Iron Precipitation Project (IPP)

This project is carried out by Mengyuan Cai, Minghao Qiu, and Yichen Xu, instructed by Prof. Dr. rer. nat. Dipl.-Hydr. Külls and M. Eng. v.Grafenstein.

<latex>NO_3^-</latex>

The task is to determine the reason and the quantity of iron precipitation in a given water sample from an aquifer, and, perhaps, provide some possible solutions.

Ion balance and activity

In order to examine the result given by the document, ion balances and activity of ions are recalculated.

The calculation example for ion balance of Brunnen 07 Filter 1 Time 1(abbreviated as F1T1) is given as follows.

Ion	Molar mass (mg/l)	Mass concentration (mg/l)
Anion		
Chloride(Cl^-)	35.453	16.1
Nitrite(NO_2^-)	46.006	0.01
Nitrate(NO_3^-)	62.005	0.10
Sulfate(SO_4^{2-})	96.063	16.5
Bicarbonate(HCO_3^-)	61.017	297.2
Cation		
Sodium(Na^+)	22.990	9.05
Ammonium(NH_4^+)	18.038	0.10
Potassium(K^+)	39.098	1.70
Calcium(Ca^{2+})	40.078	96.7
Magnesium(Mg^{2+})	24.305	6.60
Ferrous(Fe^{2+})	55.845	0.5

To calculate the ion balance, anion and cation equivalent concentrations are needed.

Anion equivalent concentration $$AEC=\sum_{i=1}^n \frac{c_i*Z_i}{M_i}$$ $$=\frac{c_{Cl^-}*Z_{Cl^-}}{M_{Cl^-}}+\frac{c_{NO_2^-}*Z_{NO_2^-}}{M_{NO_2^-}}+\frac{c_{NO_3^-}*Z_{NO_3^-}}{M_{NO_3^-}}+\frac{c_{SO_4^{2-}}*Z_{SO_4^{2-}}}{M_{SO_4^{2-}}}+\frac{c_{HCO_3^-}*Z_{HCO_3^-}}{M_{HCO_3^-}}$$ $$=5.670\ meq/l$$

Cation equivalent concentration $$CEC=\sum_{i=1}^n \frac{c_i*Z_i}{M_i}$$ $$=\frac{c_{Na^+}*Z_{Na^+}}{M_{Na^+}}+\frac{c_{NH_4^+}*Z_{NH_4^+}}{M_{NH_4^+}}+\frac{c_{K^+}*Z_{K^+}}{M_{K^+}}+\frac{c_{Ca^{2+}}*Z_{Ca^{2+}}}{M_{Ca^{2+}}}+\frac{c_{Mg^{2+}}*Z_{Mg^{2+}}}{M_{Mg^{2+}}}+\frac{c_{Fe^{2+}}*Z_{Fe^{2+}}}{M_{Fe^{2+}}}$$ $$=5.829\ meq/l$$

In which c=mass concentration of ion, Z=charge of ion, M=molar mass of ion.

$$Ion\ balance=\frac{AEC-CEC}{AEC+CEC}=-1.383\%$$

To calculate activity of ions, ion strength and activity coefficients for monovalent and bivalent ions are needed.

Ion strength $$I=\frac{1}{2} \sum_{i=1}^n c_i*z_i$$ $$=c_{Cl^-}*Z_{Cl^-}+c_{NO_2^-}*Z_{NO_2^-}+c_{NO_3^-}*Z_{NO_3^-}+c_{SO_4^{2-}}*Z_{SO_4^{2-}}+c_{HCO_3^-}*Z_{HCO_3^-}$$
$$+c_{Na^+}*Z_{Na^+}+c_{NH_4^+}*Z_{NH_4^+}+c_{K^+}*Z_{K^+}+c_{Ca^{2+}}*Z_{Ca^{2+}}+c_{Mg^{2+}}*Z_{Mg^{2+}}+c_{Fe^{2+}}*Z_{Fe^{2+}}$$ $$=8.6148*10^{-3}\ eq/l$$

In which c=molar concentration of ion.

To calculate the activity coefficient, Debye-Hückel equation is used.

$$log{\gamma_i}=-\frac{A*Z_i^2*\sqrt{I}}{1+a_i*B*\sqrt{I}}$$

In which A=0.4960, B=0.3258*10^{-8} at 10°C, and the values of a_i are shown as follows.

a_0 (*10^8)	**Ion**
2.5	NH_4^+
3	K^-, Cl^-, NO_3^-
4	SO_4^{2+}
4.0-4.5	Na^+, HCO_3^-
6	Ca^{2+}, Fe^{2+}
8	Mg^{2+}
9	Fe^{3+}

Since the a_i value of NO_2^- is missing in the table, the a_i value of NO_3^- is used instead. Moreover, the a_i value of Na^+, HCO_3^- is chosen as 4.25 since the error caused by the a_i value is not significant.

The calculated activity coefficients of ions are as follows.

Activity coefficient γ	
NH_4^+	0.90614759
K^-, Cl^-, NO_3^-, NO_2^-	0.90738638
SO_4^{2+}	0.68505193
Na^+, HCO_3^-	0.91034496
Ca^{2+}, Fe^{2+}	0.69844622
Mg^{2+}	0.71076069
Fe^{3+}	0.71655243

Results of activity of ions are as follows.

Ion	**Activity (mol/l)**
Chloride(Cl^-)	$4.12064*10^{-4}$
Nitrite(NO_2^-)	$1.97232*10^{-7}$

Ion	Activity (mol/l)
Nitrate(NO_3^-)	$1.46341*10^{-6}$
Sulfate(SO_4^{2-})	$1.17666*10^{-4}$
Bicarbonate(HCO_3^-)	$4.43408*10^{-3}$
Sodium(Na^+)	$3.58357*10^{-4}$
Ammonium(NH_4^+)	$5.02355*10^{-6}$
Potassium(K^+)	$3.94536*10^{-5}$
Calcium(Ca^{2+})	$1.68521*10^{-3}$
Magnesium(Mg^{2+})	$1.93006*10^{-4}$
Ferrous(Fe^{2+})	$6.25344*10^{-6}$

The results of all calculations are as follows.

The results of ion balance calculations are as follows.

Br7 T1	Br7 T2	Br7 T4	
-2.74%	-1.83%	-2.39%	
F1 T1	**F1 T2**	**F1 T3**	**F1 T4**
-1.38%	-1.56%	-1.95%	-2.25%
F2 T1	**F2 T2**	**F2 T3**	**F2 T4**
-2.24%	-2.90%	-2.14%	-2.25%

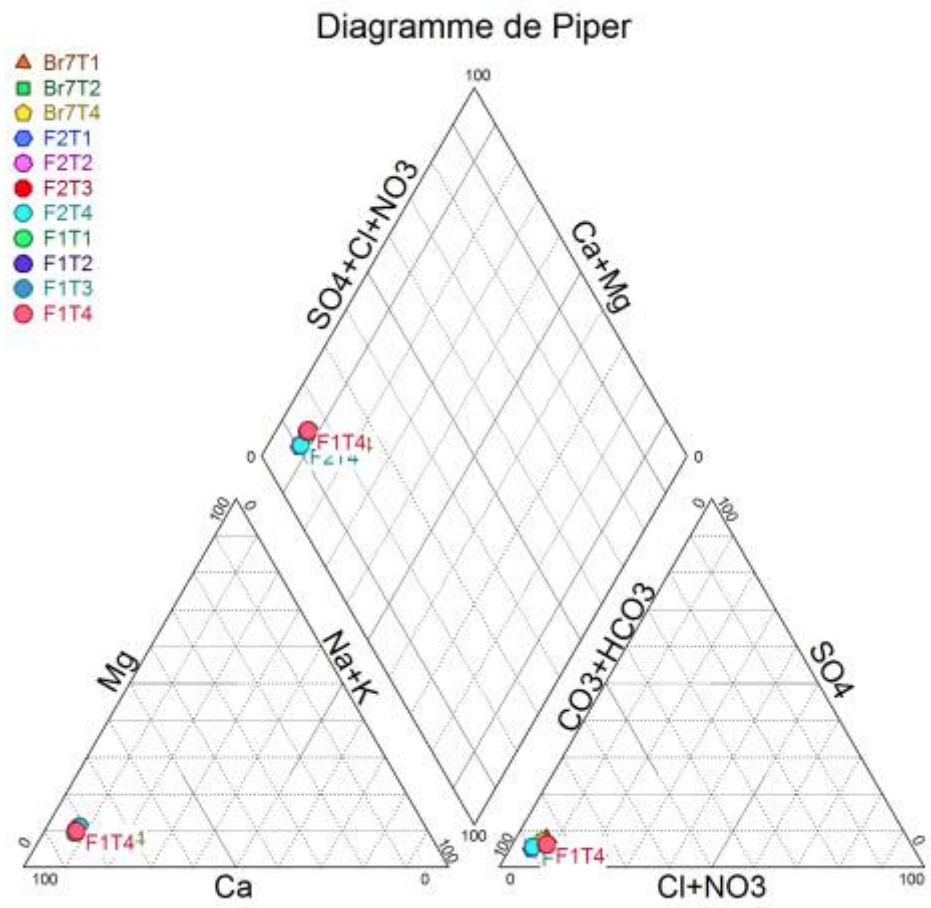
The results of activity calculations are as follows.

Activity a (mol/l)	Br7 T1	Br7 T2	Br7 T4	
Chloride(Cl^-)	$3.33531*10^{-4}$	$3.13601*10^{-4}$	$3.15872*10^{-4}$	
Nitrite(NO_2^-)	$1.97714*10^{-7}$	$1.98089*10^{-7}$	$1.97902*10^{-7}$	
Nitrate(NO_3^-)	$2.14177*10^{-5}$	$5.14414*10^{-5}$	$5.13927*10^{-5}$	
Sulfate(SO_4^{2-})	$1.54051*10^{-4}$	$1.35587*10^{-4}$	$1.35823*10^{-4}$	
Bicarbonate(HCO_3^-)	$4.24256*10^{-3}$	$4.18718*10^{-3}$	$4.24633*10^{-3}$	
Sodium(Na^+)	$4.00871*10^{-4}$	$3.50689*10^{-4}$	$3.38858*10^{-4}$	
Ammonium(NH_4^+)	$5.03583*10^{-6}$	$6.05480*10^{-6}$	$7.05706*10^{-6}$	
Potassium(K^+)	$2.62886*10^{-5}$	$4.14890*10^{-5}$	$4.28469*10^{-5}$	
Calcium(Ca^{2+})	$1.63862*10^{-3}$	$1.57850*10^{-3}$	$1.61396*10^{-3}$	
Magnesium(Mg^{2+})	$2.27352*10^{-4}$	$2.12972*10^{-4}$	$2.25064*10^{-4}$	
Iron(Fe^{2+})	$1.23654*10^{-5}$	$1.43509*10^{-5}$	$1.40513*10^{-5}$	
Activity a (mol/l)	**F1 T1**	**F1 T2**	**F1 T3**	**F1 T4**
Chloride(Cl^-)	$4.12064*10^{-4}$	$4.19508*10^{-4}$	$4.19766*10^{-4}$	$4.17044*10^{-4}$
Nitrite(NO_2^-)	$1.97232*10^{-7}$	$1.97122*10^{-7}$	$1.97243*10^{-7}$	$1.97167*10^{-7}$
Nitrate(NO_3^-)	$1.46341*10^{-6}$	$1.46259*10^{-6}$	$1.46349*10^{-6}$	$1.46292*10^{-6}$
Sulfate(SO_4^{2-})	$1.17666*10^{-4}$	$1.21687*10^{-4}$	$1.20544*10^{-4}$	$1.20367*10^{-4}$
Bicarbonate(HCO_3^-)	$4.43408*10^{-3}$	$4.45861*10^{-3}$	$4.37015*10^{-3}$	$4.39542*10^{-3}$
Sodium(Na^+)	$3.58357*10^{-4}$	$3.53420*10^{-4}$	$3.57187*10^{-4}$	$3.59829*10^{-4}$
Ammonium(NH_4^+)	$5.02355*10^{-6}$	$5.02066*10^{-6}$	$5.02383*10^{-6}$	$5.02183*10^{-6}$
Potassium(K^+)	$3.94536*10^{-5}$	$3.71120*10^{-5}$	$3.71348*10^{-5}$	$3.78165*10^{-5}$

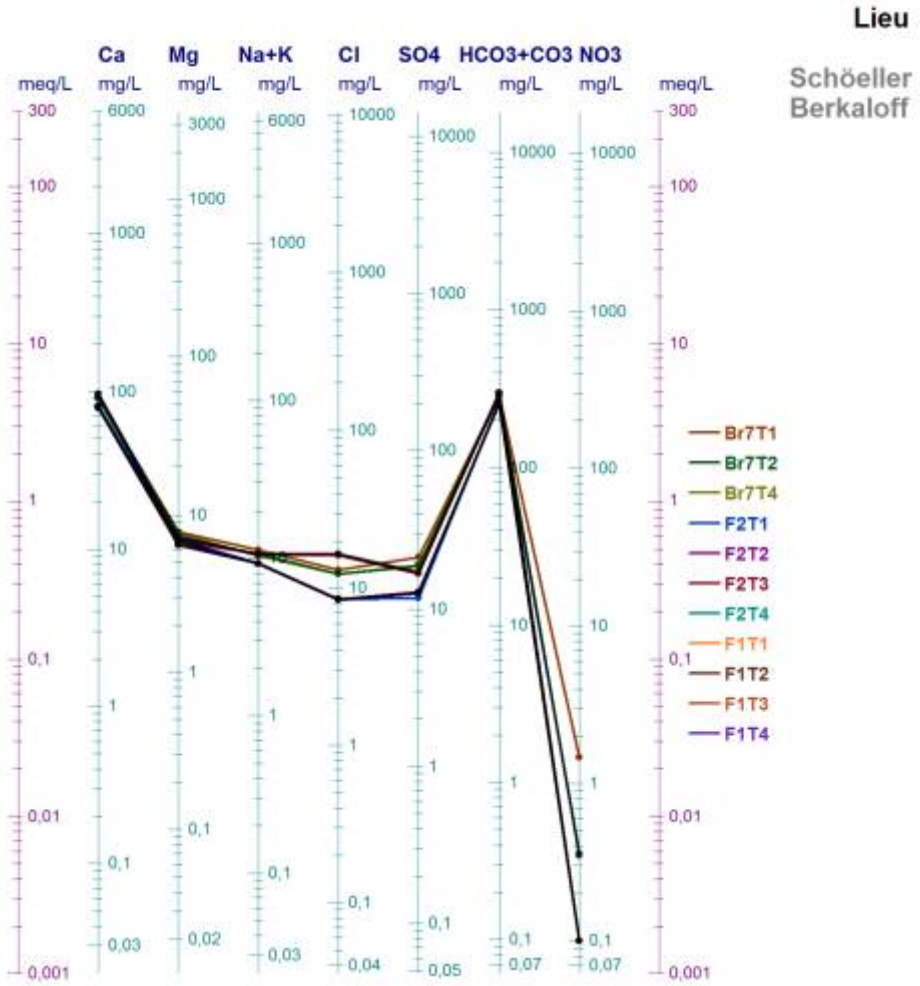
Activity a (mol/l)	**F1 T1**	**F1 T2**	**F1 T3**	**F1 T4**
Calcium(Ca^{2+})	$1.68521*10^{-3}$	$1.68547*10^{-3}$	$1.67681*10^{-3}$	$1.69200*10^{-3}$
Magnesium(Mg^{2+})	$1.93006*10^{-4}$	$2.12817*10^{-4}$	$2.01813*10^{-4}$	$2.05078*10^{-4}$
Iron(Fe^{2+})	$6.25344*10^{-6}$	$1.12347*10^{-5}$	$1.12583*10^{-5}$	$1.12434*10^{-5}$
Activity a (mol/l)	**F2 T1**	**F2 T2**	**F2 T3**	**F2 T4**
Chloride(Cl^{-})	$2.17596*10^{-4}$	$2.14859*10^{-4}$	$2.17818*10^{-4}$	$2.20081*10^{-4}$
Nitrite(NO_2^{-})	$1.98207*10^{-7}$	$1.99200*10^{-7}$	$1.99308*10^{-7}$	$1.99263*10^{-7}$
Nitrate(NO_3^{-})	$5.29430*10^{-6}$	$1.47801*10^{-6}$	$1.47881*10^{-6}$	$1.47847*10^{-6}$
Sulfate(SO_4^{2-})	$1.13653*10^{-4}$	$1.22435*10^{-4}$	$1.23461*10^{-4}$	$1.22466*10^{-4}$
Bicarbonate(HCO_3^{-})	$4.03852*10^{-3}$	$3.93684*10^{-3}$	$3.92003*10^{-3}$	$3.93779*10^{-3}$
Sodium(Na^{+})	$3.09254*10^{-4}$	$2.98214*10^{-4}$	$3.02365*10^{-4}$	$3.01897*10^{-4}$
Ammonium(NH_4^{+})	$5.05292*10^{-6}$	$5.05517*10^{-6}$	$7.58737*10^{-6}$	$7.58544*10^{-6}$
Potassium(K^{+})	$3.59861*10^{-5}$	$4.06768*10^{-5}$	$4.21038*10^{-5}$	$4.06905*10^{-5}$
Calcium(Ca^{2+})	$1.86997*10^{-3}$	$1.84082*10^{-3}$	$1.80729*10^{-3}$	$1.82069*10^{-3}$
Magnesium(Mg^{2+})	$2.61300*10^{-4}$	$2.57208*10^{-4}$	$2.45161*10^{-4}$	$2.47395*10^{-4}$
Iron(Fe^{2+})	$1.31731*10^{-6}$	$2.10847*10^{-5}$	$2.20841*10^{-5}$	$2.17499*10^{-5}$

Visualization

This is the Piper Diagram of all samples. It shows that all the water samples have a relatively high consistency, which means the water at the sampling site is highly homogeneous.



This is the Schoeller Diagram of all samples. It shows that although the water is highly homogeneous, there are differences between the Cl^- and SO_4^{2-} concentration of Filter 1 and Filter 2.



Redox potential

Due to the absence of data of Fe^{3+} concentration, assumptions are needed when doing the following calculations. Thus, 3 assumptions are made as follows.

1. Since every device has its detecting limit, it is possible that the Fe^{3+} could be just below the detecting threshold.

2. Since there is iron precipitation in the water sample, it is also possible that all the iron precipitation contains Fe^{3+}, which are all previously dissolved in the water.

3. It is reasonable to assume that the Fe^{3+} concentration is dissolved part of $Fe(OH)_3$ in the water at equilibrium.

According to the calculations, the first two assumptions are not likely to be true because the pe value is too high, which is high enough to cause the dissociation of water itself. Therefore, only the methodology of calculation and result is given as follows.

F1 T1 is taken as an example.

$$[Fe^{3+}]=\frac{K_{sp}}{[OH^-]^3}=\frac{1.1*10^{-36}}{10^{-(14.534617-7.2)*3}}=1.1098*10^{-14}\ mol/l$$

In which $K_{sp}=1.1*10^{-36}$ is the solubility product at 18°C because the solubility product at 10°C is not available, and $10^{-14.534617}$ is the ion product of water at 10°C.

$$pe=pe^0+\log \frac{[Fe^{3+}]}{[Fe^{2+}]}=13+\log \frac{1.1098*10^{-14}}{6.25344*10^{-6}}=4.2491$$

In which $pe^0=13$ is the standard pe at 25°C because the standard pe at 10°C is not available.

The results of all redox potential calculations are as follows.

Br7 T1	**Br7 T2**	**Br7 T4**	
3.3530	3.2884	3.2975	
F1 T1	**F1 T2**	**F1 T3**	**F1 T4**
4.2491	3.9947	3.9938	3.9943
F2 T1	**F2 T2**	**F2 T3**	**F2 T4**
4.9256	3.7213	3.7012	3.7078

Carbon balance

In order to obtain the activity of CO_3^{2-}, which might be responsible for the precipitation of Calcite, Dolomite, and Siderite, the carbon balance is calculated.

The calculation example of carbon balance of F1 T1 is given as follows.

$$CO_2(g) + H_2O \rightleftharpoons H_2CO_3$$

$$K_0=\frac {[H_2CO_3]}{[CO_2]}=5.37*10^{-2}$$

$$H_2CO_3 \rightleftharpoons H^+ + HCO_3^-$$

$$K_1=\frac {[H^+][HCO_3^-]}{[H_2CO_3]}=3.47*10^{-7}$$

$$HCO_3^- \rightleftharpoons H^+ + CO_3^{2-}$$

$$K_2=\frac {[H^+][CO_3^{2-}]}{[HCO_3^-]}=2.75*10^{-11}$$

The activity of HCO_3^- is calculated previously.

$$[HCO_3^-]=4.43408*10^{-3}\ mol/l$$

Therefore, $$[CO_2(g)]=1.50*10^{-2}\ mol/l$$

$$[H_2CO_3]=8.07*10^{-4}\ mol/l$$

$$[CO_3^{2-}]=1.94*10^{-6}\ mol/l$$

The results of all carbon balance calculations are as follows.

Activity a (mol/l)	**Br7 T1**	**Br7 T2**	**Br7 T4**
$[CO_2(g)]$	$9.07*10^{-3}$	$8.95*10^{-3}$	$9.08*10^{-3}$

Activity a (mol/l)	**Br7 T1**	**Br7 T2**	**Br7 T4**
$[H_2CO_3]$	$4.87*10^{-4}$	$4.81*10^{-4}$	$4.88*10^{-4}$
$[CO_3^{2-}]$	$2.94*10^{-6}$	$2.90*10^{-6}$	$2.94*10^{-6}$

Activity a (mol/l)	**F1 T1**	**F1 T2**	**F1 T3**	**F1 T4**
$[CO_2(g)]$	$1.50*10^{-2}$	$1.51*10^{-2}$	$1.48*10^{-2}$	$1.49*10^{-2}$
$[H_2CO_3]$	$8.07*10^{-4}$	$8.11*10^{-4}$	$7.95*10^{-4}$	$8.00*10^{-4}$
$[CO_3^{2-}]$	$1.94*10^{-6}$	$1.95*10^{-6}$	$1.91*10^{-6}$	$1.92*10^{-6}$
Activity a (mol/l)	**F2 T1**	**F2 T2**	**F2 T3**	**F2 T4**
$[CO_2(g)]$	$8.63*10^{-3}$	$8.42*10^{-3}$	$8.38*10^{-3}$	$8.42*10^{-3}$
$[H_2CO_3]$	$4.64*10^{-4}$	$4.52*10^{-4}$	$4.50*10^{-4}$	$4.52*10^{-4}$
$[CO_3^{2-}]$	$2.79*10^{-6}$	$2.72*10^{-6}$	$2.71*10^{-6}$	$2.72*10^{-6}$

Saturation indices(SI)

It is clear that not all compounds that exist in the water can form a precipitation. Therefore, only saturation indices(SI) of those that are possible to form a precipitation need to be determined. The compounds that can form a precipitation are $CaCO_3$, $MgCO_3$, $FeCO_3$, $Fe(OH)_2$, and $Fe(OH)_3$. However, for the water samples from Filter 1 and Filter 2, when calculating the redox potential, $Fe(OH)_3$ is assumed as at equilibrium. Thus, the SI of $Fe(OH)_3$ of those samples are 0. As for Brunnen 07, the SI of $Fe(OH)_3$ can be calculated.

The calculation example of saturation indices of F1 T1 is given as follows.

$CaCO_3$ is taken as an example.

$$SI_{CaCO_3}=\log \frac{[Ca^{2+}][CO_3^{2+}]}{K_{sp}}=0.1435$$

In which $K_{sp}=10^{-8.36}$ is the solubility product of Calcite at 10°C.

The results of all saturation indices of F1 T1 are as follows.

Compounds	**Saturation indices SI**
$CaCO_3$	0.1435
$MgCO_3$	-4.5726
$CaSO_4$	-2.4880
$FeCO_3$	0.0519
$Fe(OH)_2$	-5.6880

The results of all saturation indices calculations are as follows.

Saturation indices SI	**Br7 T1**	**Br7 T2**	**Br7 T4**
$CaCO_3$	0.1121	0.0902	0.1059
$MgCO_3$	-4.5206	-4.5547	-4.5247
$CaSO_4$	-2.7379	-2.5455	-2.5254
$FeCO_3$	0.3288	0.3878	0.3847
$Fe(OH)_2$	-8.3919	-8.3272	-8.3364

Saturation indices SI	Br7 T1	Br7 T2	Br7 T4
$Fe(OH)_3$	-0.7451	-1.0856	-0.9650

Saturation indices SI	F1 T1	F1 T2	F1 T3	F1 T4
$CaCO_3$	0.1435	0.1459	0.1350	0.1414
$MgCO_3$	-4.5726	-4.5278	-4.5595	-4.5501
$CaSO_4$	-2.4880	-2.4734	-2.4797	-2.4764
$FeCO_3$	0.0519	0.3087	0.3009	0.3029
$Fe(OH)_2$	-5.6880	-5.4335	-5.4326	-5.4332
Saturation indices SI	**F2 T1**	**F2 T2**	**F2 T3**	**F2 T4**
$CaCO_3$	0.1481	0.1302	0.1203	0.1255
$MgCO_3$	-4.4816	-4.4995	-4.5222	-4.5163
$CaSO_4$	-2.4579	-2.4324	-2.4368	-2.4371
$FeCO_3$	-0.6651	0.5281	0.5463	0.5417
$Fe(OH)_2$	-9.3644	-8.1601	-8.1400	-8.1466

Modeling

Modeling with PHREEQC

After calculating all the data manually, a program called 'PHREEQC' is used to establish the models.

These models are used to investigate:

1)the saturation indices of different minerals that can exist in the water samples;

2)the sensitivity of the minerals to the change of temperature, pH, and pe;

3)the results of mixing two water samples from F1 and F2 in different ratio.

(Due to the problems of PHREEQC about calculations in redox reactions, the sensitivity related to pe level will not be taken into consideration. Moreover, the results of mixing are only relative data.)

Saturation indices

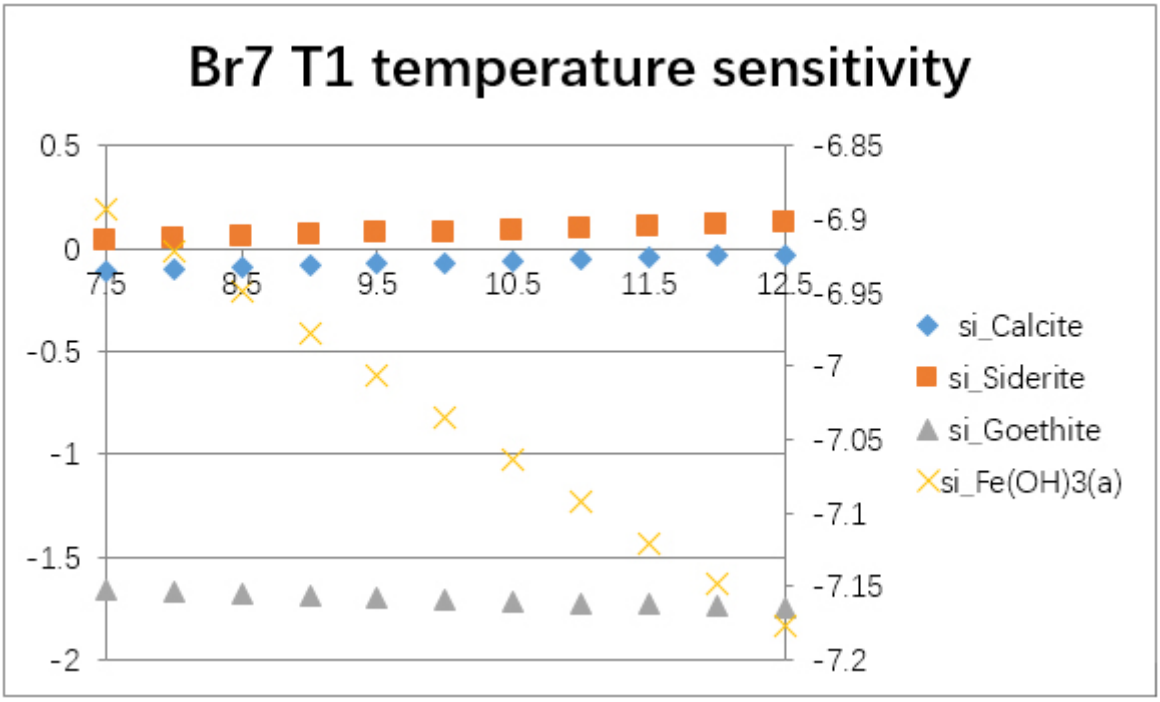
pH=7.2	pe=2	Calcite	Dolomite	Gypsum	Anhydrite	Siderite	Goethite	Fe(OH)3(a)	Jarosite
Br7	T1	-0.0692	-1.1042	-2.1038	-2.5752	0.0763	-1.7034	-7.0254	-32.3761
	T2	-0.0908	-1.1600	-2.1727	-2.6445	0.1360	-2.0420	-7.3626	-33.2996
	T4	-0.0747	-1.1128	-2.1640	-2.6353	0.1324	-1.9237	-7.2461	-32.9336
F1	T1	-0.0276	-1.0977	-2.2038	-2.6709	-0.1941	-0.9141	-6.2508	-30.0733
	T2	-0.0240	-1.0463	-2.1902	-2.6562	0.0638	-0.9159	-6.2566	-30.0808
	T3	-0.0346	-1.0882	-2.1958	-2.6618	0.0582	-0.9158	-6.2565	-30.0876
	T4	-0.0283	-1.0726	-2.1931	-2.6591	0.0596	-0.9159	-6.2565	-30.0823

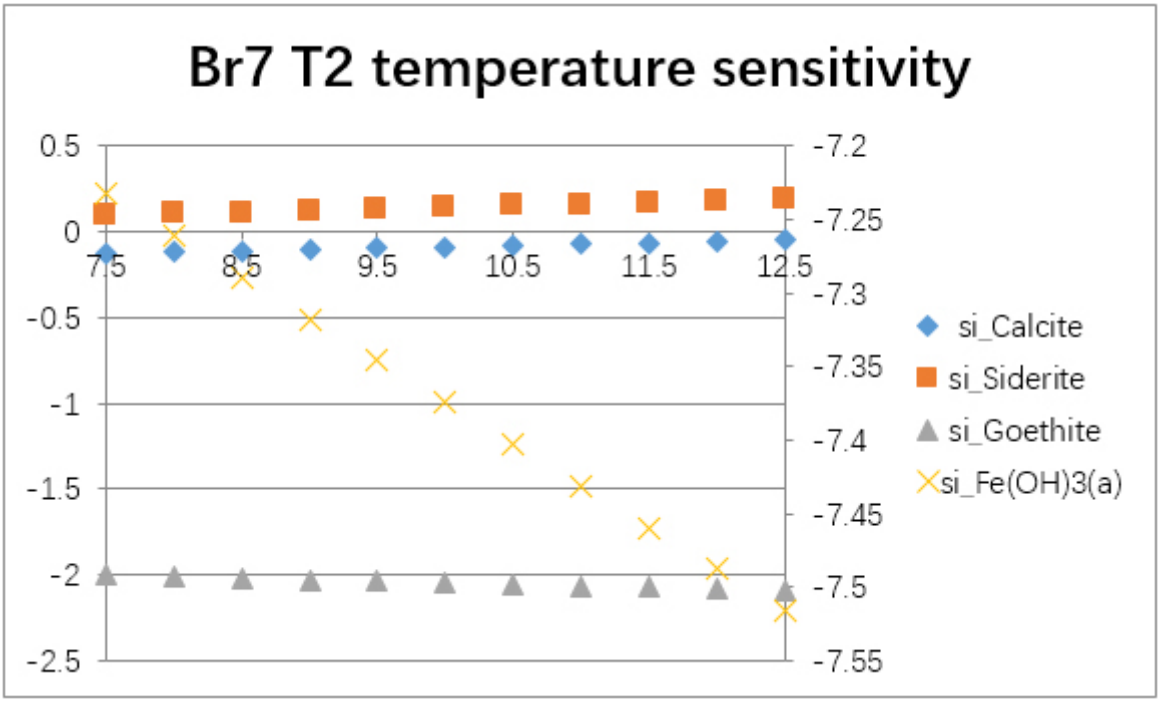
pH=7.2	pe=2	Calcite	Dolomite	Gypsum	Anhydrite	Siderite	Goethite	Fe(OH)3(a)	Jarosite
F2	T1	-0.1374	-1.2231	-2.3982	-2.8642	-1.0161	-3.9137	-9.2543	-39.3805
	T2	-0.1566	-1.2634	-2.3707	-2.8379	0.1779	-3.9119	-9.2486	-39.2515
	T3	-0.1656	-1.2943	-2.3726	-2.8397	0.1972	-3.9118	-9.2485	-39.2252
	T4	-0.1608	-1.2839	-2.3738	-2.8410	0.1918	-3.9118	-9.2485	-39.2486

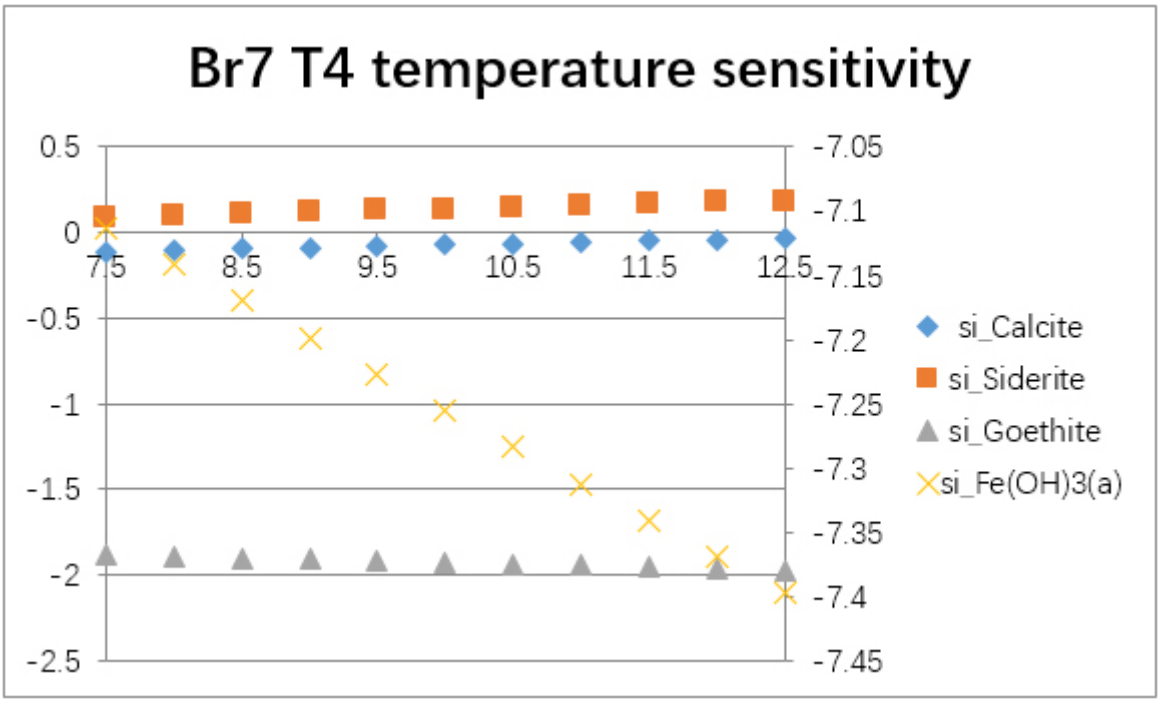
Sensitivity

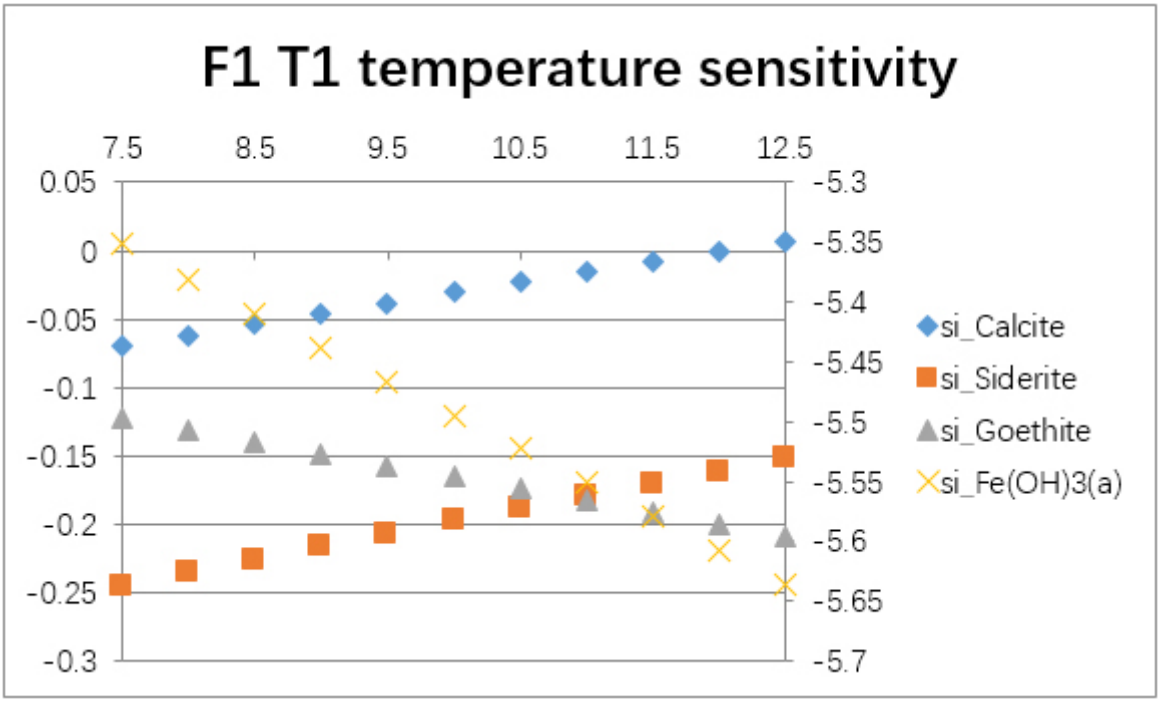
The temperature sensitivity of all water samples are shown as follows.

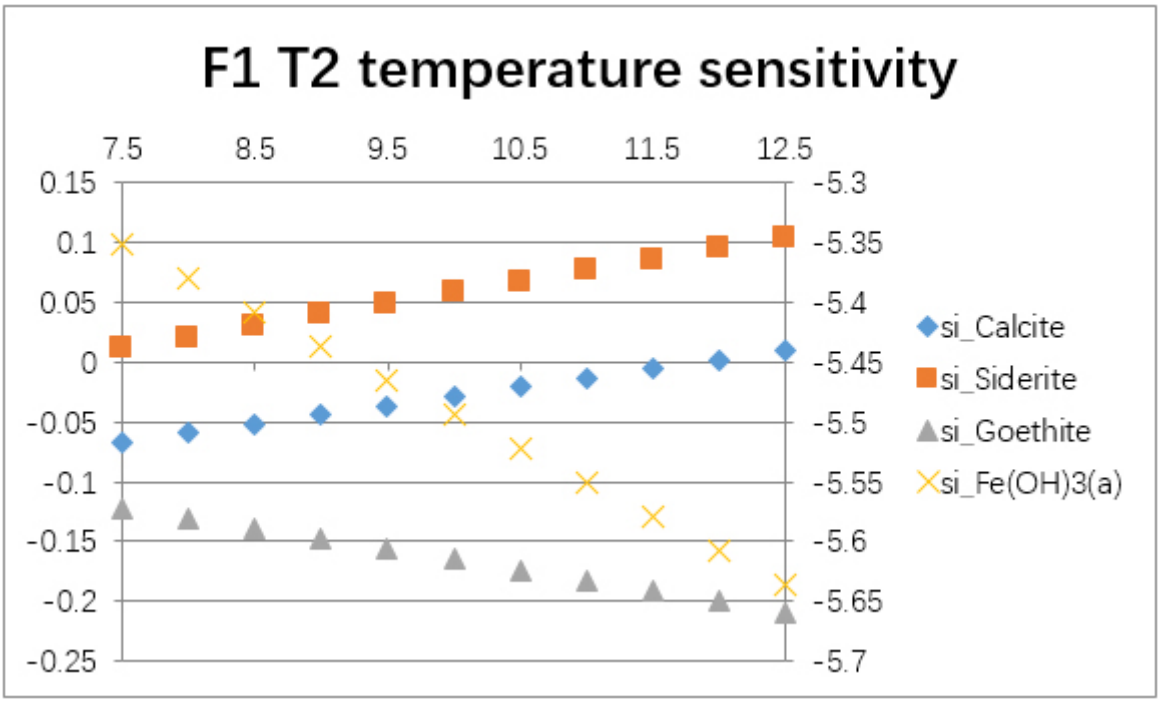
(For each graph, the x-axis is temperature, and the y-axes are saturation indices. The saturation indices of $Fe(OH)_3(a)$ should be read from the secondary axis.)

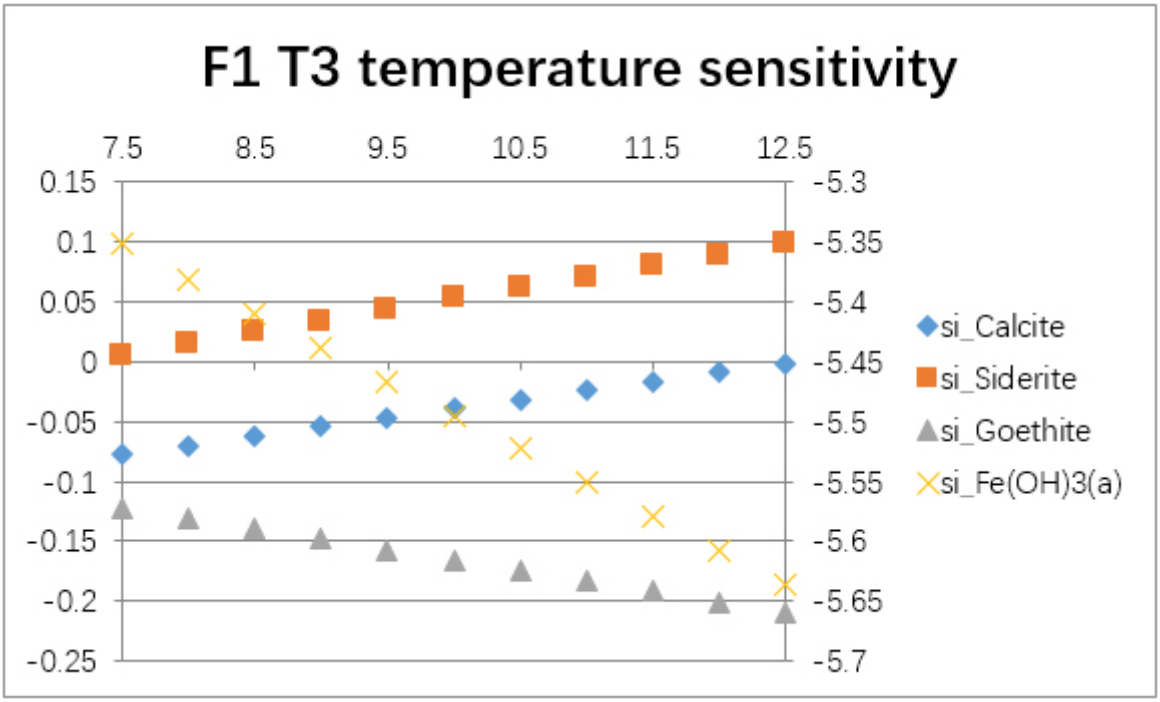


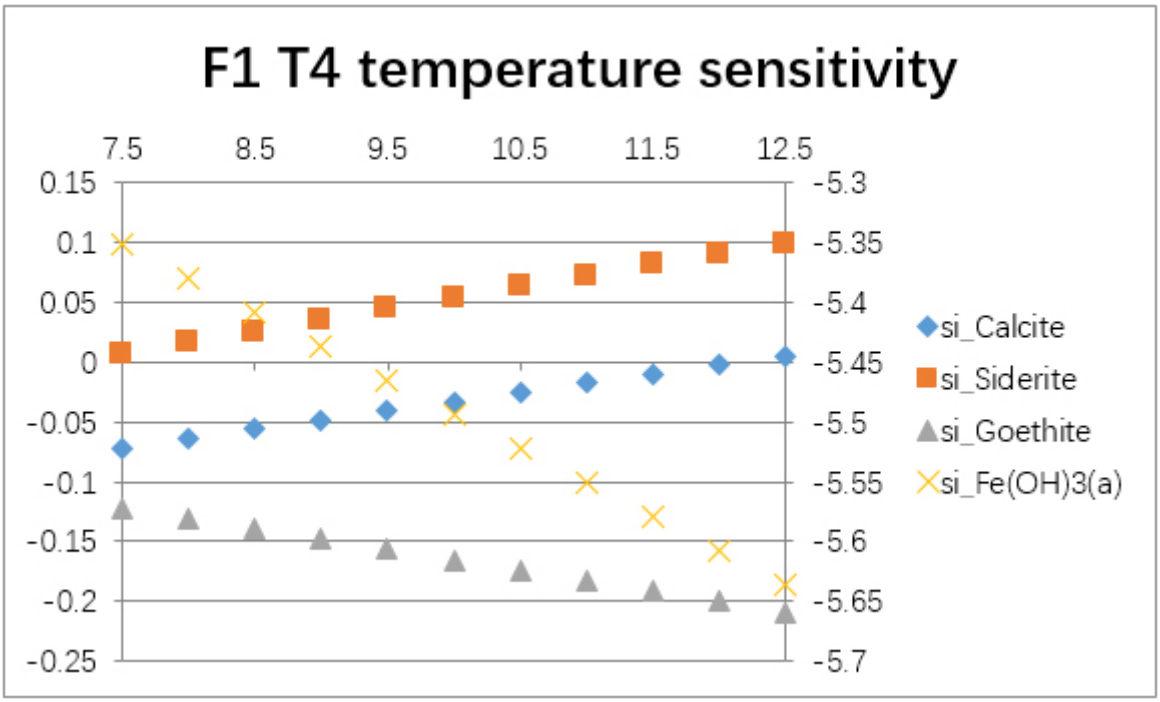

Br7 T2 temperature sensitivity
0.5
0
-0.5
-1
-1.5
-2
-2.5
7.5
8.5
9.5
10.5
11.5
12.5
-7.2
-7.25
-7.3
-7.35
-7.4
-7.45
-7.5
-7.55
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)

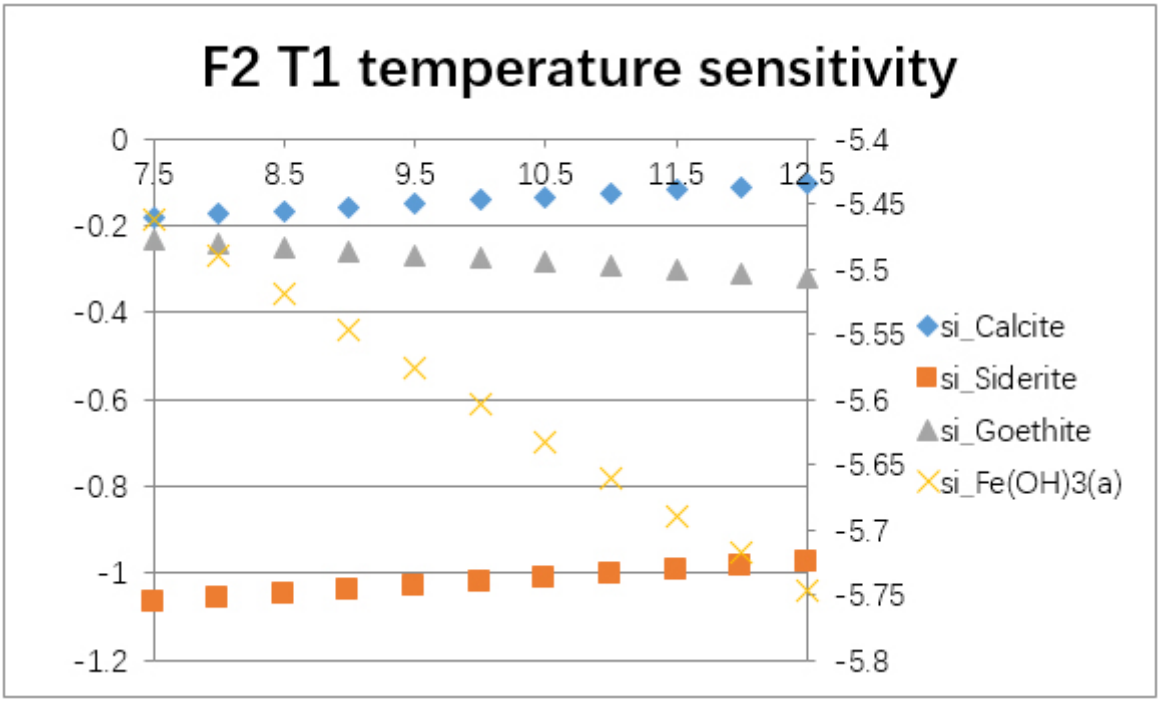

Br7 T4 temperature sensitivity
0.5
0
-0.5
-1
-1.5
-2
-2.5
7.5
8.5
9.5
10.5
11.5
12.5
-7.05
-7.1
-7.15
-7.2
-7.25
-7.3
-7.35
-7.4
-7.45
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)

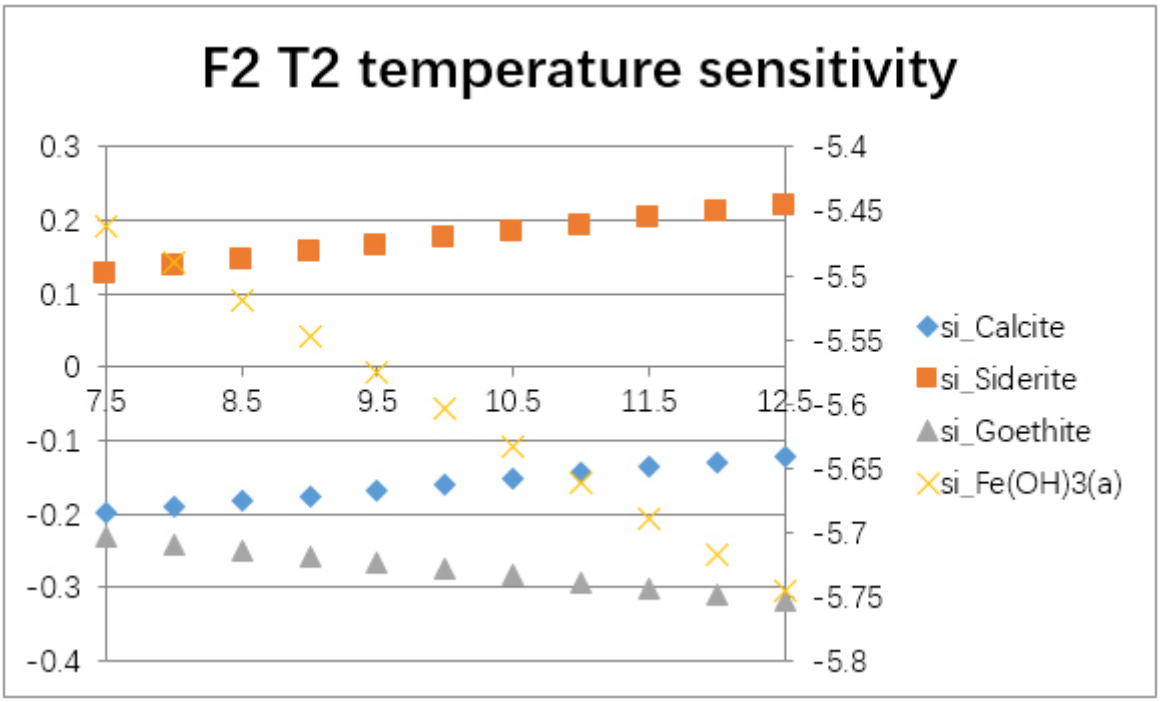

F1 T1 temperature sensitivity
7.5
8.5
9.5
10.5
11.5
12.5
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.25
-0.3
-5.3
-5.35
-5.4
-5.45
-5.5
-5.55
-5.6
-5.65
-5.7
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)

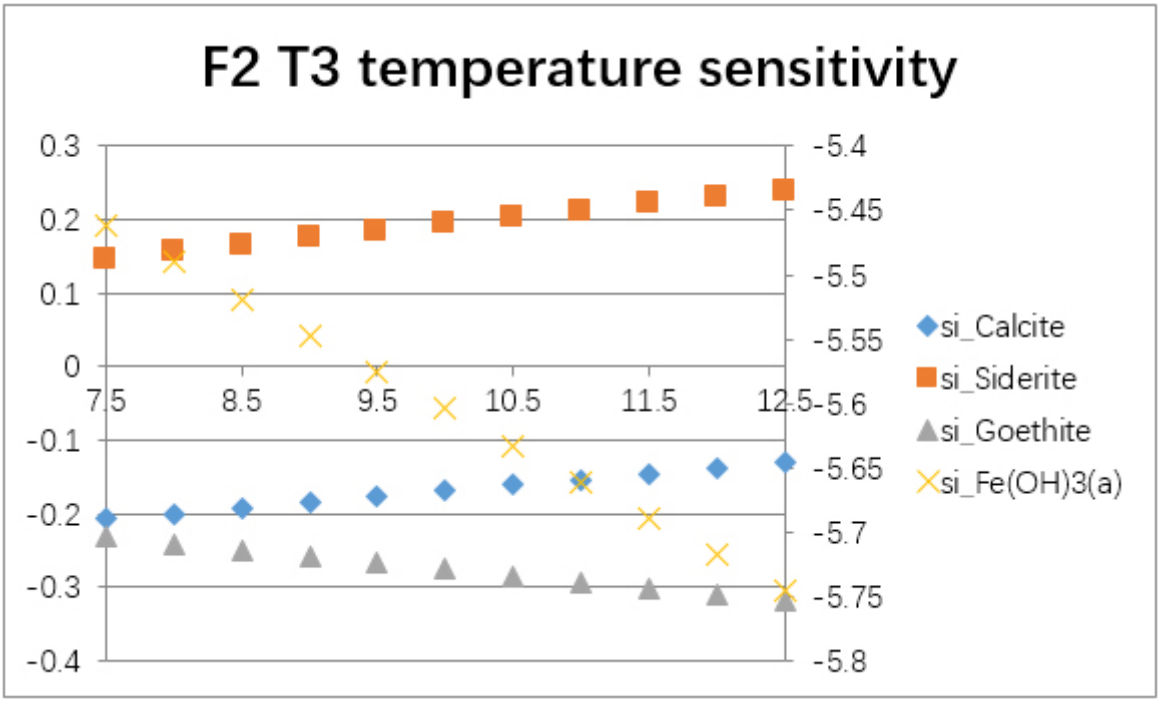

F1 T2 temperature sensitivity
7.5
8.5
9.5
10.5
11.5
12.5
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.25
-5.3
-5.35
-5.4
-5.45
-5.5
-5.55
-5.6
-5.65
-5.7
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)

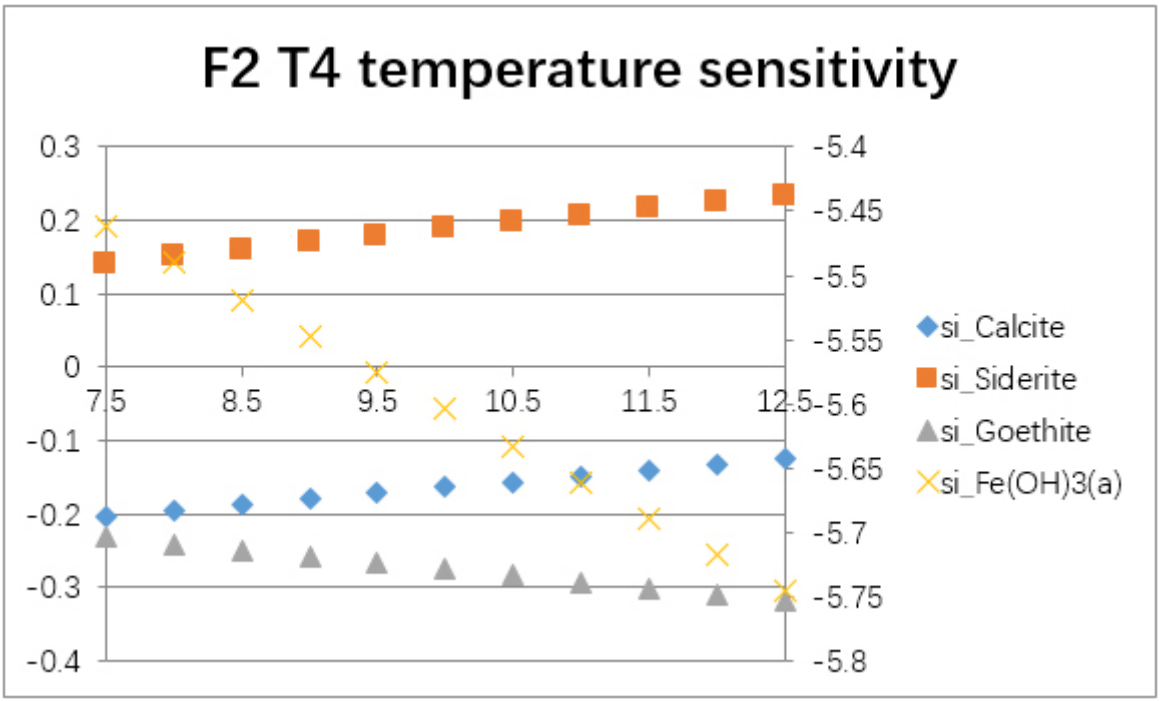

F1 T3 temperature sensitivity
7.5
8.5
9.5
10.5
11.5
12.5
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.25
-5.3
-5.35
-5.4
-5.45
-5.5
-5.55
-5.6
-5.65
-5.7
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)


F1 T4 temperature sensitivity
7.5
8.5
9.5
10.5
11.5
12.5
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
-0.25
-5.3
-5.35
-5.4
-5.45
-5.5
-5.55
-5.6
-5.65
-5.7
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)


F2 T1 temperature sensitivity
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
7.5
8.5
9.5
10.5
11.5
12.5
-5.4
-5.45
-5.5
-5.55
-5.6
-5.65
-5.7
-5.75
-5.8
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)


F2 T2 temperature sensitivity
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
7.5
8.5
9.5
10.5
11.5
12.5
-5.4
-5.45
-5.5
-5.55
-5.6
-5.65
-5.7
-5.75
-5.8
si_Calcite
si_Siderite
si_Goethite
si_Fe(OH)3(a)





The pH sensitivity of all water samples are shown as follows.

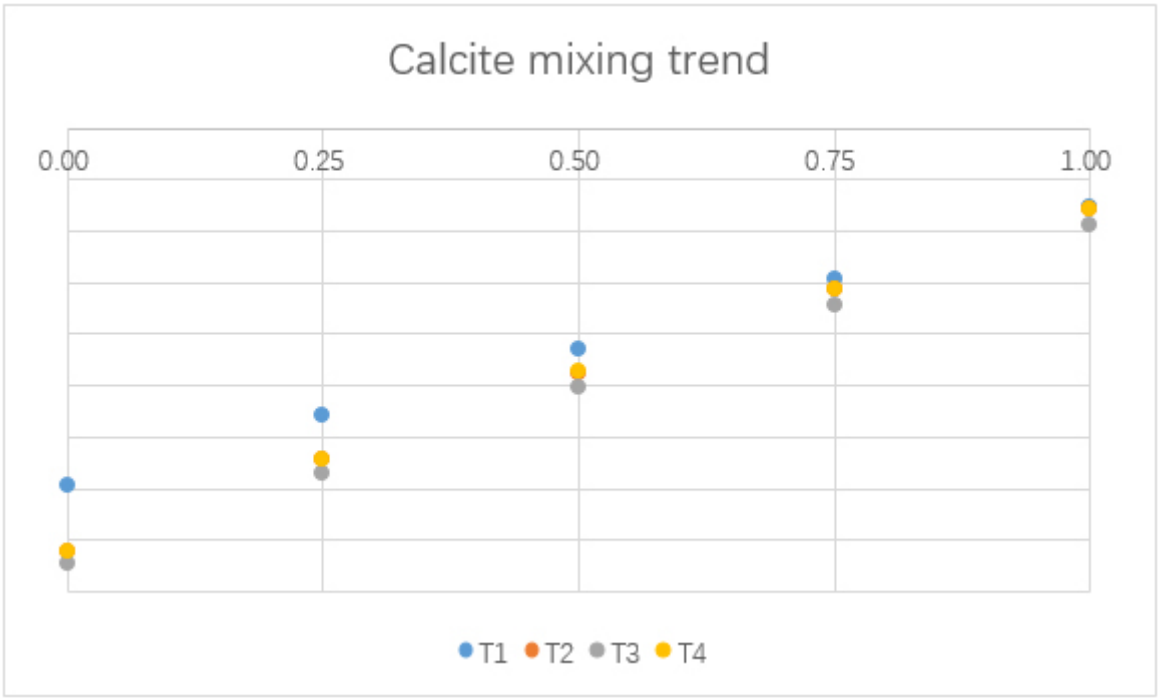
Site	Time	pH	si_Calcite	si_Siderite	si_Goethite	si_Fe(OH)3(a)
Br7	T1	6.8	-0.4679	-0.3159	-1.9537	-7.2758
		7.0	-0.2684	-0.1189	-1.8176	-7.1397
		7.2	-0.0692	0.0763	-1.7034	-7.0254
		7.4	0.1295	0.2689	-1.6127	-6.9348
	T2	6.8	-0.4895	-0.2562	-2.2924	-7.6130
		7.0	-0.2900	-0.0592	-2.1563	-7.4769
		7.2	-0.0908	0.1360	-2.0420	-7.3626
		7.4	0.1079	0.3286	-1.9514	-7.2720
	T4	6.8	-0.4733	-0.2598	-2.1739	-7.4963
		7.0	-0.2739	-0.0628	-2.0379	-7.3603
		7.2	-0.0747	0.1324	-1.9237	-7.2461
		7.4	0.1240	0.3249	-1.8331	-7.1555
Site	**Time**	**pH**	**si_Calcite**	**si_Siderite**	**si_Goethite**	**si_Fe(OH)3(a)**
F1	T1	6.8	-0.4262	-0.5860	-0.4180	-5.7547
		7.0	-0.2268	-0.3892	-0.2827	-5.6194
		7.2	-0.0276	-0.1941	-0.1693	-5.5060
		7.4	0.1711	-0.0019	-0.0796	-5.4163
	T2	6.8	-0.4226	-0.3280	-0.4188	-5.7594
		7.0	-0.2231	-0.1312	-0.2836	-5.6243
		7.2	-0.0240	0.0638	-0.1705	-5.5111
		7.4	0.1746	0.2561	-0.0809	-5.4216
	T3	6.8	-0.4332	-0.3337	-0.4194	-5.7600
		7.0	-0.2338	-0.1368	-0.2843	-5.6249
		7.2	-0.0346	0.0582	-0.1711	-5.5118
		7.4	0.1640	0.2506	-0.0816	-5.4223
	T4	6.8	-0.4269	-0.3323	-0.4190	-5.7596
		7.0	-0.2274	-0.1355	-0.2839	-5.6245
		7.2	-0.0283	0.0596	-0.1707	-5.5113
		7.4	0.1703	0.2519	-0.0812	-5.4218

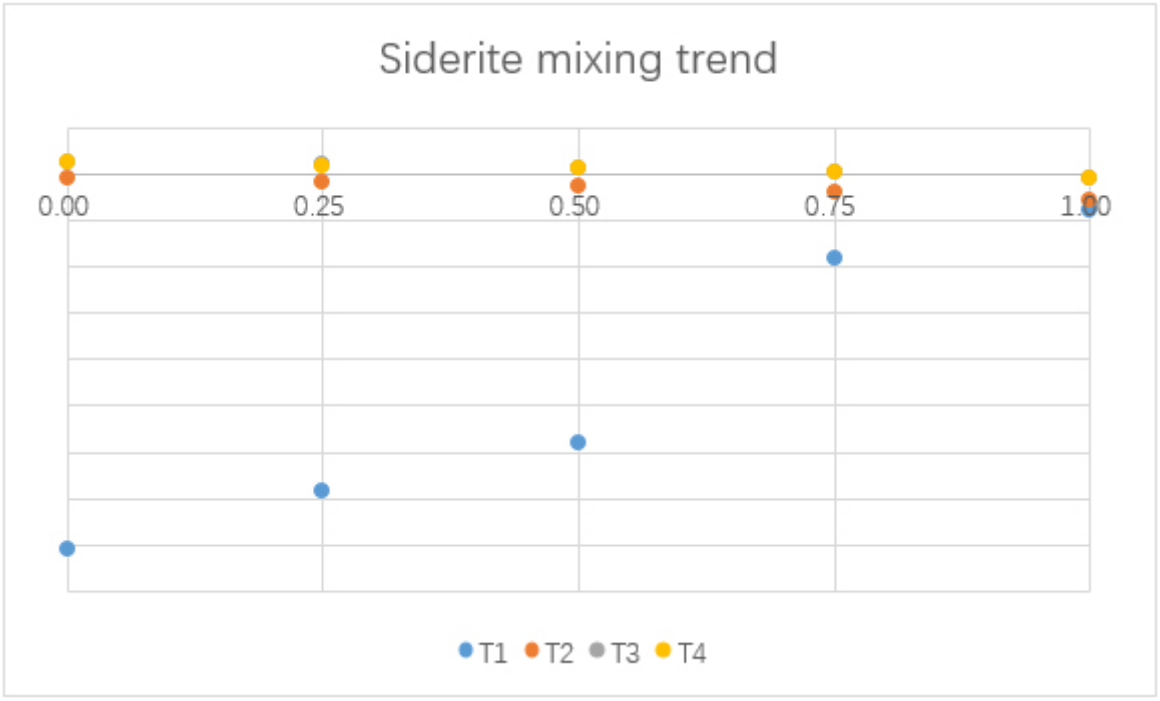
Site	Time	pH	si_Calcite	si_Siderite	si_Goethite	si_Fe(OH)3(a)
F2	T1	6.8	-0.5361	-1.4085	-0.5283	-5.8690
		7.0	-0.3366	-1.2115	-0.3935	-5.7341
		7.2	-0.1374	-1.0161	-0.2806	-5.6213
		7.4	0.0614	-0.8234	-0.1914	-5.5320
	T2	6.8	-0.5553	-0.2146	-0.5270	-5.8637
		7.0	-0.3558	-0.0175	-0.3920	-5.7287
		7.2	-0.1566	0.1779	-0.2789	-5.6156
		7.4	0.0421	0.3707	-0.1895	-5.5262
	T3	6.8	-0.5643	-0.1953	-0.5271	-5.8638
		7.0	-0.3648	0.0018	-0.3921	-5.7288
		7.2	-0.1656	0.1972	-0.2790	-5.6157
		7.4	0.0331	0.3900	-0.1896	-5.5263
	T4	6.8	-0.5595	-0.2007	-0.5271	-5.8637
		7.0	-0.3600	-0.0036	-0.3920	-5.7287
		7.2	-0.1608	0.1918	-0.2790	-5.6157
		7.4	0.0379	0.3846	-0.1896	-5.5262

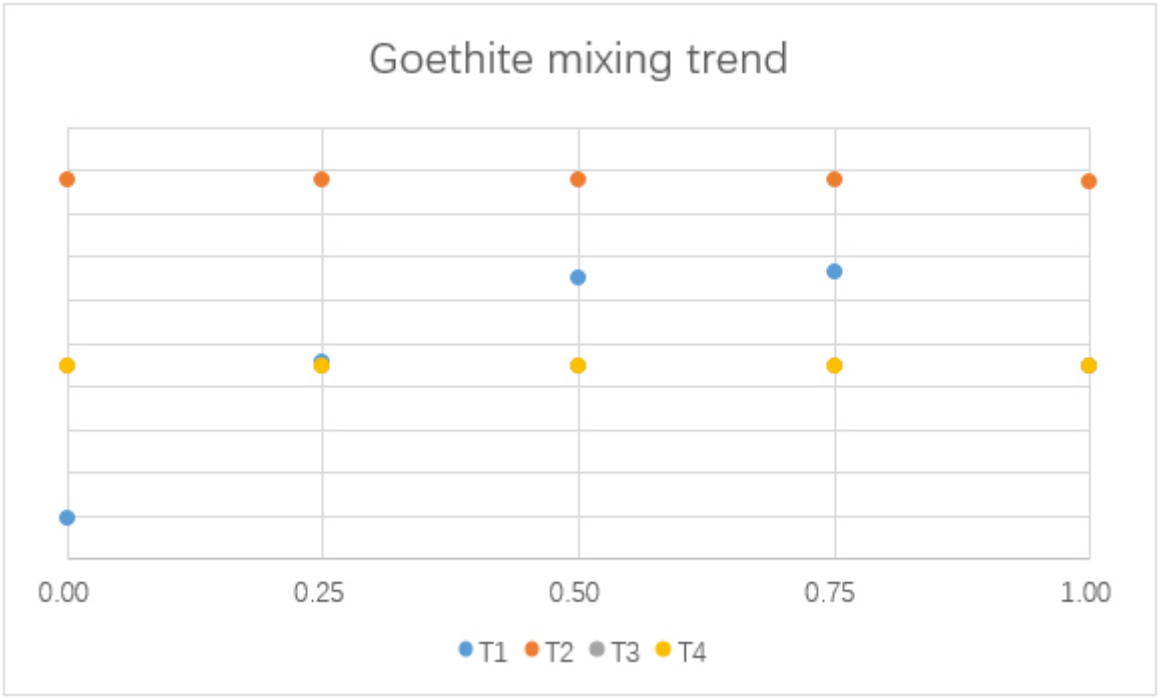
Mixing

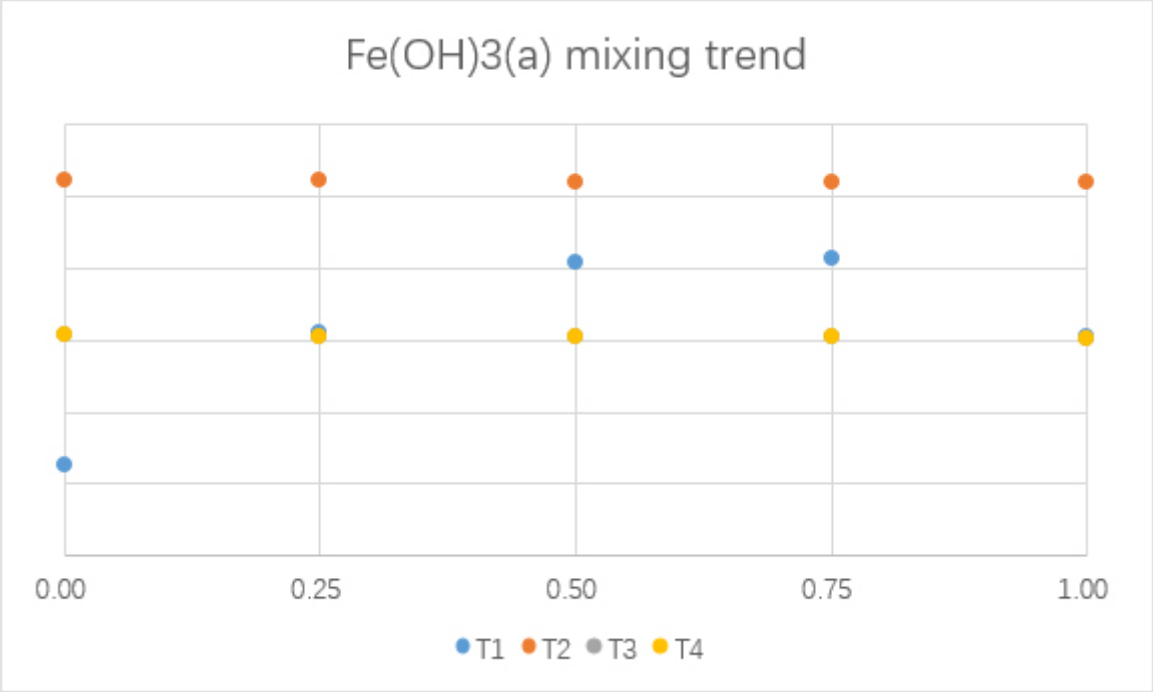
To understand the consequence of the mixing of water from F1 and F2, different simulations with different mixing ratios are made.

(For each graph, the x-axis is ratio of F1 to total mixing water.)




Siderite mixing trend
0.00
0.25
0.50
0.75
1.00
T1
T2
T3
T4


Goethite mixing trend
0.00
0.25
0.50
0.75
1.00
T1
T2
T3
T4



Modeling with aqion

Another computer modeling software called 'aqion' is also used. The results are as follows.

Br7		**T1**	**T2**	**T4**
pe		8.08	2.07	2.09
Eh	mV	454	116	117
Fe	mg/L	0.000273	0.5	0.48
Fe(2)	mg/L	5.31E-07	0.5	0.48
Fe(3)	mg/L	0.000273	0.000268	0.000269
NH4	mg/L	-	0.12	0.14
NO2	mg/L	0.404	0.26	0.26
NO3	mg/L	0.916	5.85E-13	6.42E-13
Fe(OH)3(a)	mg/L	3.67	1.57	1.3
Siderite	mg/L	0	0	0
CO2	mmol/L	0.77	0.76	0.77
HCO3-	mmol/L	4.59	4.53	4.6

F1		**T1**	**T2**	**T3**	**T4**
pe		2.03	1.84	1.83	1.83
Eh	mV	114	103	103	103
Fe	mg/L	0.5	0.777	0.787	0.784
Fe(2)	mg/L	0.5	0.777	0.786	0.784
Fe(3)	mg/L	0.000278	0.000282	0.000282	0.000282
NH4	mg/L	-	-	-	-
NO2	mg/L	-	-	-	-
NO3	mg/L	-	-	-	-
Fe(OH)3(a)	mg/L	0.172	0.172	0.0951	0.0377
Siderite	mg/L	0	0.256	0.236	0.241
CO2	mmol/L	0.8	0.8	0.79	0.79

F1		**T1**	**T2**	**T3**	**T4**
HCO3-	mmol/L	4.82	4.84	4.75	4.77

F2		**T1**	**T2**	**T3**	**T4**
pe		8.35	1.79	1.79	1.79
Eh	mV	470	101	100	100
Fe	mg/L	0.000284	0.868	0.863	0.858
Fe(2)	mg/L	2.40E-07	0.868	0.863	0.858
Fe(3)	mg/L	0.000284	0.00028	0.000279	0.000279
NH4	mg/L	-	-	0.15	0.15
NO2	mg/L	0.033	-	-	-
NO3	mg/L	0.316	-	-	-
Fe(OH)3(a)	mg/L	2.85	1.28	0.344	0.0951
Siderite	mg/L	0	0.856	0.99	0.958
CO2	mmol/L	0.71	0.7	0.7	0.7
HCO3-	mmol/L	4.27	4.16	4.15	4.17

Data

The original data and softwares are contained in the folder and extra page materials.