

Supporting information

Table S1: PhreeqC input data

Input*	E1a	E1b	E2	E3	E3.1	E4	E4.1	E5	E5.1	E6	E6.1
pH	6.1	6.5	6.5	6.7	6.5	7.1	7.5	7.9	7.6	7.9	7.9
pe	4.6	4.3	4.2	4.1	3.6	3.3	2.9	2.8	2.7	2.8	3.3
density	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
temp	19.5	19.3	19.3	17.5	17.5	16.2	16.1	15.2	15.3	14.1	13.3
Na	2500	2500	2500	2500	2500	2500	2500	2400	2500	2500	2500
Mg	166	163	165	165	165	164	164	164	166	166	165
Si	4.9	4.8	4.8	4.7	4.7	4.8	4.7	4.7	4.6	4.6	4.6
K	200	200	200	200	200	200	200	200	200	200	200
Ca	1200	1200	1200	1200	1200	1200	1200	1200	1200	1200	1200
Li	3.2	3.2	3.2	3.3	3.3	3.2	3.1	3.1	3.2	3.1	3.2
B	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.8	0.9
Cl	4400	4500	4500	4500	4500	4500	4500	4500	4500	4500	4500
S(6)	2100	2200	2200	2200	2200	2200	2200	2200	2200	2200	2200
Fe(II)	6.6	6.6	5.6	5.7	4.5	3.9	3.4	0.9	0.4	0.2	0.0
Alkal.**	820	828	796	790	810	804	808	804	816	760	770

\* units ppm

\*\* Alkalinity as CaCO<sub>3</sub>

Table S2: PhreeqC output data

Phase	SI*	Log IAP**	Log K (202 K,1 atm)
<b>E1a</b>			
Ferrihydrite	0.13	5.02	4.89
Goethite	5.83	5.03	-0.80
Hematite	13.64	10.05	-3.58
<b>E1b</b>			
Ferrihydrite	1.06	5.95	4.89
Goethite	6.74	5.95	-0.79
Hematite	15.47	11.90	-3.57
Siderite	0.34	-10.51	-10.85
<b>E2</b>			
Ferrihydrite	1.01	5.90	4.89
Goethite	6.70	5.90	-0.79
Hematite	15.38	11.81	-3.57
Siderite	0.30	-10.56	-10.85
<b>E3</b>			
Ferrihydrite	1.45	6.34	4.89
Goethite	7.07	6.35	-0.73
Hematite	16.12	12.69	-3.42

Siderite	0.47	-10.37	-10.84
<b>Phase</b>	<b>SI*</b>	<b>Log IAP**</b>	<b>Log K (202 K,1 atm)</b>
<b>E3.1</b>			
Ferrihydrite	0.33	5.22	4.89
Goethite	5.95	5.23	-0.73
Hematite	13.88	10.45	-3.42
Siderite	0.19	-10.65	-10.84
<b>Phase</b>	<b>SI*</b>	<b>Log IAP**</b>	<b>Log K (202 K,1 atm)</b>
<b>E4</b>			
Ferrihydrite	1.70	6.60	4.89
Goethite	7.28	6.60	-0.68
Hematite	16.52	13.20	-3.32
Siderite	0.68	-10.15	-10.83
<b>Phase</b>	<b>SI*</b>	<b>Log IAP**</b>	<b>Log K (202 K,1 atm)</b>
<b>E4.1</b>			
Ferrihydrite	2.20	7.09	4.89
Goethite	7.77	7.09	-0.67
Hematite	17.50	14.19	-3.31
Siderite	0.97	-9.86	-10.83
<b>Phase</b>	<b>SI*</b>	<b>Log IAP**</b>	<b>Log K (202 K,1 atm)</b>
<b>E5</b>			
Ferrihydrite	2.81	7.70	4.89
Goethite	8.34	7.70	-0.64
Hematite	18.64	15.40	-3.24
Siderite	0.68	-10.14	-10.83
<b>Phase</b>	<b>SI*</b>	<b>Log IAP**</b>	<b>Log K (202 K,1 atm)</b>
<b>E5.1</b>			
Ferrihydrite	1.47	6.36	4.89
Goethite	7.01	6.36	-0.64
Hematite	15.98	12.73	-3.25
Siderite	0.16	-10.67	-10.83
<b>Phase</b>	<b>SI*</b>	<b>Log IAP**</b>	<b>Log K (202 K,1 atm)</b>
<b>E6</b>			
Ferrihydrite	2.02	6.91	4.89
Goethite	7.51	6.91	-0.60
Hematite	16.98	13.83	-3.15
Siderite	0.06	-10.76	-10.82
<b>Phase</b>	<b>SI*</b>	<b>Log IAP**</b>	<b>Log K (202 K,1 atm)</b>
<b>E6.1***</b>			
Ferrihydrite	1.35	6.24	4.89
Goethite	6.81	6.24	-0.57
Hematite	15.57	12.48	-3.08

\* Saturation index =  $\log_{10}(\text{fugacity})$

\*\* Ion activity product

\*\*\* Last sampling point with Fe(II)