

Supplementary Materials

Table S1. The calculations of water-rock interaction.

Line group	O(quality)	O(atoms)	D(quality)	D(atoms)	W(O)	W(D)	O	D	R(O)	R(D)
Line 1	5	10	5	500	7.7	-47	7.3372727	-46.95006	8.2	-88.5
	1	2	1	100	7.7	-47	6.37	-46.75228	8.2	-88.5
	0.1	0.2	0.1	10	7.7	-47	4.375	-44.72545	8.2	-88.5
	0.05	0.1	0.05	5	7.7	-47	4.0727273	-42.83	8.2	-88.5
	0.01	0.02	0.01	1	7.7	-47	3.7882353	-34.49	8.2	-88.5
	0.001	0.002	0.001	0.1	7.7	-47	3.7179641	-24.25455	8.2	-88.5
Line 2	5	10	5	500	9.9	-62	9.2281818	-61.88719	7	-72
	1	2	1	100	9.9	-62	7.4366667	-61.4404	7	-72
	0.1	0.2	0.1	10	9.9	-62	3.7416667	-56.86182	7	-72
	0.05	0.1	0.05	5	9.9	-62	3.1818182	-52.58	7	-72
	0.01	0.02	0.01	1	9.9	-62	2.654902	-33.74	7	-72
	0.001	0.002	0.001	0.1	9.9	-62	2.5247505	-10.61818	7	-72
Line 3	5	10	5	500	-15.6	-115	-13.84455	-114.8143	8.2	-88.5
	1	2	1	100	-15.6	-115	-9.163333	-114.079	8.2	-88.5
	0.1	0.2	0.1	10	-15.6	-115	0.4916667	-106.5436	8.2	-88.5
	0.05	0.1	0.05	5	-15.6	-115	1.9545455	-99.49667	8.2	-88.5
	0.01	0.02	0.01	1	-15.6	-115	3.3313725	-68.49	8.2	-88.5
	0.001	0.002	0.001	0.1	-15.6	-115	3.6714571	-30.43636	8.2	-88.5
Line 4	5	10	5	500	-15.6	-115	-13.95364	-114.7814	7	-72
	1	2	1	100	-15.6	-115	-9.563333	-113.9156	7	-72
	0.1	0.2	0.1	10	-15.6	-115	-0.508333	-105.0436	7	-72
	0.05	0.1	0.05	5	-15.6	-115	0.8636364	-96.74667	7	-72

	0.01	0.02	0.01	1	-15.6	-115	2.154902	-60.24	7	-72
	0.001	0.002	0.001	0.1	-15.6	-115	2.4738523	-15.43636	7	-72
Line 5	5	10	5	500	7.7	-47	7.1227273	-46.91259	8.2	-88.5
	1	2	1	100	7.7	-47	5.5833333	-46.56644	8.2	-88.5
	0.1	0.2	0.1	10	7.7	-47	2.4083333	-43.01909	8.2	-88.5
	0.05	0.1	0.05	5	7.7	-47	1.9272727	-39.70167	8.2	-88.5
	0.01	0.02	0.01	1	7.7	-47	1.4745098	-25.105	8.2	-88.5
	0.001	0.002	0.001	0.1	7.7	-47	1.3626747	-7.190909	8.2	-88.5
Line 6	5	10	5	500	9.9	-62	9.0136364	-61.84972	7	-72
	1	2	1	100	9.9	-62	6.65	-61.25455	7	-72
	0.1	0.2	0.1	10	9.9	-62	1.775	-55.15545	7	-72
	0.05	0.1	0.05	5	9.9	-62	1.0363636	-49.45167	7	-72
	0.01	0.02	0.01	1	9.9	-62	0.3411765	-24.355	7	-72
	0.001	0.002	0.001	0.1	9.9	-62	0.1694611	6.4454545	7	-72
	10	20	10	1000	1.4	-79.66667	1.3404762	-79.5738	7	-72
Line 7	5	10	5	500	7.0666667	-67.88889	6.4378788	-67.72686	7	-72
	1	2	1	100	7.0666667	-67.88889	4.7611111	-67.08514	7	-72
	0.1	0.2	0.1	10	7.0666667	-67.88889	1.3027778	-60.50899	7	-72
	0.05	0.1	0.05	5	7.0666667	-67.88889	0.7787879	-54.35907	7	-72
	0.01	0.02	0.01	1	7.0666667	-67.88889	0.2856209	-27.29944	7	-72
	0.001	0.002	0.001	0.1	7.0666667	-67.88889	0.1638057	5.910101	7	-72
Line 8	5	10	5	500	4.8	-72.6	4.3772727	-72.42856	7	-72
	1	2	1	100	4.8	-72.6	3.25	-71.7496	7	-72
	0.1	0.2	0.1	10	4.8	-72.6	0.925	-64.79182	7	-72
	0.05	0.1	0.05	5	4.8	-72.6	0.5727273	-58.285	7	-72
	0.01	0.02	0.01	1	4.8	-72.6	0.2411765	-29.655	7	-72

	0.001	0.002	0.001	0.1	4.8	-72.6	0.1592814	5.4818182	7	-72
	10	20	10	1000	7.0666667	-67.88889	6.7373016	-67.80779	7	-72
	5	10	5	500	1.4	-79.66667	1.2863636	-79.48112	7	-72
	1	2	1	100	1.4	-79.66667	0.9833333	-78.7463	7	-72
	0.1	0.2	0.1	10	1.4	-79.66667	0.3583333	-71.21606	7	-72
Line 9	0.05	0.1	0.05	5	1.4	-79.66667	0.2636364	-64.17389	7	-72
	0.01	0.02	0.01	1	1.4	-79.66667	0.1745098	-33.18833	7	-72
	0.001	0.002	0.001	0.1	1.4	-79.66667	0.152495	4.8393939	7	-72
	10	20	10	1000	4.8	-72.6	4.5785714	-72.5142	7	-72
	5	10	5	500	-15.6	-115	-14.16818	-114.7439	7	-72
	1	2	1	100	-15.6	-115	-10.35	-113.7298	7	-72
	0.1	0.2	0.1	10	-15.6	-115	-2.475	-103.3373	7	-72
Line 10	0.05	0.1	0.05	5	-15.6	-115	-1.281818	-93.61833	7	-72
	0.01	0.02	0.01	1	-15.6	-115	-0.158824	-50.855	7	-72
	0.001	0.002	0.001	0.1	-15.6	-115	0.1185629	1.6272727	7	-72

Note: O(quality) and O(atoms) respectively mean the quality and atom numbers of oxygen. D(quality) and D(atoms) respectively mean the quality and atom numbers of hydrogen. W(O) and W(D) respectively mean the numbers of oxygen and hydrogen in fluid. R(O) and R(D) respectively mean the numbers of oxygen and hydrogen in rocks. O and D respectively mean the final values of oxygen and hydrogen after water-rock exchange.