4599 |
| Ca++ | 3.984e-05 | 1.595 | 0.6216 | -4.6062 |
| Na(CO3)- | 2.749e-05 | 2.278 | 0.8809 | -4.6160 |
| SO4-- | 2.203e-05 | 2.113 | 0.6114 | -4.8707 |
| Fe(CO3) | 9.728e-06 | 1.126 | 1.0000 | -5.0120 |
| Mg(HCO3)+ | 5.386e-06 | 0.4590 | 0.8829 | -5.3228 |
| CaCO3 | 5.209e-06 | 0.5207 | 1.0000 | -5.2832 |
| Ca(HCO3)+ | 5.059e-06 | 0.5107 | 0.8829 | -5.3500 |
| H3(SiO4)- | 4.843e-06 | 0.4600 | 0.8809 | -5.3700 |
| Mg(CO3) | 4.531e-06 | 0.3816 | 1.0000 | -5.3438 |
| NaCl | 2.710e-06 | 0.1582 | 1.0000 | -5.5671 |
| Na(SO4)- | 1.883e-06 | 0.2239 | 0.8809 | -5.7803 |
| OH- | 1.722e-06 | 0.02924 | 0.8809 | -5.8191 |
| FeCO3OH- | 6.026e-07 | 0.07995 | 0.8809 | -6.2751 |
| Fe++ | 1.941e-07 | 0.01082 | 0.6216 | -6.9185 |
| Mg(SO4) | 7.364e-08 | 0.008852 | 1.0000 | -7.1329 |
| Ca(SO4) | 6.449e-08 | 0.008768 | 1.0000 | -7.1905 |
| Fe(CO3)2-- | 6.415e-08 | 0.01127 | 0.6114 | -7.4065 |
| MgCl+ | 5.792e-08 | 0.003456 | 0.8829 | -7.2913 |
| FeHCO3+ | 3.996e-08 | 0.004663 | 0.8829 | -7.4525 |
| KCl | 3.162e-08 | 0.002355 | 1.0000 | -7.5000 |
| Si2O2(OH)5- | 2.139e-08 | 0.003701 | 0.8809 | -7.7248 |
| K(SO4)- | 1.829e-08 | 0.002468 | 0.8809 | -7.7930 |
| Al(OH)4- | 1.782e-08 | 0.001691 | 0.8809 | -7.8041 |
| Mg(OH)+ | 1.139e-08 | 0.0004698 | 0.8829 | -7.9977 |

(only species > 1e-8 molal listed)

Exchanging species molality moles act. coef. activity log activity

| | | | | | |
|--------|---------|---------|--------|--------|---------|
| >X:Na | 0.4376 | 0.4376 | 1.0811 | 0.4731 | -0.3251 |
| >X:K | 0.1117 | 0.1117 | 1.0811 | 0.1208 | -0.9180 |
| >X2:Ca | 0.09595 | 0.09595 | 2.1621 | 0.2074 | -0.6831 |
| >X2:Mg | 0.09189 | 0.09189 | 2.1621 | 0.1987 | -0.7018 |

Mineral saturation states

| | log Q/K | | log Q/K |
|------------------|--------------|------------------|---------|
| Berthierine_Lorr | 11.4764s/sat | Chabazite | -0.5833 |
| Chamosite | 3.5114s/sat | Phillipsite_Ca | -0.5911 |
| Smectite_MX80(5) | 3.5036s/sat | Pyrophyllite | -0.6000 |
| Smectite_MX80(3) | 3.1190s/sat | Vaterite | -0.6038 |
| HBeidellite-Na | 3.0852s/sat | Cristobalite | -0.6057 |
| Sudoite | 2.9058s/sat | Ferryhydrite | -0.6142 |
| HBeidellite-Ca | 2.7372s/sat | Beidellite-Mg | -0.6444 |
| HBeidellite-Mg | 2.6453s/sat | Boehmite | -0.6721 |
| HBeidellite-K | 2.0663s/sat | Paragonite | -0.6758 |
| Amesite-Fe | 2.0133s/sat | Gibbsite | -0.7321 |
| Beidellite_SBI-d | 1.8089s/sat | Laumontite | -0.7541 |
| Hematite | 1.4894s/sat | HMontmorillonite | -0.7640 |
| HMontmorillonite | 1.3916s/sat | CaCO3:H2O(s) | -0.8533 |
| Muscovite | 1.3139s/sat | Analcime | -0.9020 |
| HMontmorillonite | 1.1753s/sat | Dawsonite | -0.9343 |
| Clinochlore | 1.1735s/sat | Amesite | -0.9612 |
| Phillipsite_Na | 0.8205s/sat | Minnesotaite | -0.9890 |
| HMontmorillonite | 0.6723s/sat | Montmorillonite- | -1.0268 |
| HMontmorillonite | 0.6095s/sat | Illite-Al | -1.0525 |
| Illite-Fell | 0.5557s/sat | SiO2(am) | -1.0722 |
| HMontmorillonite | 0.5496s/sat | HSaponite-Na | -1.1461 |
| Magnesite(nat) | 0.5009s/sat | Beidellite-Ca | -1.2027 |
| Montmorillonite- | 0.4128s/sat | Saponite-FeNa | -1.2734 |
| Phillipsite_K | 0.4111s/sat | Pyrrhotite | -1.3886 |

Montmorillonite- 0.3686s/sat Montmorillonite- -1.3943
 Microcline 0.3459s/sat Troilite -1.4216
 Heulandite_Na 0.3397s/sat Celadonite-Mg -1.5173
 HMontmorillonite 0.2491s/sat Montmorillonite- -1.5542
 Dolomite 0.2351s/sat Saponite-FeK -1.5545
 Diaspore 0.1049s/sat HSaponite-Ca -1.5664
 Siderite 0.0000 sat Ripidolite_Cca-- -1.5772
 Kaolinite 0.0000 sat HSaponite-Mg -1.6582
 Quartz 0.0000 sat Beidellite_SBld- -1.6809
 Pyrite 0.0000 sat Acmite -1.7305
 Calcite 0.0000 sat Saponite-FeMg -1.7541
 Celadonite-Fe -0.0934 Clinoptilolite_C -1.7894
 Cronstedtite-Th -0.1070 Saponite-Na -1.8472
 Saponite_SapCa(4 -0.1136 Saponite-K -1.9529
 Goethite -0.1536 Ferrihydrite(am) -1.9642
 Aragonite -0.1691 Gismondine -1.9865
 Sanidine -0.2316 FeAl2O4(s) -1.9917
 Saponite-FeCa -0.2325 Scolecite -2.0043
 Greenalite -0.2741 Albite-high -2.0392
 Heulandite_Ca -0.3255 illite-FeIII -2.1296
 Beidellite-Na -0.3292 Saponite-Mg -2.1525
 Magnesite(syn) -0.3347 HSaponite-K -2.2373
 Magnetite -0.3903 Mordenite_Oregon -2.4693
 Beidellite-K -0.4347 Mordenite_Ca -2.4870
 Illite-Mg -0.4401 Illite_lmt-- -2.4985
 Montmorillonite- -0.4537 C(cr) -2.6494
 HMontmorillonite -0.4902 Vermiculite-Na -2.6979
 Lepidocrocite -0.5284 Saponite-Ca -2.7208
 Montmorillonite- -0.5362 Vermiculite-Mg -2.7954
 SmectiteMX80 -0.5387 Illite/smectitel -2.8973
 Montmorillonite- -0.5592 Dickite -2.9755
 Albite-low -0.5685 Maghemite(disord -2.9769
 (only minerals with log Q/K > -3 listed)

| Gases | partial press. (bar) | fugacity | fug. coef. | log fug. |
|--------|-------------------------|-----------|------------|----------|
| H2O(g) | 0.01829 | 0.01829 | 1.000* | -1.7377 |
| CO2(g) | 0.002399 | 0.002399 | 1.000* | -2.6200 |
| H2(g) | 3.119e-08 | 3.119e-08 | 1.000* | -7.5059 |
| CH4(g) | 4.483e-09 | 4.483e-09 | 1.000* | -8.3484 |
| H2S(g) | 1.667e-09 | 1.667e-09 | 1.000* | -8.7780 |
| CO(g) | 2.398e-14 | 2.398e-14 | 1.000* | -13.6202 |
| HCl(g) | 4.150e-19 | 4.150e-19 | 1.000* | -18.3819 |
| SO2(g) | 5.503e-25 | 5.503e-25 | 1.000* | -24.2594 |
| Cl2(g) | 2.108e-64 | 2.108e-64 | 1.000* | -63.6761 |
| O2(g) | 5.879e-72 | 5.879e-72 | 1.000* | -71.2307 |

*no data, gas taken to be ideal

| | In fluid Original basis total moles | Sorbed moles | mg/kg | moles | mg/kg |
|----------|--|-----------------|----------|--------|----------|
| H2O | -8.03 | 55.5 | 9.99e+05 | | |
| Al+++ | 7.75 | 1.81e-08 | 0.000487 | | |
| CO3-- | 1.56 | 0.0151 | 902. | | |
| Ca++ | 1.59 | 5.02e-05 | 2.01 | 0.0959 | 3.84e+03 |
| Cl- | 0.000734 | 0.000734 | 26.0 | | |
| Fe++ | 0.877 | 1.06e-05 | 0.593 | | |
| H+ | -21.6 | 0.0149 | 14.9 | | |
| H4(SiO4) | 41.0 | 0.000144 | 13.8 | | |
| K+ | 0.112 | 0.000185 | 7.24 | 0.112 | 4.36e+03 |

| | | | | | |
|-------------------------------|--------|-----------|-----------|--------|----------|
| Mg ⁺⁺ | 0.0920 | 6.59e-05 | 1.60 | 0.0919 | 2.23e+03 |
| Na ⁺ | 0.453 | 0.0156 | 358. | 0.438 | 1.00e+04 |
| O ₂ (aq) | -2.92 | -1.14e-08 | -0.000365 | | |
| SO ₄ ⁻⁻ | 1.67 | 2.41e-05 | 2.31 | | |
| >X:Na | 0.925 | | | | |

| Sorbed | fraction | log fraction |
|--------|----------|--------------|
|--------|----------|--------------|

| | | |
|------------------|--------|--------|
| Ca ⁺⁺ | 0.9995 | -0.000 |
| K ⁺ | 0.9983 | -0.001 |
| Mg ⁺⁺ | 0.9993 | -0.000 |
| Na ⁺ | 0.9656 | -0.015 |

| Elemental composition | In fluid | | Sorbed | |
|-----------------------|-------------|-------|--------|-------|
| | total moles | moles | mg/kg | mg/kg |

| | | | | | |
|------------------------------------|-----------|-----------|-----------|---------|-----------|
| Al ⁺⁺⁺ | 7.747 | 1.808e-08 | 0.0004873 | | |
| CO ₃ ⁻⁻ | 1.556 | 0.01505 | 902.1 | | |
| Ca ⁺⁺ | 1.594 | 5.018e-05 | 2.009 | 0.09595 | 3840. |
| Cl ⁻ | 0.0007342 | 0.0007342 | 26.00 | | |
| Fe ⁺⁺ | 0.8766 | 1.064e-05 | 0.5932 | | |
| H ⁺ | -37.61 | 111.0 | 1.118e+05 | | |
| H ₄ (SiO ₄) | 41.03 | 0.0001440 | 13.82 | | |
| K ⁺ | 0.1119 | 0.0001854 | 7.241 | 0.1117 | 4363. |
| Mg ⁺⁺ | 0.09196 | 6.585e-05 | 1.598 | 0.09189 | 2231. |
| Na ⁺ | 0.4532 | 0.01560 | 358.1 | 0.4376 | 1.005e+04 |
| O ₂ | -13.86 | 55.51 | 8.869e+05 | | |
| SO ₄ ⁻⁻ | 1.667 | 2.407e-05 | 2.310 | | |

Appendix 4

Input file of GWB 15 of 2004 reference model using ThermoChimie v.10a and the new cation exchange data

```
# React script, saved Thu May 13 2021 by Iwang
data = ThermoChimie_GWB_oxygen_v10a.tdat verify
surface_data = "Iwang PW IonEx Lander GT.sdat"
exchange_capacity IonEx = 1.11 eq
conductivity = conductivity-USGS.dat
temperature = 16 C
H2O      = 1 free kg
swap Calcite for Ca++
Calcite   = .15 free kg
swap Pyrite for O2(aq)
Pyrite    = 100 free g
swap Siderite for Fe++
Siderite  = 5 free g
swap Kaolinite for Al+++
Kaolinite = 1000 free g
Na+       = .01417 total mol
Mg++      = 5.41e-5 total mol
K+        = .000168 total mol
SO4--     = 2.31 total mg/kg
balance on H+
Cl-       = 26 total mg/kg
swap CO2(g) for CO3--
CO2(g)    = .00158489319 fugacity
swap Quartz for H4(SiO4)
Quartz    = 2000 free g
slide log fugacity of CO2(g) to -2.2
alter >X:K beta = .04698941
alter >X2:Ca beta = .143548943
alter >X2:Mg beta = .209893988
extrapolate
precip = off
```

Appendix 5

A part of output running the Input file of GWB 15 of 2004 reference model using ThermoChimie v.10a with the new cation exchange data (Appendix 4)

Step # 30 Xi = 0.3000

Temperature = 16.0 C Pressure = 1.013 bar
 pH = 8.489 log fO2 = -71.231
 Eh = -0.2776 volts pe = -4.8390
 Ionic strength = 0.016217 molal
 Activity of water = 0.999974
 Solvent mass = 0.99999 kg
 Solution mass = 1.0013 kg
 Mineral mass = 3.2549 kg
 Fluid density = 0.999 g/cm3
 compressibility = 4.556e-05 /bar
 expansivity = 0.0001844 /C
 viscosity = 0.011 poise
 Chlorinity = 0.000000 molal
 Dissolved solids = 1306 mg/kg sol'n
 Elect. conductivity = 1373.03 uS/cm (or umho/cm)
 Hardness = 11.60 mg/kg sol'n as CaCO3
 carbonate = 11.60 mg/kg sol'n as CaCO3
 non-carbonate = 0.00 mg/kg sol'n as CaCO3
 Carbonate alkalinity = 760.17 mg/kg sol'n as CaCO3
 Water type = Na-HCO3
 Bulk volume = 2.22e+03 cm3
 Fluid volume = 1.00e+03 cm3
 Mineral volume = 1.22e+03 cm3
 Inert volume = 0.00 cm3
 Porosity = 45.2 %
 Permeability = 5.90e-07 cm2
 Mass reacted = 0.0368 g
 IonEx sorbing surface:
 Exchange capacity = 1.11 eq

| Reactants | moles remaining | moles reacted | grams reacted | cm3 reacted | rxn rate (mol/kg sec) |
|-----------------------|-----------------|---------------|---------------|-------------|-----------------------|
| CO2(g) (sliding fug.) | | 0.0008368 | 0.03683 | -- | -- |

| Minerals in system | moles | log moles | grams | volume (cm3) |
|--------------------|---------|-----------|-------|--------------|
| Calcite | 1.498 | 0.176 | 149.9 | 55.32 |
| Kaolinite | 3.874 | 0.588 | 1000. | 384.8 |
| Pyrite | 0.8335 | -0.079 | 100.0 | 19.95 |
| Quartz | 33.29 | 1.522 | 2000. | 755.3 |
| Siderite | 0.04316 | -1.365 | 5.000 | 1.268 |
| (total) | | 3255. | 1217. | |

| Aqueous species | molality | mg/kg sol'n | act. coef. | log act. |
|-----------------|-----------|-------------|------------|----------|
| Na+ | 0.01546 | 355.0 | 0.8829 | -1.8649 |
| HCO3- | 0.01454 | 885.7 | 0.8809 | -1.8927 |
| Cl- | 0.0007314 | 25.90 | 0.8809 | -3.1909 |
| CO3-- | 0.0002506 | 15.02 | 0.6113 | -3.8148 |
| K+ | 0.0001854 | 7.239 | 0.8829 | -3.7860 |
| H4(SiO4) | 0.0001391 | 13.35 | 1.0000 | -3.8568 |
| Na(HCO3) | 0.0001136 | 9.533 | 1.0000 | -3.9445 |

| | | | | |
|-------------|-----------|-----------|--------|---------|
| CO2 | 0.0001044 | 4.591 | 1.0000 | -3.9811 |
| Mg++ | 5.580e-05 | 1.355 | 0.6216 | -4.4599 |
| Ca++ | 3.980e-05 | 1.593 | 0.6216 | -4.6067 |
| Na(CO3)- | 2.753e-05 | 2.282 | 0.8809 | -4.6152 |
| SO4-- | 2.203e-05 | 2.113 | 0.6113 | -4.8708 |
| Fe(CO3) | 9.728e-06 | 1.126 | 1.0000 | -5.0120 |
| Mg(HCO3)+ | 5.390e-06 | 0.4593 | 0.8829 | -5.3225 |
| CaCO3 | 5.209e-06 | 0.5207 | 1.0000 | -5.2832 |
| Ca(HCO3)+ | 5.056e-06 | 0.5105 | 0.8829 | -5.3503 |
| H3(SiO4)- | 4.846e-06 | 0.4602 | 0.8809 | -5.3697 |
| Mg(CO3) | 4.537e-06 | 0.3820 | 1.0000 | -5.3432 |
| NaCl | 2.711e-06 | 0.1583 | 1.0000 | -5.5668 |
| Na(SO4)- | 1.884e-06 | 0.2240 | 0.8809 | -5.7801 |
| OH- | 1.723e-06 | 0.02926 | 0.8809 | -5.8189 |
| FeCO3OH- | 6.029e-07 | 0.08000 | 0.8809 | -6.2748 |
| Fe++ | 1.939e-07 | 0.01081 | 0.6216 | -6.9190 |
| Mg(SO4) | 7.364e-08 | 0.008852 | 1.0000 | -7.1329 |
| Ca(SO4) | 6.441e-08 | 0.008757 | 1.0000 | -7.1911 |
| Fe(CO3)2-- | 6.424e-08 | 0.01128 | 0.6113 | -7.4060 |
| MgCl+ | 5.792e-08 | 0.003457 | 0.8829 | -7.2912 |
| FeHCO3+ | 3.994e-08 | 0.004661 | 0.8829 | -7.4527 |
| KCl | 3.163e-08 | 0.002355 | 1.0000 | -7.5000 |
| Si2O2(OH)5- | 2.141e-08 | 0.003703 | 0.8809 | -7.7245 |
| K(SO4)- | 1.828e-08 | 0.002468 | 0.8809 | -7.7930 |
| Al(OH)4- | 1.783e-08 | 0.001692 | 0.8809 | -7.8039 |
| Mg(OH)+ | 1.139e-08 | 0.0004701 | 0.8829 | -7.9974 |

(only species > 1e-8 molal listed)

Exchanging species molality moles act. coef. activity log activity

| | | | | | |
|--------|--------|--------|---------|--------|---------|
| >X:Na | 0.5254 | 0.5254 | 0.90089 | 0.4733 | -0.3248 |
| >X:K | 0.1341 | 0.1341 | 0.90089 | 0.1208 | -0.9180 |
| >X2:Ca | 0.1150 | 0.1150 | 1.8018 | 0.2072 | -0.6836 |
| >X2:Mg | 0.1103 | 0.1103 | 1.8018 | 0.1987 | -0.7018 |

Mineral saturation states

| | log Q/K | | log Q/K |
|------------------|--------------|------------------|---------|
| Berthierine_Lorr | 11.4765s/sat | Chabazite | -0.5833 |
| Chamosite | 3.5114s/sat | Phillipsite_Ca | -0.5911 |
| Smectite_MX80(5) | 3.5039s/sat | Pyrophyllite | -0.6000 |
| Smectite_MX80(3) | 3.1193s/sat | Vaterite | -0.6038 |
| HBeidellite-Na | 3.0854s/sat | Cristobalite | -0.6057 |
| Sudoite | 2.9069s/sat | Ferryhydrite | -0.6143 |
| HBeidellite-Ca | 2.7372s/sat | Beidellite-Mg | -0.6443 |
| HBeidellite-Mg | 2.6454s/sat | Boehmite | -0.6721 |
| HBeidellite-K | 2.0664s/sat | Paragonite | -0.6753 |
| Amesite-Fe | 2.0133s/sat | Gibbsite | -0.7321 |
| Beidellite_SBI-d | 1.8090s/sat | Laumontite | -0.7541 |
| Hematite | 1.4892s/sat | HMontmorillonite | -0.7635 |
| HMontmorillonite | 1.3923s/sat | CaCO3:H2O(s) | -0.8533 |
| Muscovite | 1.3141s/sat | Analcime | -0.9016 |
| Clinochlore | 1.1763s/sat | Dawsonite | -0.9338 |
| HMontmorillonite | 1.1757s/sat | Amesite | -0.9590 |
| Phillipsite_Na | 0.8210s/sat | Minnesotaite | -0.9890 |
| HMontmorillonite | 0.6725s/sat | Montmorillonite- | -1.0265 |
| HMontmorillonite | 0.6100s/sat | Illite-Al | -1.0522 |
| Illite-Fell | 0.5560s/sat | SiO2(am) | -1.0722 |
| HMontmorillonite | 0.5499s/sat | HSaponite-Na | -1.1443 |
| Magnesite(nat) | 0.5014s/sat | Beidellite-Ca | -1.2027 |
| Montmorillonite- | 0.4134s/sat | Saponite-FeNa | -1.2722 |

Phillipsite_K 0.4114s/sat Pyrrhotite -1.3886
 Montmorillonite- 0.3691s/sat Montmorillonite- -1.3940
 Microcline 0.3461s/sat Troilite -1.4216
 Heulandite_Na 0.3408s/sat Celadonite-Mg -1.5165
 HMontmorillonite 0.2493s/sat Saponite-FeK -1.5533
 Dolomite 0.2356s/sat Montmorillonite- -1.5540
 Diaspore 0.1049s/sat HSaponite-Ca -1.5647
 Siderite 0.0000 sat Ripidolite_Cca-- -1.5756
 Kaolinite 0.0000 sat HSaponite-Mg -1.6565
 Quartz 0.0000 sat Beidellite_SBlD- -1.6809
 Pyrite 0.0000 sat Acmite -1.7301
 Calcite 0.0000 sat Saponite-FeMg -1.7530
 Celadonite-Fe -0.0931 Clinoptilolite_C -1.7894
 Cronstedtite-Th -0.1071 Saponite-Na -1.8454
 Saponite_SapCa(4) -0.1118 Saponite-K -1.9511
 Goethite -0.1537 Ferrihydrite(am) -1.9643
 Aragonite -0.1691 Gismondine -1.9865
 Sanidine -0.2314 FeAl2O4(s) -1.9917
 Saponite-FeCa -0.2314 Scolecite -2.0043
 Greenalite -0.2741 Albite-high -2.0387
 Heulandite_Ca -0.3255 illite-FeIII -2.1294
 Beidellite-Na -0.3290 Saponite-Mg -2.1507
 Magnesite(syn) -0.3342 HSaponite-K -2.2356
 Magnetite -0.3905 Mordenite_Oregon -2.4691
 Beidellite-K -0.4346 Mordenite_Ca -2.4870
 Illite-Mg -0.4397 Illite_lmt-- -2.4981
 Montmorillonite- -0.4532 C(cr) -2.6491
 HMontmorillonite -0.4899 Vermiculite-Na -2.6958
 Lepidocrocite -0.5285 Saponite-Ca -2.7192
 Montmorillonite- -0.5358 Vermiculite-Mg -2.7936
 SmectiteMX80 -0.5384 Illite/smectitel -2.8971
 Montmorillonite- -0.5589 Dickite -2.9755
 Albite-low -0.5681 Maghemite(disord -2.9771
 (only minerals with log Q/K > -3 listed)

| Gases | partial press. (bar) | fugacity | fug. coef. | log fug. |
|--------|-------------------------|-----------|------------|----------|
| H2O(g) | 0.01829 | 0.01829 | 1.000* | -1.7377 |
| CO2(g) | 0.002399 | 0.002399 | 1.000* | -2.6200 |
| H2(g) | 3.120e-08 | 3.120e-08 | 1.000* | -7.5058 |
| CH4(g) | 4.489e-09 | 4.489e-09 | 1.000* | -8.3478 |
| H2S(g) | 1.668e-09 | 1.668e-09 | 1.000* | -8.7779 |
| CO(g) | 2.398e-14 | 2.398e-14 | 1.000* | -13.6201 |
| HCl(g) | 4.148e-19 | 4.148e-19 | 1.000* | -18.3822 |
| SO2(g) | 5.497e-25 | 5.497e-25 | 1.000* | -24.2598 |
| Cl2(g) | 2.105e-64 | 2.105e-64 | 1.000* | -63.6767 |
| O2(g) | 5.874e-72 | 5.874e-72 | 1.000* | -71.2310 |

*no data, gas taken to be ideal

| | In fluid | Sorbed | | |
|----------------|-------------|----------|----------|----------------|
| Original basis | total moles | moles | mg/kg | moles mg/kg |
| H2O | -8.03 | 55.5 | 9.99e+05 | |
| Al+++ | 7.75 | 1.81e-08 | 0.000488 | |
| CO3-- | 1.56 | 0.0151 | 903. | |
| Ca++ | 1.61 | 5.01e-05 | 2.01 | 0.115 4.60e+03 |
| Cl- | 0.000734 | 0.000734 | 26.0 | |
| Fe++ | 0.877 | 1.06e-05 | 0.593 | |
| H+ | -21.6 | 0.0149 | 15.0 | |
| H4(SiO4) | 41.0 | 0.000144 | 13.8 | |

| | | | | | |
|--------|-------|-----------|-----------|-------|----------|
| K+ | 0.134 | 0.000185 | 7.24 | 0.134 | 5.24e+03 |
| Mg++ | 0.110 | 6.59e-05 | 1.60 | 0.110 | 2.68e+03 |
| Na+ | 0.541 | 0.0156 | 358. | 0.525 | 1.21e+04 |
| O2(aq) | -2.92 | -1.14e-08 | -0.000365 | | |
| SO4-- | 1.67 | 2.41e-05 | 2.31 | | |
| >X:Na | 1.11 | | | | |

Sorbed fraction log fraction

| | | |
|------|--------|--------|
| Ca++ | 0.9996 | -0.000 |
| K+ | 0.9986 | -0.001 |
| Mg++ | 0.9994 | -0.000 |
| Na+ | 0.9712 | -0.013 |

Elemental composition In fluid Sorbed
total moles moles mg/kg moles mg/kg

| | | | | | |
|----------|-----------|-----------|-----------|--------|-----------|
| Al+++ | 7.747 | 1.809e-08 | 0.0004876 | | |
| CO3-- | 1.556 | 0.01506 | 902.7 | | |
| Ca++ | 1.613 | 5.014e-05 | 2.007 | 0.1150 | 4603. |
| Cl- | 0.0007342 | 0.0007342 | 26.00 | | |
| Fe++ | 0.8766 | 1.064e-05 | 0.5932 | | |
| H+ | -37.61 | 111.0 | 1.118e+05 | | |
| H4(SiO4) | 41.03 | 0.0001440 | 13.82 | | |
| K+ | 0.1343 | 0.0001854 | 7.241 | 0.1341 | 5235. |
| Mg++ | 0.1103 | 6.588e-05 | 1.599 | 0.1103 | 2677. |
| Na+ | 0.5410 | 0.01561 | 358.3 | 0.5254 | 1.206e+04 |
| O2 | -13.86 | 55.51 | 8.869e+05 | | |
| SO4-- | 1.667 | 2.407e-05 | 2.310 | | |