Supplementary Materials 3- Tables with saturation index (SI) of water simulation

Table S45: SI>0 in the GRN Simulation. The numbers of simulations are referred to the sampling period and pe to the redox potential

GRN												
Simulation	**pH**	**pe**	**Al_2O_3**	**Boehmite**	**Diaspore**	**Ferrihydrite**	**Gibbsite**	**Goethite**	**Hematite**	**Kaolinite**	**Magnetite**	**Lepidocrocite**
12	6.4	0.88	-	0.90	2.60	-	1.19	0.62	3.64	2.91	5.68	-
13	7.08	0.39	-	0.65	2.35	-	0.93	2.16	6.72	2.41	10.12	1.28
14	7.01	3.79	-	0.79	2.49	2.36	1.07	5.06	12.53	2.69	15.49	4.18
15	6.63	4.62	-	1.03	2.74	1.80	1.32	4.50	11.41	3.18	13.35	3.62
16	7.14	1.66	-	0.31	2.01	-	0.59	2.13	6.66	1.73	8.69	1.25
17	6.6	3.33	0.25	1.37	3.08	1.37	1.66	4.07	10.54	3.86	13.38	3.19
18	6.43	3.25	-	1.16	2.86	0.24	1.45	2.94	8.29	3.44	10.25	2.06
19	6.22	3.83	-	0.44	2.14	0.19	0.72	2.89	8.19	1.99	9.73	2.01

Table S46: SI>0 in SR10A Simulation. The numbers of simulations are referred to the sampling period and pe to the redox potential.

SR10A											
Simulation	**pH**	**pe**	**Al_2O_3**	**Boehmite**	**Diaspore**	**Gibbsite**	**Goethite**	**Kaolinite**	**Magnetite**	**Lepidocrocite**	**Hematite**
14	7.7	0.45	-	0.21	1.92	0.50	2.50	1.54	10.45	1.62	7.40
15	5.96	4.20	2.35	1.23	2.93	1.51	1.76	3.57	6.22	0.88	5.92
16	6.09	4.93	0.57	0.87	2.58	1.16	2.58	2.86	7.82	1.70	7.56
17	6.28	2.00	-	0.90	2.60	1.18	-	2.91	2.41	-	2.13
18	5.90	3.83	-	0.16	1.87	0.45	0.62	1.45	3.22	-	3.63
19	6.29	3.33	0.27	1.15	2.85	1.44	1.49	3.42	5.93	0.61	5.37
20	6.09	4.06	0.39	0.92	2.62	1.21	1.14	2.96	4.35	0.26	4.67

Table S47: SI>0 in S113 simulation. The numbers of simulations are referred to the sampling period and pe to the redox potential.

S113													
Simulation	**pH**	**pe**	**Alunite**	**Ferrihydrite**	**Gibbsite**	**Goethite**	**Hematite**	**Diaspore**	**Boehmite**	**Magnetite**	**Lepidocrocite**	**Kaolinite**	**Al_2O_3**
19	6.2	0.49	-	-	0.86	-	-	2.28	0.57	-	-	2.27	-
20	5.53	4.30	0.31	-	0.25	0.55	3.49	1.66	-	2.91	-	1.04	-
21	6.88	5.64	0.15	1.16	1.58	3.86	10.12	3.00	1.30	10.17	2.98	3.71	0.10
22	7.3	5.62	-	1.61	1.16	4.31	11.03	2.58	0.88	11.11	3.43	2.87	-
23	7.48	5.64	-	1.73	0.89	4.43	11.26	2.30	0.60	11.27	3.55	2.31	-
24	6.84	5.76	0.21	0.70	1.56	3.40	9.21	2.98	1.27	8.71	2.52	3.66	0.05
25	7.06	5.76	-	1.16	1.38	3.86	10.13	2.80	1.09	9.87	2.98	3.30	-

Table S18: SI>0 in SR8 simulation. The numbers of simulations are referred to the sampling period and pe to the redox potential.

SR8														
Simulation	**pH**	**pe**	**Calcite**	**Dolomite**	**Boehmite**	**Diaspore**	**Ferrihydrite**	**Gibbsite**	**Goethite**	**Magnetite**	**Lepidocrocite**	**Kaolinite**	**Hematite**	**Al_2O_3**
5	8.36	1.66	0.91	0.56	-	-	-	-	-	-	-	-	-	-
8	7.71	1.06	0.34	-	-	-	-	-	-	-	-	-	-	-
10	8.43	1.66	0.54	-	-	-	-	-	-	-	-	-	-	-
11	7.32	0.17	0.08	-	-	-	-	-	-	-	-	-	-	-
14	7.83	0.45	0.48	-	0.25	1.96	1.62	0.54	4.32	15.77	3.44	1.62	11.04	-
15	7.57	4.45	0.06	-	0.87	2.57	2.20	1.16	4.90	13.77	4.02	2.85	12.19	-
16	7.06	2.54	-	-	0.76	2.46	0.71	1.05	3.41	11.72	2.53	2.63	9.21	-
17	6.76	1.66	-	-	1.33	3.03	-	1.62	2.17	9.19	1.29	3.77	6.74	0.16
18	7.2	2.74	-	-	1.14	2.84	2.19	1.42	4.89	15.82	4.01	3.39	12.18	-
19	7.02	3.18	-	-	1.09	2.79	0.50	1.37	3.20	10.48	2.32	3.29	8.79	-
20	6.63	3.64	-	-	1.20	2.90	0.30	1.49	3.00	9.83	2.12	3.52	8.40	-

Table S49: SI>0 in S2EST simulation. The numbers of simulations are referred to the sampling period and pe to the redox potential.

S2EST Simulation	pH	pe	Calcite	Dolomite	Al_2O_3	Alunite	Boehmite	Diaspore	Gibbsite	Goethite	Hematite	Kaolinite	Magnetite
10	9.97	2	0.78	0.45	-	-	-	-	-	-	-	-	-
18	5.36	0.5	-	-	-	3.19	0.47	2.17	0.75	-	-	2.05	-
19	4.9	6.3	-	-	-	2.91	-	1.62	0.20	0.30	3.00	0.95	0.78
20	4.9	5.3	-	-	-	0.16	-	0.87	-	-	1.86	-	0.03
21	5.57	2	-	-	0.66	5.93	1.58	3.28	1.87	-	-	4.28	-
22	5.46	4.4	-	-	-	4.31	1.02	2.72	1.31	0.22	2.84	3.16	1.90
23	5.49	5.5	-	-	-	4.10	0.93	2.63	1.22	1.39	5.19	2.98	4.27

Table S50: SI>0 in S1N simulation The numbers of simulations are referred to the sampling period and pe to the redox potential.

S1N																			
Simulation	**pH**	**pe**	**Calcite**	**Dolomite**	**Al_2O_3**	**Alunite**	**Boehmite**	**Diaspore**	**Ferrihydrite**	**Gibbsite**	**Goethite**	**Hematite**	**Kaolinite**	**Magnetite**	**Lepidocrocite**	**SbO_2**	**Romeite**	**Schafarzikite**	**Tripuhyite**
1	7.4	2.5	-	-	-	-	-	-	-	-	-	-	-	-	-	0.01	-	-	-
3	7.2	1.7	-	-	-	-	-	-	-	-	-	-	-	-	-	1.45	-	-	-
4	10.9	1.2	1.24	0.96	-	-	-	-	-	-	-	-	-	-	-	-	1.44	-	-
5	7.9	1.7	-	-	-	-	-	-	-	-	-	-	-	-	-	0.29	-	-	-
6	7.2	1.7	-	-	-	-	-	-	-	-	-	-	-	-	-	1.28	-	-	-
7	7.0	1.7	-	-	-	-	-	-	-	-	-	-	-	-	-	1.78	-	-	-
8	7.7	2.1	-	-	-	-	-	-	-	-	-	-	-	-	-	0.16	-	-	-
9	8.7	1.6	0.71	0.13	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
11	7.0	1.7	-	-	-	-	-	-	-	-	-	-	-	-	-	1.25	-	-	-
13	7.3	1.7	-	-	-	-	-	-	-	-	-	-	-	-	-	0.66	-	-	-
14	9.4	1.0	1.30	0.97	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
15	6.6	1.5	-	-	-	-	-	-	-	-	-	-	-	-	-	2.12	-	-	-
16	8.2	0.0	0.36	-	-	-	-	-	-	-	-	-	-	-	-	1.02	-	-	-
17	11.3	-3.8	0.63	0.71	-	-	-	-	-	-	-	-	-	-	-	-	1.69	-	-
18	10.9	-3.5	0.94	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
19	9.3	0.5	0.81	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
20	7.0	0.5	-	-	-	-	0.36	2.07	-	0.65	0.74	3.87	1.84	5.87		1.62	-	0.36	
21	7.8	4.8	-	-	0.04	-	1.27	2.97	2.08	1.56	4.78	11.95	3.65	12.83	3.90	-	-	-	0.79
22	7.5	4.6	-	-	0.21	-	1.36	3.06	1.76	1.64	4.46	11.31	3.83	12.30	3.58	-	-	-	1.01
23	9.7	0.0	1.22	0.85	-	-	0.59	2.29	1.88	0.87	4.58	11.56	1.83	15.19	3.70	-	-	-	
24	6.8	4.4	-	-	1.57	0.40	2.03	3.74	2.24	2.32	4.94	12.28	5.19	14.66	4.06	-	-	-	0.90
25	10.6	1.9	1.36	1.17	-	-	-	1.18	1.01		3.71	9.82		9.71	2.83	-	0.71	-	-
26	6.9	3.9	-	-	0.09	0.16	1.29	3.00	0.65	1.58	3.35	9.09	3.70	10.40	2.47	0.28	-	-	0.53

Table S51: SI>0 in S6N simulation The numbers of simulations are referred to the sampling period and pe to the redox potential.

S6N Simulation	pH	pe	Calcite	Al_2O_3	Alunite	Boehmite	Diaspore	Ferrihydrite	Gibbsite	Goethite	Hematite	Kaolinite	Lepidocrocite	Magnetite	SbO_2	Schafarzikite	Tripuhyite
1	7.7	2.0	0.26	-	-	-	-	-	-	-	-	-	-	-	0.52	-	-
2	7.3	2.0	-	-	-	-	-	-	-	-	-	-	-	-	1.61	-	-
3	7.4	2.0	-	-	-	-	-	-	-	-	-	-	-	-	1.33	-	-
4	8.5	2.5	0.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-
5	7.1	3.2	-	-	-	-	-	-	-	-	-	-	-	-	0.98	-	-
6	7.8	2.0	0.36	-	-	-	-	-	-	-	-	-	-	-	0.65	-	-
7	6.5	2.0	-	-	-	-	-	-	-	-	-	-	-	-	3.08	-	-
8	7.4	2.0	-	-	-	-	-	-	-	-	-	-	-	-	1.02	-	-
9	7.8	2.3	0.56	-	-	-	-	-	-	-	-	-	-	-	0.38	-	-
10	8.6	2.8	0.96	-	-	-	-	-	-	-	-	-	-	-	-	-	-
11	8.2	2.0	0.86	-	-	-	-	-	-	-	-	-	-	-	-	-	-
12	7.3	-0.3	-	-	-	-	-	-	-	-	-	-	-	-	3.45	-	-
13	8.7	-1.5	0.93	-	-	-	-	-	-	-	-	-	-	-	2.05	-	-
14	7.8	0.7	0.30	-	-	-	-	-	-	-	-	-	-	-	1.75	-	-
15	7.0	0.5	-	-	-	0.68	2.38	-	0.96	2.48	7.36	2.48	1.60	11.05	3.04	4.77	-
16	7.3	5.0	-	-	-	0.66	2.37	1.37	0.95	4.07	10.54	2.45	3.19	11.05	-	-	1.00
17	6.8	4.3	-	-	0.33	0.87	2.57	1.65	1.16	4.35	11.10	2.86	3.47	12.97	-	-	1.50
18	7.4	2.0	0.21	-	-	0.30	2.00	1.41	0.59	4.11	10.61	1.71	3.23	13.99	1.07	-	0.77
19	6.9	4.6	-	0.20	-	1.35	3.05	1.44	1.63	4.14	10.68	3.81	3.26	12.04	-	-	1.42
20	7.7	2.7	0.24	-	-	0.34	2.05	1.63	0.63	4.34	11.07	1.80	3.46	13.70	-	-	0.89
21	6.7	3.8	-	-	1.09	1.01	2.72	1.28	1.30	3.98	10.37	3.15	3.10	12.54	0.64	-	1.31

Table S52: SI>0 in S118 simulation. The numbers of simulations are referred to the sampling period and pe to the redox potential.

S118																
Simulation	**pH**	**pe**	**Alunite**	**Al_2O_3**	**Boehmite**	**Diaspore**	**Ferrihydrite**	**Gibbsite**	**Goethite**	**Hematite**	**Magnetite**	**Kaolinite**	**Lepidocrocite**	**SbO_2**	**Schafarzikite**	**Tripuhyite**
1	6.7	1.7	-	-	-	-	-	-	-	-	-	-	-	1.24	-	-
2	6.5	1.7	-	-	-	-	-	-	-	-	-	-	-	1.07	-	-
3	6.2	1.7	-	-	-	-	-	-	-	-	-	-	-	1.85	-	-
4	6.5	2.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-
5	6.0	1.7	-	-	-	-	-	-	-	-	-	-	-	0.62	-	-
6	6.4	1.7	-	-	-	-	-	-	-	-	-	-	-	2.43	-	-
7	6.9	1.7	-	-	-	-	-	-	-	-	-	-	-	0.58	-	-
8	6.7	1.9	-	-	-	-	-	-	-	-	-	-	-	1.31	-	-
9	5.9	2.5	-	-	-	-	-	-	-	-	-	-	-	2.14	-	-
10	7.9	1.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-
11	7.3	0.9	-	-	-	-	-	-	-	-	-	-	-	1.61	-	-
12	6.0	1.0	-	-	-	-	-	-	-	-	-	-	-	2.04	-	-
13	5.7	0.6	-	-	-	-	-	-	-	-	-	-	-	1.20	-	-
14	7.2	0.5	-	-	0.21	1.92	-	0.50	2.03	6.46	9.45	1.54	1.15	1.38	0.27	-
15	6.1	4.9	1.36	-	0.64	2.34	-	0.92	2.28	6.97	7.00	2.39	1.40	0.31	-	-
16	6.4	3.9	2.16	-	1.24	2.95	0.01	1.53	2.71	7.82	8.92	3.60	1.83	0.79	-	-
17	7.6	1.7	-	-	0.45	2.16	1.21	0.74	3.91	10.21	13.60	2.02	3.03	1.18	-	0.47
18	6.7	3.4	1.41	-	1.15	2.85	0.84	1.44	3.54	9.49	11.63	3.42	2.66	0.86	-	0.68
19	6.6	4.9	1.62	1.15	1.82	3.53	1.73	2.11	4.43	11.25	12.89	4.77	3.55	-	-	1.94
20	6.1	4.6	1.72	-	0.94	2.65	-	1.23	2.27	6.93	7.18	3.00	1.39	1.01	-	0.16