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Electronic Supplementary Information

for

Kinetics of iron mineral transformation under the impact of humic acid and Pb(II): Nano-scale mechanisms and implications for C and Pb(II) dynamics

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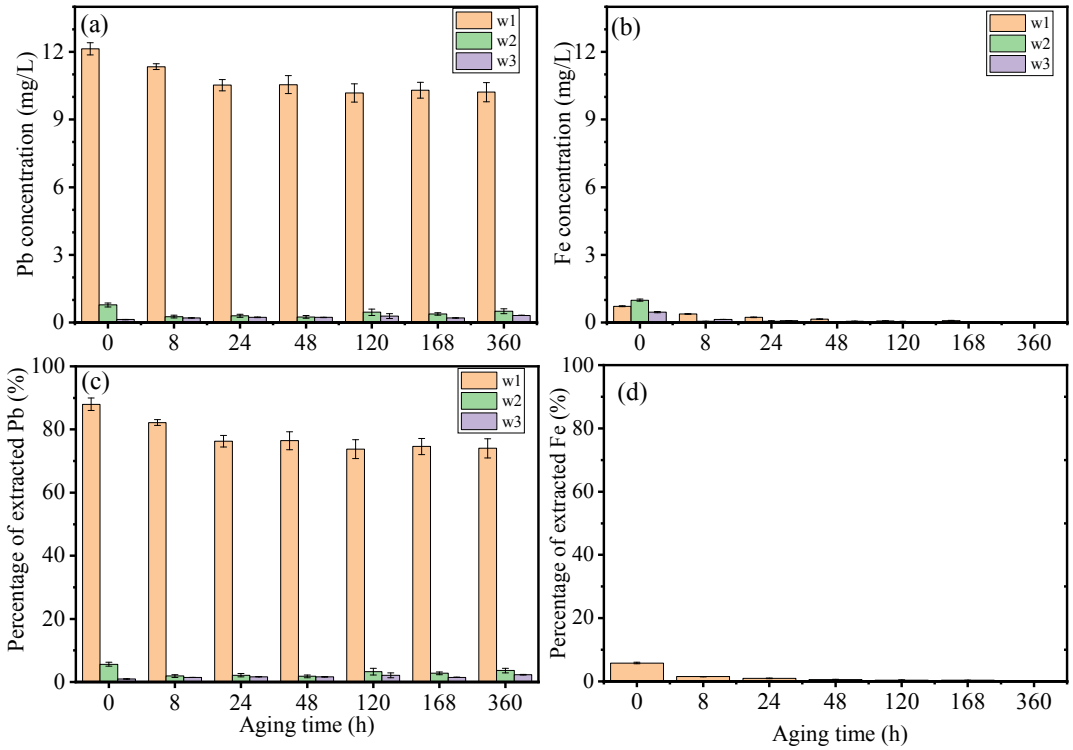

Figure S1. Concentrations of batch pH 3.0 extraction experiments at various aging time. (a) - (b), Fe, Pb concentrations of 3 - times wash at pH 3.0; (c) - (d), calculated w/w % results of 3 - times wash at pH 3.0.

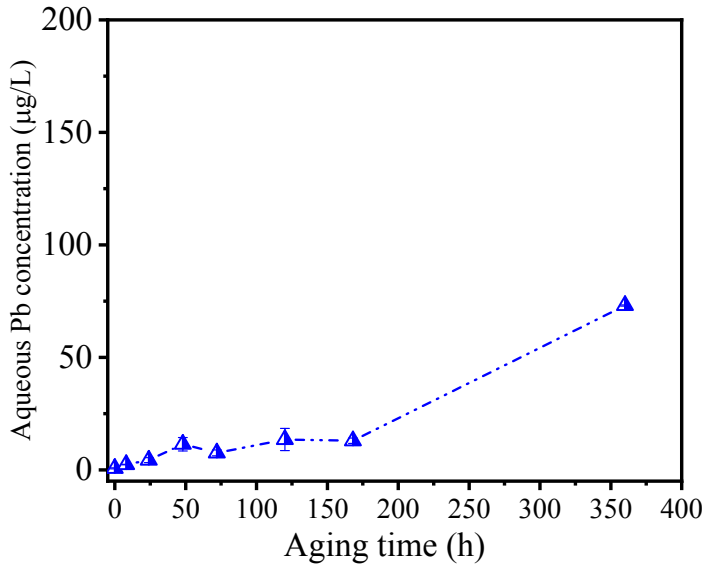

Figure S2. Concentration of aqueous Pb during the incubation experiments.

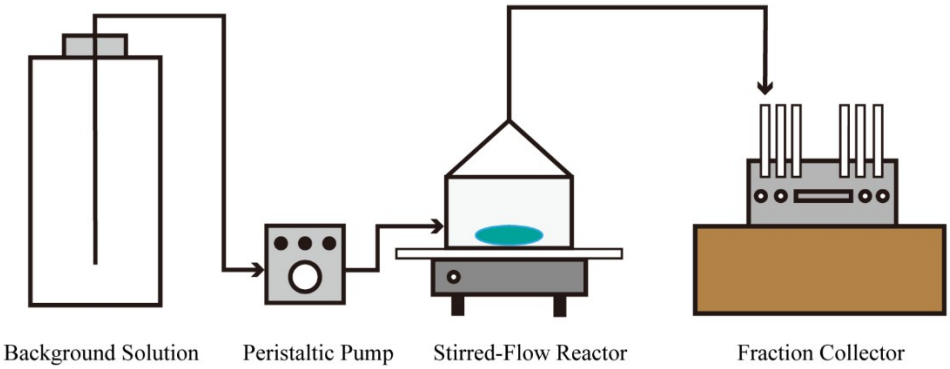

Figure S3. Experimental set up of stirred-flow experiments in this study.

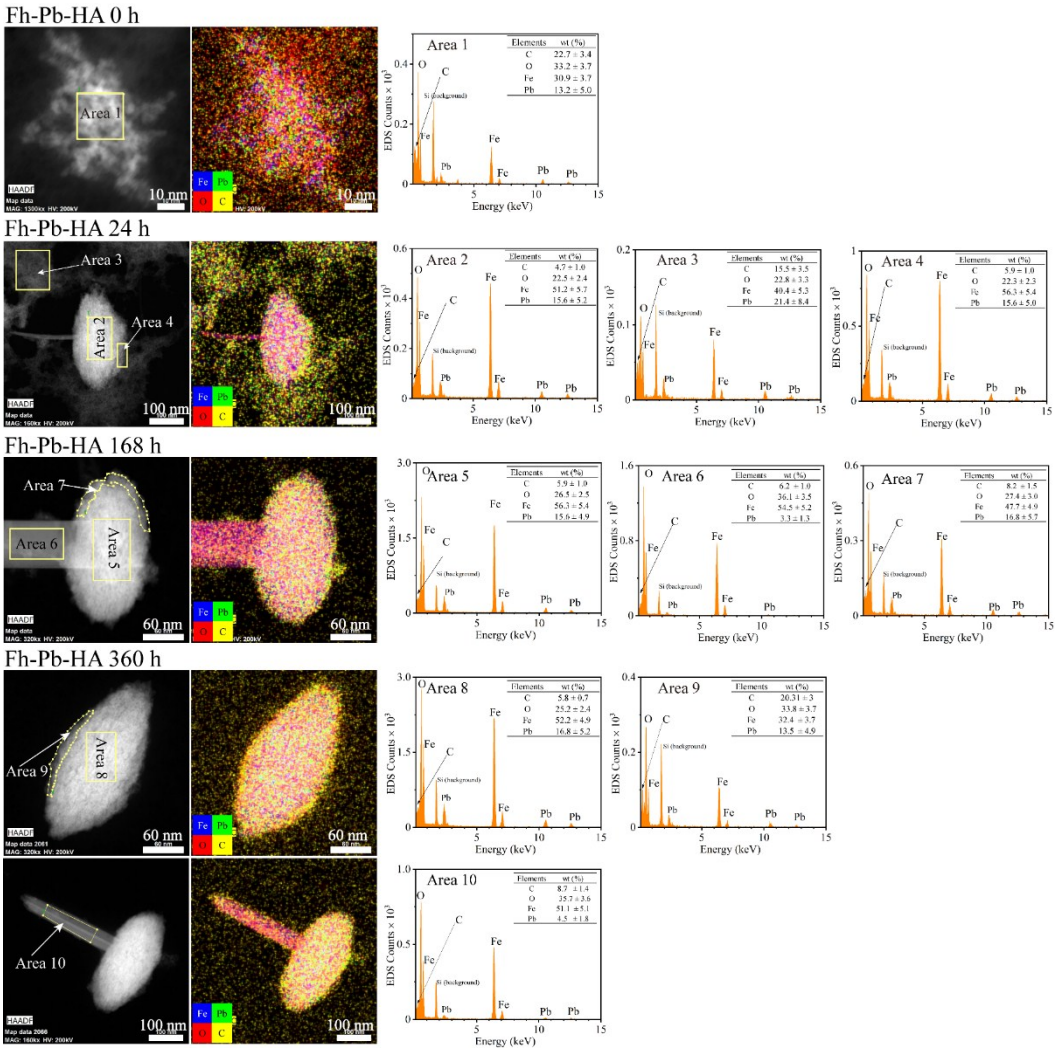

Figure S4. Time resolved EDS mapping, spectra, and quantitative results of iron oxides at various aging time.

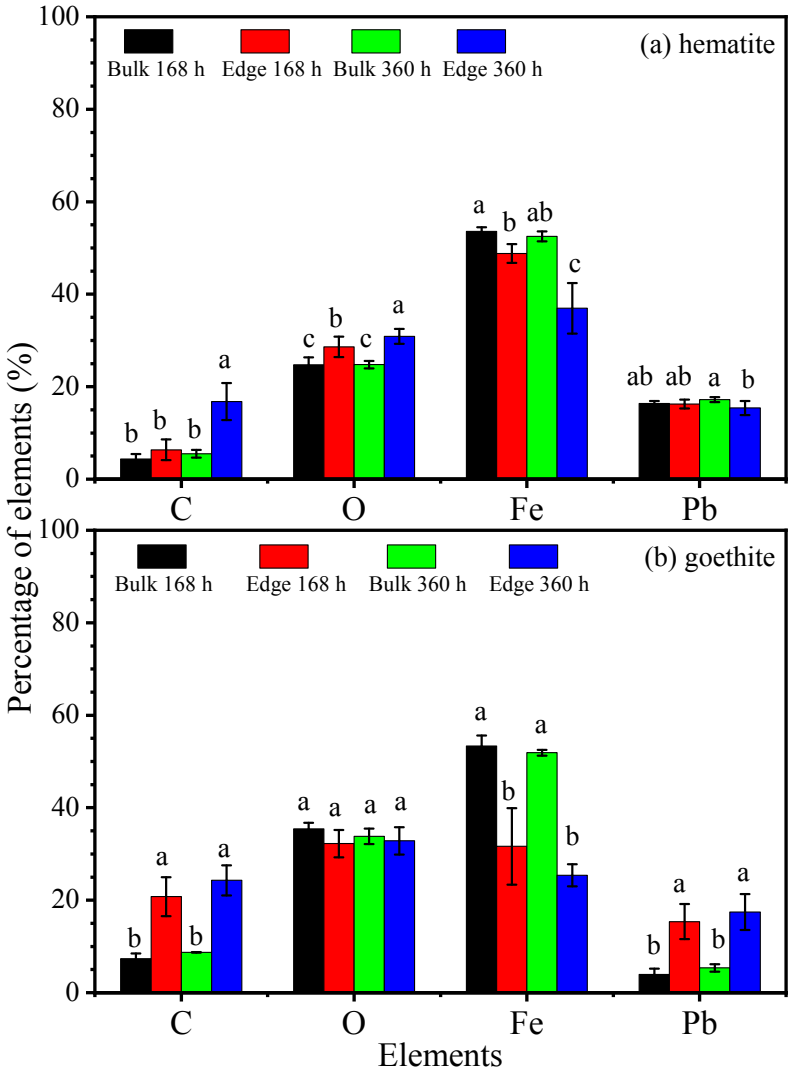

Figure S5. Hematite and goethite edge and bulk statistical analysis based on EDS quantitative results. (a) Hematite edge and bulk compositional differences at 168h and 360h; (b) Goethite edge and bulk elemental compositional differences at 168h and 360h. Statistical differences among various elements were determined by Duncan's test ($p < 0.05$). Different letters on the columns denote a significant difference at $p < 0.05$ using the DMRT (Duncan's new multiple range tests) method.

Table S1. Quantitative analysis of EDS mapping on the bulk and edge of the hematite nanoparticles after 168 h and 360 h aging time. Average values in the table were expressed as mean ± standard error of the replicates.

Hematite

Fh-Pb-HA 168 h

Hematite bulk	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	4.5	25.2	53.9	16.4
2	4.4	24.6	54.5	16.6
3	5.6	26.5	52.4	15.6
4	2.9	22.6	53.6	16.9
Average	4.4 ± 1.1	24.7 ± 1.6	53.6 ± 0.9	16.4 ± 0.6
Hematite edge	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	5.9	25.8	51.0	17.2
2	9.2	28.3	45.8	16.7
3	8.2	27.4	47.7	16.8
4	4.2	30.3	49.8	15.7
5	4.3	31.3	49.7	14.8
Average	6.4 ± 2.3	28.6 ± 2.2	48.8 ± 2.1	16.2 ± 1.0

Fh-Pb-HA 360 h

Hematite bulk	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	5.8	25.2	52.2	16.8
2	5.4	24.7	52.7	17.2
3	4.7	24.9	53.5	16.9
4	4.7	23.6	54.1	17.7
5	5.0	25.2	52.3	17.5
6	5.8	25.9	51.8	16.5
7	7.1	23.9	50.9	18.0
Average	5.5 ± 0.8	24.8 ± 0.8	52.5 ± 1.1	17.2 ± 0.5
Hematite edge	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	20.3	33.8	32.4	13.5
2	18.0	31.6	35.2	15.1
3	14.4	29.1	41.0	15.6
4	15.7	31.6	38.5	14.2
5	11.9	29.8	43.4	14.9
6	13.8	29.5	40.4	16.3
7	23.4	30.8	27.8	18.1
Average	16.8 ± 4.0	30.9 ± 1.6	37.0 ± 5.5	15.4 ± 1.5

Table S2. Quantitative analysis of EDS mapping on the bulk and edge of the goethite nanoparticles after 168 h and 360 h aging time. Average values in the table were expressed as mean ± standard error of the replicates.

Goethite

Fh-Pb-HA 168 h

Goethite bulk	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	6.8	34.4	56.9	2.0
2	8.2	37.1	50.8	4.0
3	8.8	33.1	52.1	6.0
4	6.0	35.6	54.9	3.5
5	6.7	36.2	53.5	3.7
6	8.6	35.6	50.9	5.0
7	6.2	36.1	54.5	3.3
Average	7.3 ± 1.2	35.4 ± 1.3	53.3 ± 2.2	3.9 ± 1.3
Goethite edge	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	15.1	31.9	43.2	9.9
2	22.3	34.7	25.9	17.1
3	18.0	31.8	36.6	13.7
4	25.8	35.1	22.8	16.3
5	22.7	27.7	29.7	19.9
Average	20.8 ± 4.2	32.2 ± 3.0	31.6 ± 8.3	15.4 ± 3.8

Fh-Pb-HA 360 h

Goethite bulk	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	8.8	32.6	52.4	6.1
2	8.7	35.7	51.2	4.5
3	8.7	33.1	52.1	5.5
Average	8.7 ± 0.1	33.8 ± 1.7	51.9 ± 0.6	5.4 ± 0.8
Goethite edge	C (wt %)	O (wt %)	Fe (wt %)	Pb (wt %)
1	24.0	30.8	25.2	20.0
2	27.7	36.2	23.1	13.0
3	21.2	31.5	27.9	19.4
Average	24.3 ± 3.3	32.8 ± 2.9	25.4 ± 2.4	17.5 ± 3.9

Table S3. Calculation of Pb saturation index (pH 10.0, 10 mM $NaNO_3$) by Visual Minteq 3.0 after 360 h aging.

Mineral	Saturation Index
Cerrusite	-2.133
Hydrocerrusite	-5.669
Litharge	-6.453
Massicot	-6.653
Natron	-4.886
$Pb(OH)_2(s)$	-1.914
$Pb_{10}(OH)_6O(CO_3)_6(s)$	-58.291
$Pb_2O(OH)_2(s)$	-13.717
$Pb_2OCO_3(s)$	-8.538
$Pb_3O_2CO_3(s)$	-13.88
$PbO{:}0.3H_2O(s)$	-6.744
Thermonatrite	-6.833