# Re-oxidation of chromium(III) products formed under different biogeochemical regimes: Supporting Information

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**Supplementary Information Figures**

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**Figure SI-2** Nitrite and sulfate in the 7 columns for the entire period of the re-oxidation experiment (left panel), and the first 100 days (right panel). The x-axis shows days adjusted to the start of the re-oxidation phase in each of the columns. The y-axis has concentrations reported relative to influent values (Equation 1). Note the differences in the y-axis scale for each of the ions. Concentration values are listed in Tables SI-3 to SI-7).

**Figure SI-3** Comparison of conditions in (a) denitrifying column N-D1, and in (b) and in the sulfate-amended low activity column S-L1, during the initial period (200 days) after oxidative conditions were introduced. The x-axis shows days adjusted to the start of re-oxidation in each of the columns. The y-axes have concentrations reported relative to influent values (Equation 1). Negative nitrate values indicate consumption of influent nitrate during re-oxidation. The dashed line is drawn at day 42, when conditions where switched from a nitrogen headspace to ambient atmospheric conditions.

**Figure SI-4** DIC, nitrate concentrations (relative to influent as in Equation 1) and δ13C of the DIC for 250 days after oxidative conditions were introduced. The nitrate-amended columns are shown in the left panel, and the sulfate-amended columns are shown in the right panel. The dashed line indicates day 42.

**Figure SI-5** pH values in the 7 columns and influent solution for the entire period of the re-oxidation experiment. The x-axis shows days adjusted to the start of the re-oxidation phase of the experiment. pH values for the first 66 days were slightly higher due to NaOH pellets that were used to scrub $CO_2$ from the glove bag.

**Figure SI-6** Influent-subtracted concentrations of various ions in the column effluents during the pump manipulation experiments (calculated as $C=C_{effluent}-C_{influent}$). The x-axis shows days adjusted to the start of the pump manipulation. Note the differences in the y-axis scale for each of the ions.

**Figure SI-7** Effluent chromium and manganese concentrations in the denitrifying columns.

**Supplementary Information Tables**

**Table SI-1** Chromium speciation results measured using cation-exchange (IC-H) cartridges. Chromium concentrations relative to influent are shown, with percentage of Cr(VI) present displayed in parentheses. Percent values are only shown when chromium concentrations are above the method detection limit (0.01 μM).

**Table SI-2** Chromium, manganese, and iron concentrations (μg/g) in different column sections from the 0.5 N HCl extractions, compared to reference material from Hanford.

**Table SI-3** Total Cr concentrations relative to influent (μM) in the re-oxidation experiment ($Cr=Cr_{effluent}-Cr_{influent}$). NA indicates values not measured. The method detection limit for Cr concentrations relative to influent is 0.01 μM.

**Table SI-4** Total Mn concentrations relative to influent (μM) in the re-oxidation experiment ($Mn=Mn_{effluent}-Mn_{influent}$). NA indicates values not measured.

**Table SI-5** Nitrate concentrations relative to influent (μM) in the re-oxidation experiment ($Nitrate= Nitrate_{effluent}- Nitrate_{influent}$). Values were rounded to the nearest integer. NA indicates values not measured. Negative values indicate nitrate consumption due to denitrification during re-oxidation.

**Table SI-6** Nitrite concentrations relative to influent (μM) in the re-oxidation experiment ($Nitrite= Nitrite_{effluent}- Nitrite_{influent}$). Values were rounded to the nearest integer. NA indicates values not measured.

**Table SI-7** Effluent sulfate concentrations relative to influent (μM) in the re-oxidation experiment ($Sulfate=Sulfate_{effluent}- Sulfate_{influent}$). NA indicates values not measured.

**Figure SI-1** Timeline of pump manipulation experiments.

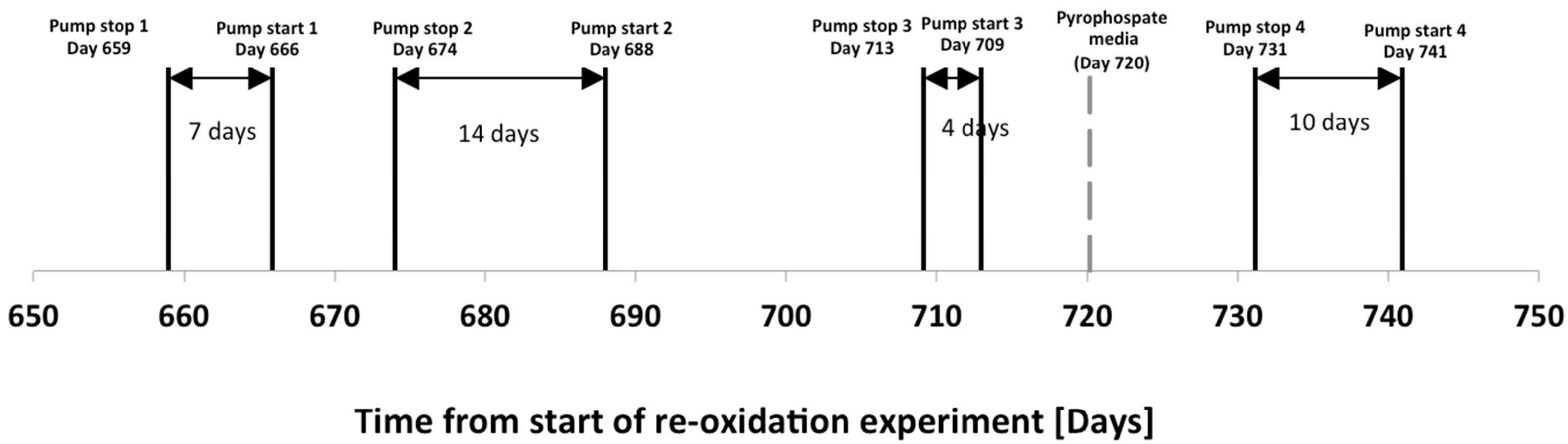
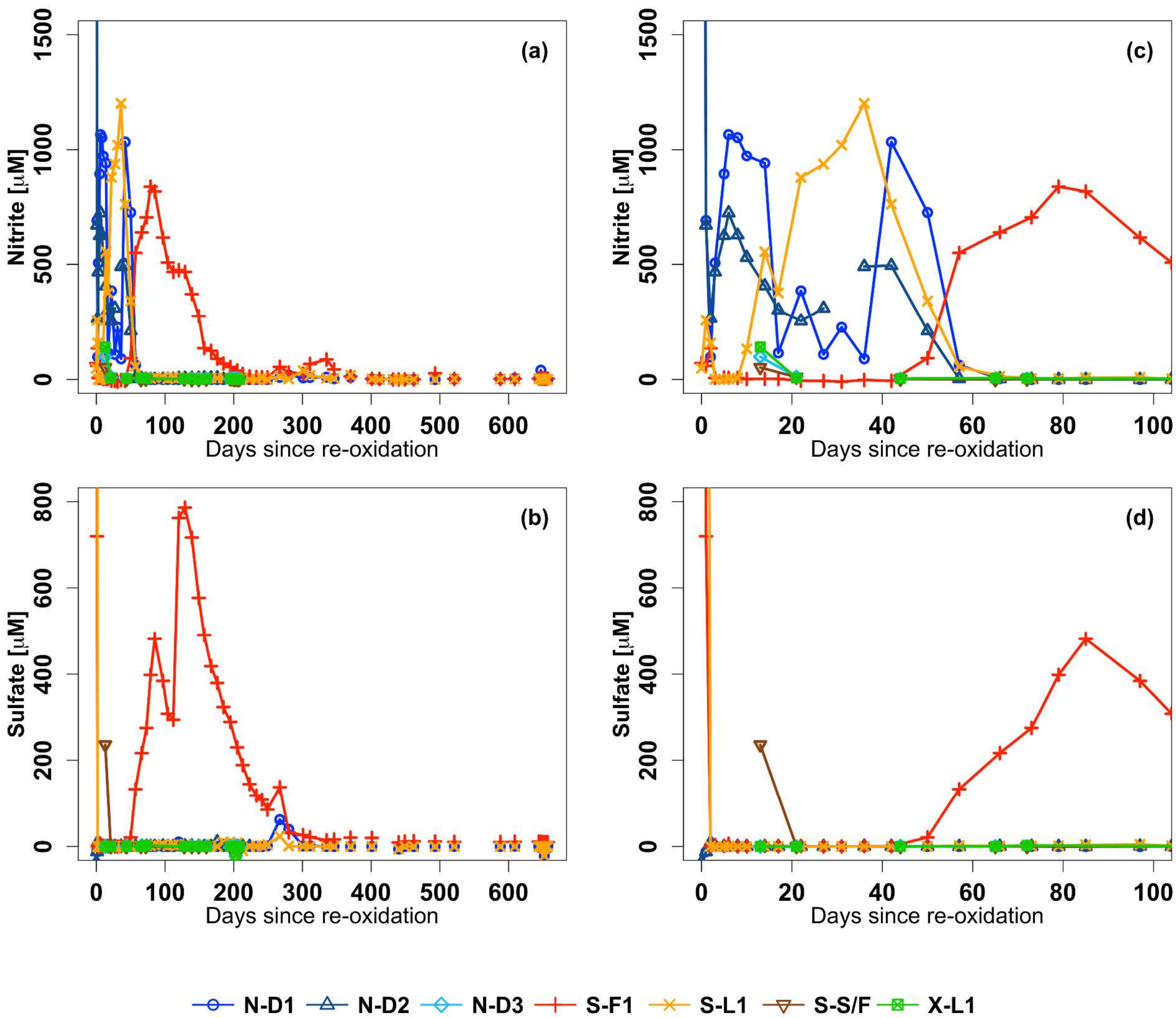


**Figure SI-2** Nitrite and sulfate in the 7 columns for the entire period of the re-oxidation experiment (left panel), and the first 100 days (right panel). The x-axis shows days adjusted to the start of the re-oxidation phase in each of the columns. The y-axis has concentrations reported relative to influent values (Equation 1). Note the differences in the y-axis scale for each of the ions. Concentration values are listed in Tables SI-3 to SI-7).



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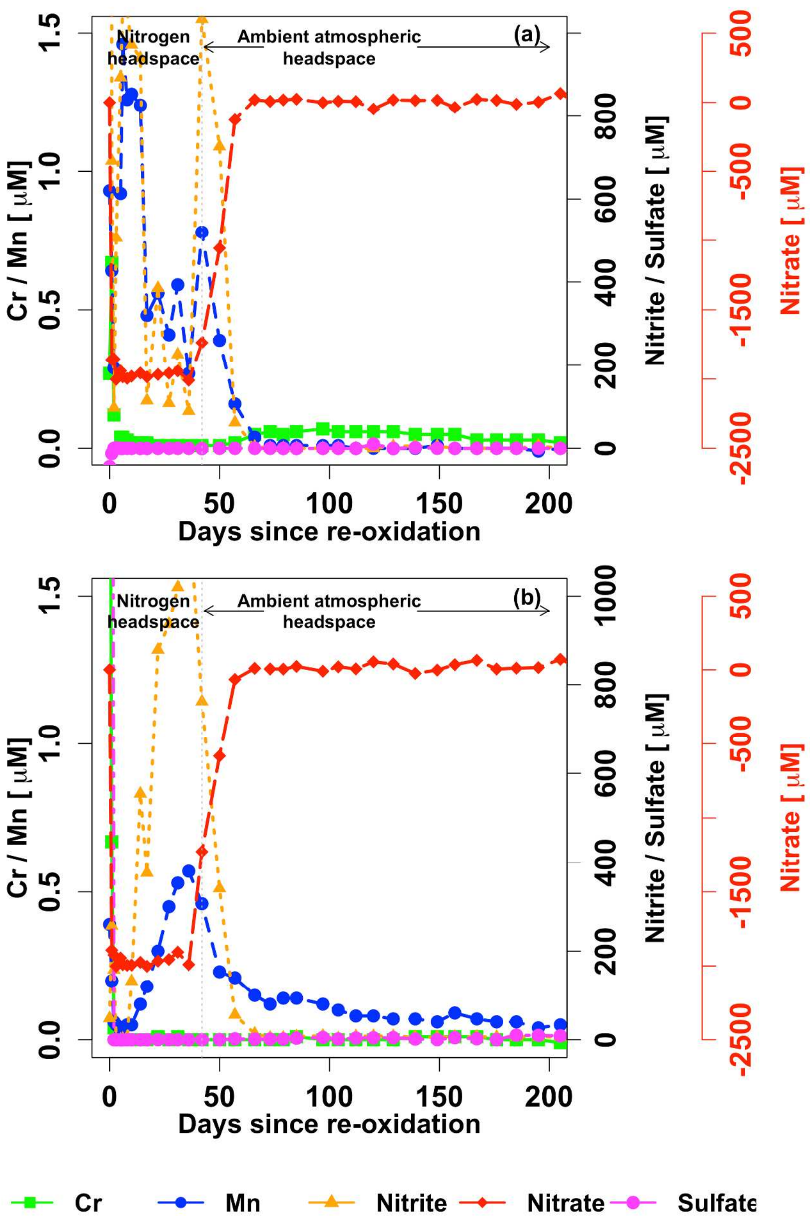

**Figure SI-4** DIC, nitrate concentrations (relative to influent as in Equation 1) and δ13C of the DIC for 250 days after oxidative conditions were introduced. The nitrate-amended columns are shown in the left panel, and the sulfate-amended columns are shown in the right panel. The dashed line indicates day 42.

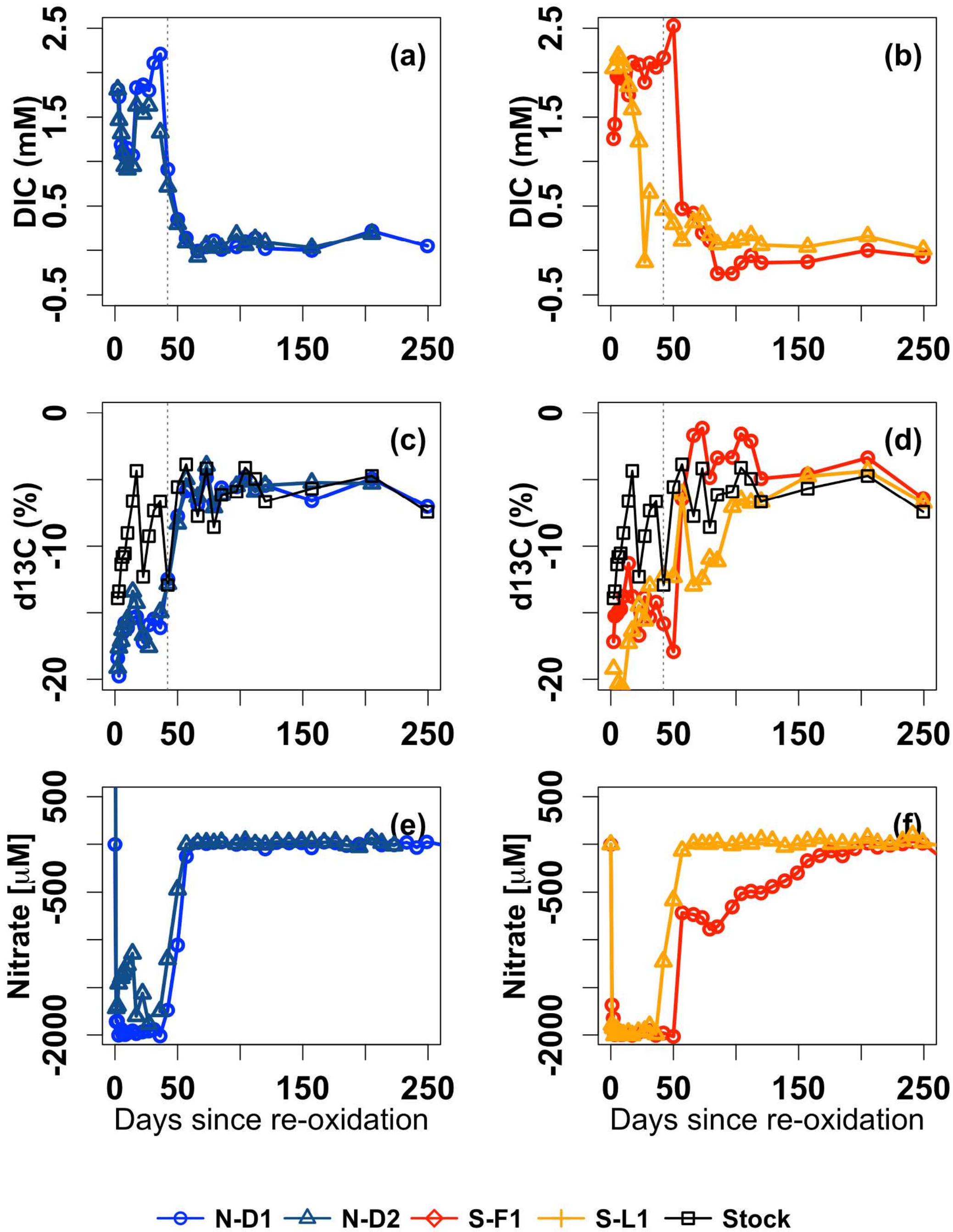

**Figure SI-5** pH values in the 7 columns and influent solution for the entire period of the re-oxidation experiment. The x-axis shows days adjusted to the start of the re-oxidation phase of the experiment. pH values for the first 66 days were slightly higher due to NaOH pellets that were used to scrub $CO_2$ from the glove bag.

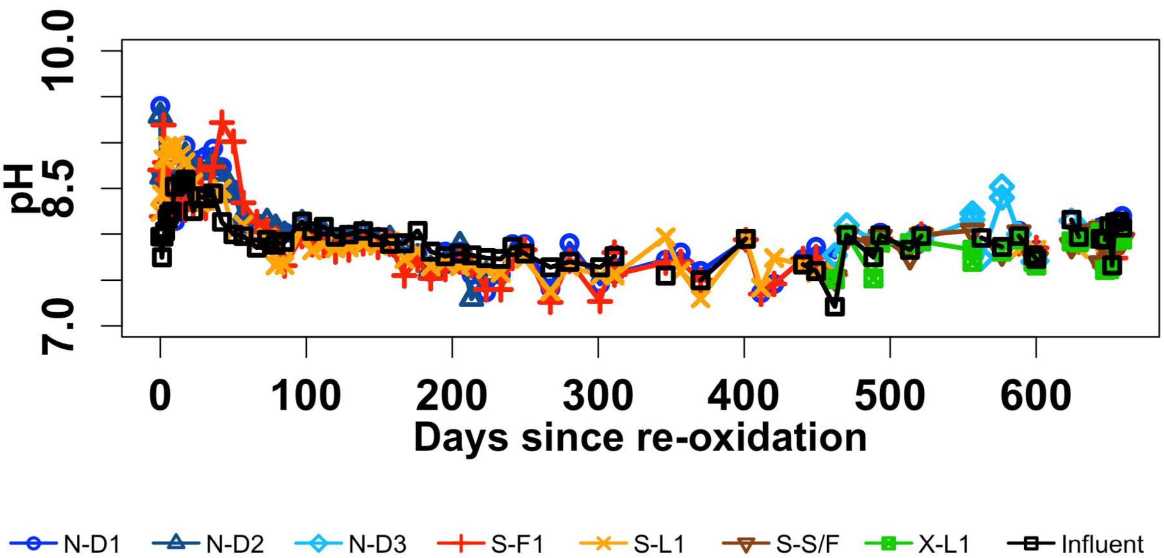

**Figure SI-6** Influent-subtracted concentrations of various ions in the column effluents during the pump manipulation experiments (calculated as $C = C_{effluent} - C_{influent}$). The x-axis shows days adjusted to the start of the pump manipulation. Note the differences in the y-axis scale for each of the ions.

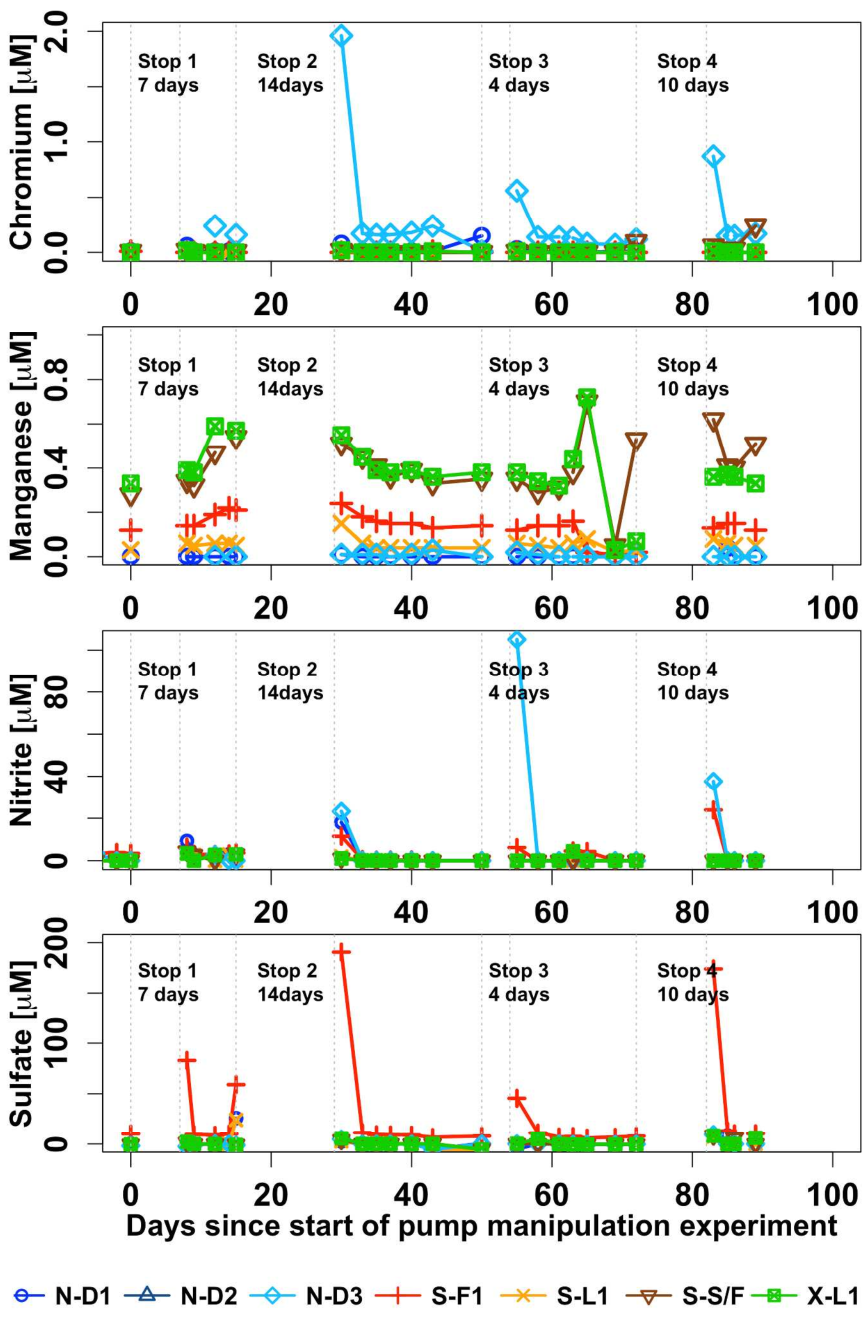


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**Figure SI-7** Effluent chromium and manganese concentrations in the denitrifying columns.

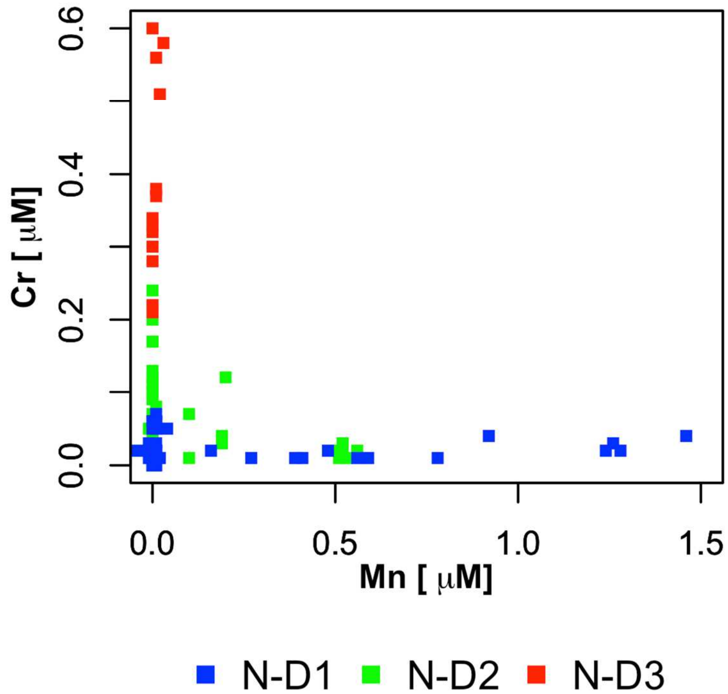
0.0
0.2
0.4
0.6
Cr [ μM]
0.0
0.5
1.0
1.5
Mn [ μM]
N-D1
N-D2
N-D3

**Table SI-1** Chromium speciation results measured using cation-exchange (IC-H) cartridges. Chromium concentrations relative to influent are shown (as $C=C_{effluent}-C_{influent}$), with percentage of Cr(VI) present displayed in parentheses. Percent values are only shown when chromium concentrations are above the method detection limit (0.01 μM).

| Days | Stage of experiment | N-D1 | N-D2 | N-D3 | S-F1 | S-L1 | S-S/F | X-L1 |
|---|---|---|---|---|---|---|---|---|
| 0 | N2 headspace | 0.27 (72%) | 0.24 (59%) | | 0.03 (26%) | 2.67 (74%) | | |
| 1 | N2 headspace | 0.67 (71%) | 0.37 (58%) | | 0.08 (39%) | 0.67 (95%) | | |
| 5 | N2 headspace | 0.04 (59%) | 0.04 (53%) | | 0.02 (39%) | 0.02 (5%) | | |
| 6 | N2 headspace | 0.04 (65%) | 0.03 (59%) | | 0.02 (46%) | 0.01 (37%) | | |
| 73 | Atmospheric headspace | 0.06 (94%) | 0.17 (92%) | | 0.00 | 0.00 | | |
| 85 | Atmospheric headspace | 0.06 (97%) | 0.12 (93%) | | 0.00 | 0.01 | | |
| 112 | Atmospheric headspace | 0.06 (95%) | 0.10 (91%) | | 0.00 | 0.00 | | |
| 120 | Atmospheric headspace | 0.06 (87%) | 0.11 (86%) | | 0.00 | 0.00 | | |
| 223 | Atmospheric headspace | 0.02 (105%) | 0.06 (77%) | | 0.00 | 0.00 | | |
| 301 | Atmospheric headspace | 0.01 (60%) | | | 0.00 | 0.00 | | |
| 335 | Atmospheric headspace | 0.00 (67%) | | | 0.00 | 0.00 | | |
| 370 | Atmospheric headspace | 0.02 (86%) | | | 0.01 (2%) | 0.00 | | |
| 462 | Atmospheric headspace | 0.01 (108%) | | 2.36 (94%) | 0.00 | 0.00 | 1.29 (98%) | 0.39 (92%) |
| 493 | Atmospheric headspace | 0.02 (112%) | | 0.51 (103%) | 0.00 | 0.00 | 0.02 (91%) | 0.01 |
| 521 | Atmospheric headspace | 0.01 | | 0.38 (90%) | 0.04 (3%) | 0.00 | 0.01 | 0.02 (89%) |
| 556 | Atmospheric headspace | 0.01 | | | 0.00 | 0.00 | | |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 563 | Atmospheric headspace | | | | | | | |
| 588 | Atmospheric headspace | 0.01 | | 0.33 (91%) | 0.00 | 0.00 | 0.01 | 0.00 |
| 624 | Atmospheric headspace | 0.01 | | 0.33 (91%) | 0.00 | 0.00 | 0.01 | 0.00 |
| 671 | Pump stop | 0.01 (33%) | | 0.24 (62%) | 0.00 | 0.00 | 0.00 | 0.00 |
| 714 | Pump stop | 0.03 (86%) | | 0.56 (87%) | 0.00 | 0.00 | 0.01 | 0.01 |

**Table SI-2** Chromium, manganese, and iron concentrations (μg/g) in different column sections from the 0.5 N HCl extractions, compared to reference material from Hanford. Fe(II) was only measured for the 1-hour extractions.

| | **1-h 0.5 N HCl extractions** | | | | **24-h 0.5 N HCl extractions`** | | |
|---|---|---|---|---|---|---|---|
| **Column section** | **Total Mn** $\mu g/g_{sediment}$ | **Total Cr** $\mu g/g_{sediment}$ | **Total Fe** $\mu g/g_{sediment}$ | **Fe(II)** $\mu g/g_{sediment}$ | **Total Mn** $\mu g/g_{sediment}$ | **Total Cr** $\mu g/g_{sediment}$ | **Total Fe** $\mu g/g_{sediment}$ |
| Untreated material | 50 ± 5.4 | 0.3 ± 0.1 | 600 ± 50 | 51 ± 1 | 69 ± 2.4 | 1 ± 0.7 | 2415 ± 108 |
| S-F2: Bottom | 23 ± 0.3 | 26 ± 0.7 | 1000 ± 6 | 113 ± 18 | 41 ± 0.3 | 29 ± 0.4 | 2600 ± 37 |
| S-F2: Middle | 40 ± 1.0 | 4 ± 0.3 | 990 ± 17 | 90 ± 5 | 55 ± 0.7 | 6 ± 0.2 | 2500 ± 51 |
| S-F2: Top | 34 ± 0.7 | 2 ± 0.2 | 890 ± 9 | 94 ± 8 | 59 ± 0.8 | 2 ± 0.2 | 2500 ± 41 |
| N-D4: Bottom | 40 ± 0.6 | 21 ± 0.6 | 580 ± 16 | 62 ± 5 | 54 ± 0.4 | 21 ± 0.2 | 3000 ± 29 |
| N-D4: Middle | 47 ± 0.8 | 7 ± 0.4 | 630 ± 12 | 61 ± 5 | 62 ± 1.1 | 6 ± 0.3 | 2100 ± 26 |
| N-D4: Top | 40 ± 0.4 | 2 ± 0.1 | 550 ± 11 | 52 ± 5 | 57 ± 0.6 | 3 ± 0.1 | 2300 ± 44 |
| S-L2: Bottom | 40 ± 0.6 | 9 ± 0.3 | 610 ± 18 | 54 ± 4 | 53 ± 0.7 | 8 ± 0.2 | 2400 ± 49 |
| S-L2: Middle | 47 ± 1.1 | 8 ± 0.3 | 630 ± 17 | 60 ± 5 | 68 ± 1.0 | 8 ± 0.2 | 2100 ± 21 |
| S-L2: Top | 47 ± 0.9 | 8 ± 0.3 | 610 ± 14 | 60 ± 4 | 67 ± 1.2 | 7 ± 0.1 | 2700 ± 20 |
| X-L2: Bottom | 45 ± 1.2 | 7 ± 0.4 | 600 ± 8 | 60 ± 6 | 58 ± 0.2 | 7 ± 0.2 | 2100 ± 13 |
| X-L2: Middle | 49 ± 0.6 | 5 ± 0.1 | 630 ± 10 | 62 ± 6 | 57 ± 1.1 | 5 ± 0.2 | 2200 ± 15 |
| X-L2: Top | 49 ± 1.2 | 6 ± 0.3 | 630 ± 17 | 60 ± 5 | 64 ± 0.5 | 6 ± 0.1 | 2100 ± 16 |

**Table SI-3** Total Cr concentrations relative to influent (μM) in the re-oxidation experiment ($Cr=Cr_{effluent}-Cr_{influent}$). NA indicates values not measured. The method detection limit for Cr concentrations relative to influent is 0.01 μM.

| Days since start of Re-oxidation | Cr (N-D1) | Cr (N-D2) | Cr (N-D3) | Cr (S-F1) | Cr (S-L1) | Cr (S-S/F) | Cr (X-L1) |
|---|---|---|---|---|---|---|---|
| 0 | 0.27 | 0.24 | NA | 0.03 | 2.67 | NA | NA |
| 1 | 0.67 | 0.37 | NA | 0.08 | 0.67 | NA | NA |
| 2 | 0.12 | 0.12 | NA | 0.04 | 0.04 | NA | NA |
| 3 | NA | 0.07 | NA | 0.02 | 0.03 | NA | NA |
| 5 | 0.04 | 0.04 | NA | 0.02 | 0.02 | NA | NA |
| 6 | 0.04 | 0.03 | NA | 0.02 | 0.01 | NA | NA |
| 8 | 0.03 | 0.02 | NA | 0.01 | 0 | NA | NA |
| 10 | 0.02 | 0.03 | NA | 0 | 0 | NA | NA |
| 13 | NA | NA | 2.35 | NA | NA | 1.29 | 0.39 |
| 14 | 0.02 | 0.02 | NA | 0 | 0 | NA | NA |
| 17 | 0.02 | 0.02 | NA | 0 | 0 | NA | NA |
| 21 | NA | NA | 0.58 | NA | NA | 0.02 | 0.58 |
| 22 | 0.01 | 0.01 | NA | 0 | 0.01 | NA | NA |
| 27 | 0.01 | 0.01 | NA | 0 | 0 | NA | NA |
| 31 | 0.01 | 0.01 | NA | 0 | 0.01 | NA | NA |
| 36 | 0.01 | 0.12 | NA | 0 | 0 | NA | NA |
| 40 | NA | NA | 0.56 | NA | NA | 0.02 | 0.56 |
| 42 | 0.01 | 0.03 | NA | 0.01 | 0 | NA | NA |
| 44 | NA | NA | 0.51 | NA | NA | 0.02 | 0 |
| 50 | 0.01 | 0.17 | NA | 0 | 0 | NA | NA |
| 57 | 0.02 | 0.24 | NA | 0 | 0 | NA | NA |
| 65 | NA | NA | 0.37 | NA | NA | NA | 0 |
| 66 | 0.05 | 0.2 | NA | 0 | 0 | NA | NA |
| 72 | NA | NA | 0.38 | NA | NA | 0.01 | 0.02 |
| 73 | 0.06 | 0.17 | NA | 0 | 0 | NA | NA |
| 79 | 0.05 | 0.13 | NA | 0 | 0 | NA | NA |
| 85 | 0.06 | 0.12 | NA | 0 | 0.01 | NA | NA |
| 97 | 0.07 | 0.12 | NA | 0 | 0 | NA | NA |
| 100 | NA | NA | NA | NA | NA | NA | NA |
| 104 | 0.06 | 0.11 | NA | 0 | 0 | NA | NA |
| 112 | 0.06 | 0.1 | NA | 0 | 0 | NA | NA |
| 114 | NA | NA | NA | NA | NA | NA | NA |
| 120 | 0.06 | 0.11 | NA | 0 | 0 | NA | NA |
| 128 | NA | NA | 0.34 | NA | NA | 0 | -0.01 |
| 129 | 0.06 | 0.1 | NA | 0 | 0 | NA | NA |
| 139 | 0.05 | 0.09 | 0.33 | 0 | 0.01 | 0.01 | 0 |
| 149 | 0.05 | 0.08 | 0.3 | 0.02 | 0.01 | 0.01 | 0 |
| 157 | 0.05 | 0.07 | NA | 0 | 0.01 | NA | NA |
| 160 | NA | NA | 0.28 | NA | NA | 0 | 0.01 |
| 167 | 0.03 | 0.06 | NA | 0 | 0.01 | NA | NA |
| 175 | NA | NA | 0.32 | NA | NA | 0 | 0 |
| 176 | 0.03 | 0.05 | NA | 0 | 0 | NA | NA |
| 183 | NA | NA | NA | NA | NA | NA | NA |
| 185 | 0.03 | 0.05 | NA | 0 | 0 | NA | NA |
| 195 | 0.03 | 0.05 | 0.21 | 0 | 0 | 0 | 0 |
| 198 | NA | NA | 0.84 | NA | NA | 0 | -0.01 |
| 201 | NA | NA | 0.6 | NA | NA | 0 | 0 |
| 203 | NA | NA | 0.22 | NA | NA | 0 | 0 |
| 205 | 0.02 | 0.04 | 0.22 | -0.01 | -0.01 | 0 | 0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 208 | NA | NA | NA | NA | NA | NA | 0 |
| 213 | 0.02 | 0.04 | NA | -0.01 | 0 | NA | NA |
| 223 | 0.02 | 0.06 | NA | -0.01 | -0.01 | NA | NA |
| 233 | 0.03 | NA | NA | 0 | 0 | NA | NA |
| 241 | 0.03 | NA | NA | 0 | 0 | NA | NA |
| 249 | 0.02 | NA | NA | 0 | 0 | NA | NA |
| 267 | 0.02 | NA | NA | 0 | -0.01 | NA | NA |
| 280 | 0.02 | NA | NA | 0.02 | 0 | NA | NA |
| 301 | 0.01 | NA | NA | 0 | 0 | NA | NA |
| 311 | 0 | NA | NA | -0.01 | -0.01 | NA | NA |
| 335 | 0 | NA | NA | -0.02 | -0.02 | NA | NA |
| 346 | 0.02 | NA | NA | 0 | 0.01 | NA | NA |
| 357 | 0.02 | NA | NA | 0 | 0.01 | NA | NA |
| 370 | 0.02 | NA | NA | 0.01 | 0 | NA | NA |
| 380 | 0.02 | NA | NA | 0.01 | 0 | NA | NA |
| 393 | 0.02 | NA | NA | 0 | 0 | NA | NA |
| 401 | 0.02 | NA | NA | 0 | 0 | NA | NA |
| 412 | 0.02 | NA | NA | 0.01 | 0 | NA | NA |
| 421 | 0.02 | NA | NA | 0.01 | 0.03 | NA | NA |
| 432 | 0.02 | NA | NA | 0.01 | 0 | NA | NA |
| 440 | 0.01 | NA | NA | 0 | 0.01 | NA | NA |
| 449 | 0.01 | NA | NA | 0 | 0 | NA | NA |
| 462 | 0.01 | NA | NA | 0 | 0 | NA | NA |
| 493 | 0.01 | NA | NA | 0 | 0 | NA | NA |
| 521 | 0 | NA | NA | 0.04 | 0 | NA | NA |
| 556 | 0 | NA | NA | 0 | 0 | NA | NA |
| 588 | 0 | NA | NA | 0 | 0 | NA | NA |
| 609 | 0.02 | NA | NA | 0 | 0 | NA | NA |
| 624 | 0.01 | NA | NA | 0 | 0 | NA | NA |
| 644 | 0.03 | NA | NA | 0 | 0 | NA | NA |
| 647 | 0 | NA | NA | -0.01 | -0.01 | NA | NA |
| 650 | 0 | NA | NA | 0 | 0 | NA | NA |
| 652 | 0.03 | NA | NA | -0.01 | -0.01 | NA | NA |
| 654 | 0.01 | NA | NA | 0 | 0 | NA | NA |
| 657 | 0.01 | NA | NA | 0 | 0 | NA | NA |

**Table SI-4** Total Mn concentrations relative to influent (μM) in the re-oxidation experiment ($Mn=Mn_{effluent}-Mn_{influent}$). NA indicates values not measured.

| Days since start of Re-oxidation | Mn (N-D1) | Mn (N-D2) | Mn (N-D3) | Mn (S-F1) | Mn (S-L1) | Mn (S-S/F) | Mn (X-L1) |
|---|---|---|---|---|---|---|---|
| 0 | 0.93 | 0.27 | NA | 0.44 | 0.39 | NA | NA |
| 1 | 0.64 | 0.2 | NA | 0.19 | 0.2 | NA | NA |
| 2 | 0.29 | 0.11 | NA | 0.09 | 0.06 | NA | NA |
| 3 | NA | 0.1 | NA | 0.08 | 0.05 | NA | NA |
| 5 | 0.92 | 0.19 | NA | 0.13 | 0.03 | NA | NA |
| 6 | 1.46 | 0.52 | NA | 0.16 | 0.04 | NA | NA |
| 8 | 1.26 | 0.52 | NA | 0.44 | 0.05 | NA | NA |
| 10 | 1.28 | 0.52 | NA | 0.54 | 0.05 | NA | NA |
| 13 | NA | NA | 0.03 | NA | NA | 0.57 | 0.87 |
| 14 | 1.24 | 0.56 | NA | 0.48 | 0.12 | NA | NA |
| 17 | 0.48 | 0.5 | NA | 0.37 | 0.18 | NA | NA |
| 21 | NA | NA | 0.03 | NA | NA | 0.64 | 0.03 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 22 | 0.56 | 0.53 | NA | 0.31 | 0.3 | NA | NA |
| 27 | 0.41 | 0.51 | NA | 0.22 | 0.45 | NA | NA |
| 31 | 0.59 | 0.1 | NA | 0.16 | 0.53 | NA | NA |
| 36 | 0.27 | 0.2 | NA | 0.11 | 0.57 | NA | NA |
| 40 | NA | NA | 0.01 | NA | NA | 0.38 | 0.01 |
| 42 | 0.78 | 0.19 | NA | 0.04 | 0.46 | NA | NA |
| 44 | NA | NA | 0.02 | NA | NA | 0.41 | 0.6 |
| 50 | 0.39 | 0 | NA | 0.06 | 0.23 | NA | NA |
| 57 | 0.16 | 0 | NA | 0.04 | 0.21 | NA | NA |
| 65 | NA | NA | 0.01 | NA | NA | NA | 0.75 |
| 66 | 0.04 | 0 | NA | 0.1 | 0.15 | NA | NA |
| 72 | NA | NA | 0.01 | NA | NA | 0.57 | 0.81 |
| 73 | 0.01 | 0 | NA | 0.34 | 0.12 | NA | NA |
| 79 | 0.01 | 0 | NA | 0.68 | 0.14 | NA | NA |
| 85 | 0.01 | 0 | NA | 1.06 | 0.14 | NA | NA |
| 97 | 0.01 | 0 | NA | 1.33 | 0.12 | NA | NA |
| 100 | NA | NA | NA | NA | NA | NA | NA |
| 104 | 0.01 | 0 | NA | 1.02 | 0.1 | NA | NA |
| 112 | 0 | 0 | NA | 0.85 | 0.08 | NA | NA |
| 114 | NA | NA | NA | NA | NA | NA | NA |
| 120 | 0 | 0 | NA | 0.89 | 0.08 | NA | NA |
| 128 | NA | NA | 0 | NA | NA | 0.44 | 0.73 |
| 129 | 0 | 0 | NA | 0.88 | 0.07 | NA | NA |
| 139 | 0 | 0 | 0 | 0.8 | 0.07 | 0.26 | 0.37 |
| 149 | 0.01 | 0.01 | 0 | 0.67 | 0.06 | 0.27 | 0.32 |
| 157 | 0 | 0 | NA | 0.76 | 0.09 | NA | NA |
| 160 | NA | NA | 0 | NA | NA | 0.26 | 0.35 |
| 167 | 0 | 0 | NA | 0.67 | 0.07 | NA | NA |
| 175 | NA | NA | 0 | NA | NA | 0.26 | 0.32 |
| 176 | 0 | 0 | NA | 0.6 | 0.06 | NA | NA |
| 183 | NA | NA | NA | NA | NA | NA | NA |
| 185 | 0 | 0 | NA | 0.51 | 0.06 | NA | NA |
| 195 | -0.01 | -0.01 | 0 | 0.43 | 0.04 | 0.29 | 0.37 |
| 198 | NA | NA | 0.01 | NA | NA | 0.26 | 0.31 |
| 201 | NA | NA | 0 | NA | NA | 0.26 | 0.28 |
| 203 | NA | NA | -0.08 | NA | NA | 0.18 | 0.22 |
| 205 | 0 | 0 | 0 | 0.42 | 0.05 | 0.29 | 0.34 |
| 208 | NA | NA | NA | NA | NA | NA | 0.3 |
| 213 | 0 | 0 | NA | 0.38 | 0.04 | NA | NA |
| 223 | 0 | 0 | NA | 0.38 | 0.04 | NA | NA |
| 233 | 0 | NA | NA | 0.34 | 0.04 | NA | NA |
| 241 | 0 | NA | NA | 0.32 | 0.04 | NA | NA |
| 249 | -0.05 | NA | NA | 0.3 | 0 | NA | NA |
| 267 | 0.01 | NA | NA | 0.34 | 0.12 | NA | NA |
| 280 | 0.01 | NA | NA | 0.34 | 0.09 | NA | NA |
| 301 | 0.02 | NA | NA | 0.35 | 0.32 | NA | NA |
| 311 | 0.01 | NA | NA | 0.34 | 0.28 | NA | NA |
| 335 | 0.01 | NA | NA | 0.33 | 0.21 | NA | NA |
| 346 | 0.01 | NA | NA | 0.32 | 0.25 | NA | NA |
| 357 | 0 | NA | NA | 0.3 | 0.18 | NA | NA |
| 370 | 0 | NA | NA | 0.28 | 0.15 | NA | NA |
| 380 | -0.01 | NA | NA | 0.27 | 0.14 | NA | NA |
| 393 | -0.01 | NA | NA | 0.26 | 0.1 | NA | NA |
| 401 | -0.02 | NA | NA | 0.2 | 0.07 | NA | NA |
| 412 | -0.01 | NA | NA | 0.23 | 0.08 | NA | NA |
| 421 | -0.01 | NA | NA | 0.17 | 0.07 | NA | NA |
| 432 | -0.01 | NA | NA | 0.16 | 0.06 | NA | NA |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 440 | -0.01 | NA | NA | 0.16 | 0.06 | NA | NA |
| 449 | 0 | NA | NA | 0.17 | 0.06 | NA | NA |
| 462 | 0 | NA | NA | 0.16 | 0.06 | NA | NA |
| 493 | 0 | NA | NA | 0.15 | 0.06 | NA | NA |
| 521 | 0 | NA | NA | 0.15 | 0.06 | NA | NA |
| 556 | 0 | NA | NA | 0.18 | 0.06 | NA | NA |
| 588 | 0 | NA | NA | 0.08 | 0.04 | NA | NA |
| 609 | 0 | NA | NA | 0.1 | 0.03 | NA | NA |
| 624 | 0 | NA | NA | 0.11 | 0.03 | NA | NA |
| 644 | 0.01 | NA | NA | 0.1 | 0.03 | NA | NA |
| 647 | 0 | NA | NA | 0.11 | 0.03 | NA | NA |
| 650 | 0 | NA | NA | 0.1 | 0.03 | NA | NA |
| 652 | -0.08 | NA | NA | 0.02 | -0.05 | NA | NA |
| 654 | 0 | NA | NA | 0.12 | 0.03 | NA | NA |
| 657 | 0 | NA | NA | 0.12 | 0.03 | NA | NA |

**Table SI-5** Nitrate concentrations relative to influent (μM) in the re-oxidation experiment (Nitrate= $\text{Nitrate}_{\text{effluent}}$- $\text{Nitrate}_{\text{influent}}$). Values were rounded to the nearest integer. NA indicates values not measured. Negative values indicate nitrate consumption due to denitrification during re-oxidation.

| Days since start of Re-oxidation | Nitrate (N-D1) | Nitrate (N-D2) | Nitrate (N-D3) | Nitrate (S-F1) | Nitrate (S-L1) | Nitrate (S-S/F) | Nitrate (X-L1) |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 2948 | NA | 0 | 0 | NA | NA |
| 1 | -1859 | -1717 | NA | -1682 | -1893 | NA | NA |
| 2 | -1855 | -1689 | NA | -1823 | -1926 | NA | NA |
| 3 | -2002 | -1457 | NA | -1996 | -2002 | NA | NA |
| 5 | -1941 | -1398 | NA | -1946 | -1946 | NA | NA |
| 6 | -1984 | -1362 | NA | -1988 | -1991 | NA | NA |
| 8 | -1995 | -1328 | NA | -1995 | -1995 | NA | NA |
| 10 | -1980 | -1264 | NA | -1993 | -1994 | NA | NA |
| 13 | NA | NA | 221 | NA | NA | -137 | -217 |
| 14 | -1957 | -1145 | NA | -1974 | -1975 | NA | NA |
| 17 | -1985 | -1800 | NA | -2002 | -2002 | NA | NA |
| 21 | NA | NA | 259 | NA | NA | 325 | 4 |
| 22 | -1967 | -1561 | NA | -1972 | -1967 | NA | NA |
| 27 | -1958 | -1884 | NA | -1958 | -1956 | NA | NA |
| 31 | -1942 | NA | NA | -1955 | -1907 | NA | NA |
| 36 | -2009 | -1748 | NA | -2003 | -1990 | NA | NA |
| 42 | -1737 | -1203 | NA | -1979 | -1227 | NA | NA |
| 44 | NA | NA | 32 | NA | NA | 34 | -18 |
| 50 | -1057 | -472 | NA | -2015 | -583 | NA | NA |
| 57 | -127 | 0 | NA | -715 | -65 | NA | NA |
| 65 | NA | NA | 197 | NA | NA | -18 | -76 |
| 66 | 19 | 17 | NA | -733 | 9 | NA | NA |
| 72 | NA | NA | 44 | NA | NA | 61 | -12 |
| 73 | 8 | 23 | NA | -765 | 5 | NA | NA |
| 79 | 18 | 16 | NA | -889 | 4 | NA | NA |
| 85 | 24 | 27 | NA | -862 | 22 | NA | NA |
| 97 | -1 | 4 | NA | -654 | -10 | NA | NA |
| 104 | 9 | 39 | NA | -515 | 20 | NA | NA |
| 112 | 7 | 3 | NA | -491 | 6 | NA | NA |
| 120 | -48 | -2 | NA | -508 | 53 | NA | NA |
| 128 | NA | NA | NA | NA | NA | 68 | 9 |
| 129 | 18 | 29 | NA | -441 | 39 | NA | NA |
| 139 | 14 | 26 | 29 | -383 | -25 | 27 | 18 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 149 | 16 | 33 | 32 | -300 | -2 | 44 | 39 |
| 157 | -37 | 33 | NA | -172 | 35 | NA | NA |
| 160 | NA | NA | 48 | NA | NA | 50 | 29 |
| 167 | 23 | 22 | NA | -119 | 64 | NA | NA |
| 176 | 16 | 33 | NA | -69 | 5 | NA | NA |
| 183 | NA | NA | NA | NA | NA | NA | NA |
| 185 | -13 | -11 | NA | -121 | 11 | NA | NA |
| 195 | 3 | -28 | 129 | -45 | 15 | 175 | 98 |
| 198 | NA | NA | NA | NA | NA | 62 | 11 |
| 201 | NA | NA | 5 | NA | NA | 28 | 30 |
| 203 | NA | NA | 42 | NA | NA | 173 | 49 |
| 205 | 65 | 60 | 68 | 13 | 70 | 30 | 19 |
| 208 | NA | NA | NA | NA | NA | NA | 39 |
| 213 | -6 | 15 | NA | -31 | 16 | NA | NA |
| 223 | -5 | -13 | NA | -9 | -1 | NA | NA |
| 233 | 22 | NA | NA | 5 | 36 | NA | NA |
| 241 | -33 | NA | NA | 29 | 96 | NA | NA |
| 249 | 26 | NA | NA | 11 | 21 | NA | NA |
| 267 | -24 | NA | NA | -172 | -28 | NA | NA |
| 280 | -42 | NA | NA | -4 | 13 | NA | NA |
| 301 | 12 | NA | NA | 77 | 51 | NA | NA |
| 311 | -75 | NA | NA | -175 | -18 | NA | NA |
| 335 | -82 | NA | NA | -244 | -52 | NA | NA |
| 346 | 5 | NA | NA | -63 | 60 | NA | NA |
| 357 | NA | NA | NA | NA | NA | NA | NA |
| 370 | 25 | NA | NA | 35 | 69 | NA | NA |
| 380 | NA | NA | NA | NA | NA | NA | NA |
| 393 | NA | NA | NA | NA | NA | NA | NA |
| 401 | -21 | NA | NA | 54 | 23 | NA | NA |
| 412 | NA | NA | NA | NA | NA | NA | NA |
| 432 | NA | NA | NA | NA | NA | NA | NA |
| 440 | -119 | NA | NA | -113 | -90 | NA | NA |
| 449 | 65 | NA | NA | 37 | 25 | NA | NA |
| 462 | 15 | NA | NA | -15 | 17 | NA | NA |
| 470 | NA | NA | NA | NA | NA | NA | NA |
| 476 | NA | NA | NA | NA | NA | NA | NA |
| 493 | 81 | NA | NA | 35 | 98 | NA | NA |
| 514 | NA | NA | NA | NA | NA | NA | NA |
| 521 | 93 | NA | NA | 32 | 35 | NA | NA |
| 577 | NA | NA | NA | NA | NA | NA | NA |
| 588 | 85 | NA | NA | 87 | 69 | NA | NA |
| 598 | NA | NA | NA | NA | NA | NA | NA |
| 609 | 120 | NA | NA | 84 | 64 | NA | NA |
| 632 | NA | NA | NA | NA | NA | NA | NA |
| 644 | 95 | NA | NA | 148 | 130 | NA | NA |
| 647 | -51 | NA | NA | 2 | 5 | NA | NA |
| 650 | 15 | NA | NA | 12 | 11 | NA | NA |
| 652 | -18 | NA | NA | -23 | -10 | NA | NA |
| 654 | 42 | NA | NA | 12 | 23 | NA | NA |
| 657 | 4 | NA | NA | -2 | 14 | NA | NA |

**Table SI-6** Nitrite concentrations relative to influent (μM) in the re-oxidation experiment (Nitrite= $Nitrite_{effluent}$- $Nitrite_{influent}$). Values were rounded to the nearest integer. NA indicates values not measured.

| Days since start of Re-oxidation | Nitrite (N-D1) | Nitrite (N-D2) | Nitrite (N-D3) | Nitrite (S-F1) | Nitrite (S-L1) | Nitrite (S-S/F) | Nitrite (X-L1) |
|---|---|---|---|---|---|---|---|
| 0 | 8488 | 6380 | NA | 71 | 48 | NA | NA |
| 1 | 692 | 672 | NA | 59 | 257 | NA | NA |
| 2 | 97 | 265 | NA | 135 | 158 | NA | NA |
| 3 | 506 | 467 | NA | 7 | 0 | NA | NA |
| 5 | 893 | 625 | NA | 9 | 0 | NA | NA |
| 6 | 1066 | 725 | NA | 7 | 2 | NA | NA |
| 8 | 1053 | 628 | NA | 7 | 6 | NA | NA |
| 10 | 972 | 530 | NA | 2 | 132 | NA | NA |
| 13 | NA | NA | 98 | NA | NA | 52 | 141 |
| 14 | 940 | 407 | NA | 3 | 554 | NA | NA |
| 17 | 115 | 302 | NA | 2 | 376 | NA | NA |
| 21 | NA | NA | 11 | NA | NA | 10 | 7 |
| 22 | 385 | 254 | NA | -5 | 878 | NA | NA |
| 27 | 109 | 310 | NA | -6 | 936 | NA | NA |
| 31 | 226 | NA | NA | -10 | 1020 | NA | NA |
| 36 | 90 | 491 | NA | -2 | 1201 | NA | NA |
| 42 | 1034 | 495 | NA | -6 | 762 | NA | NA |
| 44 | NA | NA | 2 | NA | NA | 2 | 4 |
| 50 | 726 | 211 | NA | 93 | 341 | NA | NA |
| 57 | 62 | 4 | NA | 550 | 56 | NA | NA |
| 65 | NA | NA | 0 | NA | NA | 0 | 7 |
| 66 | 4 | 3 | NA | 640 | 14 | NA | NA |
| 72 | NA | NA | 2 | NA | NA | 2 | 5 |
| 73 | 0 | 0 | NA | 706 | 4 | NA | NA |
| 79 | 0 | 0 | NA | 839 | 4 | NA | NA |
| 85 | 0 | 0 | NA | 817 | 8 | NA | NA |
| 97 | 0 | 0 | NA | 616 | 9 | NA | NA |
| 104 | 0 | 0 | NA | 508 | 3 | NA | NA |
| 112 | 0 | 0 | NA | 467 | 7 | NA | NA |
| 120 | 0 | 5 | NA | 475 | 8 | NA | NA |
| 128 | NA | NA | NA | NA | NA | 3 | 3 |
| 129 | 5 | 5 | NA | 468 | 8 | NA | NA |
| 139 | 5 | 5 | 2 | 371 | 5 | 0 | 2 |
| 149 | 5 | 5 | 0 | 275 | 5 | 0 | 0 |
| 157 | 0 | 6 | NA | 136 | 7 | NA | NA |
| 160 | NA | NA | 2 | NA | NA | 2 | 2 |
| 167 | 0 | 6 | NA | 124 | 7 | NA | NA |
| 176 | 0 | 7 | NA | 90 | 6 | NA | NA |
| 183 | NA | NA | NA | NA | NA | NA | NA |
| 185 | 0 | 0 | NA | 69 | 7 | NA | NA |
| 195 | 6 | 6 | 3 | 54 | 6 | 3 | 3 |
| 198 | NA | NA | NA | NA | NA | 3 | 3 |
| 201 | NA | NA | 4 | NA | NA | 0 | 0 |
| 203 | NA | NA | 0 | NA | NA | 3 | 4 |
| 205 | 0 | 0 | 3 | 39 | 6 | 0 | 0 |
| 208 | NA | NA | 0 | NA | NA | 0 | 0 |
| 213 | 0 | 0 | NA | 24 | 6 | NA | NA |
| 223 | 0 | 0 | NA | 13 | 0 | NA | NA |
| 233 | 0 | NA | NA | 10 | 0 | NA | NA |
| 241 | 0 | NA | NA | 10 | 6 | NA | NA |
| 249 | 0 | NA | NA | 9 | 0 | NA | NA |
| 267 | 10 | NA | NA | 55 | 13 | NA | NA |
| 280 | 19 | NA | NA | 30 | 2 | NA | NA |
| 301 | 7 | NA | NA | 25 | 38 | NA | NA |
| 311 | 9 | NA | NA | 67 | 18 | NA | NA |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 335 | 10 | NA | NA | 87 | 5 | NA | NA |
| 346 | 4 | NA | NA | 44 | 5 | NA | NA |
| 357 | NA | NA | NA | NA | NA | NA | NA |
| 370 | 9 | NA | NA | 14 | 18 | NA | NA |
| 380 | NA | NA | NA | NA | NA | NA | NA |
| 393 | NA | NA | NA | NA | NA | NA | NA |
| 401 | 2 | NA | NA | 3 | 2 | NA | NA |
| 412 | 0 | NA | NA | 2 | 0 | NA | NA |
| 432 | 0 | NA | NA | 0 | 0 | NA | NA |
| 440 | 0 | NA | NA | 0 | 0 | NA | NA |
| 449 | 0 | NA | NA | 0 | 0 | NA | NA |
| 462 | 0 | NA | NA | 0 | 0 | NA | NA |
| 470 | NA | NA | NA | NA | NA | NA | NA |
| 476 | NA | NA | NA | NA | NA | NA | NA |
| 493 | 0 | NA | NA | 27 | 0 | NA | NA |
| 514 | NA | NA | NA | NA | NA | NA | NA |
| 521 | 2 | NA | NA | 2 | 2 | NA | NA |
| 577 | NA | NA | NA | NA | NA | NA | NA |
| 588 | 2 | NA | NA | 2 | 2 | NA | NA |
| 598 | NA | NA | NA | NA | NA | NA | NA |
| 609 | 5 | NA | NA | 3 | 2 | NA | NA |
| 632 | NA | NA | NA | NA | NA | NA | NA |
| 644 | 4 | NA | NA | 4 | 3 | NA | NA |
| 647 | 40 | NA | NA | 4 | 3 | NA | NA |
| 650 | 4 | NA | NA | 4 | 0 | NA | NA |
| 652 | 0 | NA | NA | 3 | 0 | NA | NA |
| 654 | 0 | NA | NA | 3 | 0 | NA | NA |
| 657 | 0 | NA | NA | 4 | 0 | NA | NA |

**Table SI-7** Effluent sulfate concentrations relative to influent (μM) in the re-oxidation experiment (Sulfate=$Sulfate_{effluent}$- $Sulfate_{influent}$). NA indicates values not measured.

| Days since start of Re-oxidation | Sulfate (N-D1) | Sulfate (N-D2) | Sulfate (N-D3) | Sulfate (S-F1) | Sulfate (S-L1) | Sulfate (S-S/F) | Sulfate (X-L1) |
|---|---|---|---|---|---|---|---|
| 0 | -44 | -37 | NA | 6742 | 7210 | NA | NA |
| 1 | -12 | -12 | NA | 720 | 2993 | NA | NA |
| 2 | 0 | 9 | NA | 0 | 0 | NA | NA |
| 3 | 2 | 0 | NA | 3 | 0 | NA | NA |
| 5 | 0 | 0 | NA | 1 | 0 | NA | NA |
| 6 | 0 | 0 | NA | 7 | 0 | NA | NA |
| 8 | 0 | 0 | NA | 0 | 0 | NA | NA |
| 10 | 0 | 0 | NA | 0 | 0 | NA | NA |
| 13 | NA | NA | 0 | NA | NA | 236 | 0 |
| 14 | 0 | 0 | NA | 1 | 0 | NA | NA |
| 17 | 0 | 0 | NA | 1 | 0 | NA | NA |
| 21 | NA | NA | 0 | NA | NA | 0 | 0 |
| 22 | 0 | 0 | NA | 1 | 0 | NA | NA |
| 27 | 0 | 0 | NA | 0 | 0 | NA | NA |
| 31 | 0 | NA | NA | 0 | 0 | NA | NA |
| 36 | 0 | 0 | NA | 1 | 0 | NA | NA |
| 42 | -1 | 0 | NA | 1 | 0 | NA | NA |
| 44 | NA | NA | 1 | NA | NA | 0 | 0 |
| 50 | 0 | 0 | NA | 21 | 0 | NA | NA |
| 57 | 0 | 0 | NA | 133 | 2 | NA | NA |
| 65 | NA | NA | 0 | NA | NA | 0 | 0 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 66 | 0 | 0 | NA | 217 | 1 | NA | NA |
| 72 | NA | NA | 0 | NA | NA | 0 | 3 |
| 73 | 0 | 0 | NA | 274 | 1 | NA | NA |
| 79 | 0 | 0 | NA | 398 | 1 | NA | NA |
| 85 | 0 | 0 | NA | 482 | 4 | NA | NA |
| 97 | 0 | 1 | NA | 384 | 5 | NA | NA |
| 104 | 0 | 0 | NA | 308 | 2 | NA | NA |
| 112 | 0 | 0 | NA | 293 | 4 | NA | NA |
| 120 | 10 | 4 | NA | 762 | 4 | NA | NA |
| 128 | NA | NA | NA | NA | NA | 0 | 0 |
| 129 | -1 | 1 | NA | 786 | 5 | NA | NA |
| 139 | 2 | 1 | 0 | 717 | 1 | 0 | 0 |
| 149 | 0 | 0 | 0 | 577 | 0 | 0 | 0 |
| 157 | 0 | 0 | NA | 491 | 5 | NA | NA |
| 160 | NA | NA | 0 | NA | NA | 0 | 0 |
| 167 | 0 | 0 | NA | 418 | 2 | NA | NA |
| 176 | 0 | 11 | NA | 380 | 0 | NA | NA |
| 183 | NA | NA | NA | NA | NA | NA | NA |
| 185 | 0 | 0 | NA | 324 | 10 | NA | NA |
| 195 | 0 | 0 | 0 | 288 | 10 | 0 | 0 |
| 198 | NA | NA | NA | NA | NA | 0 | 0 |
| 201 | NA | NA | 0 | NA | NA | 0 | 0 |
| 203 | NA | NA | -22 | NA | NA | -22 | -21 |
| 205 | 0 | 0 | 0 | 230 | 9 | 0 | 0 |
| 208 | NA | NA | -1 | NA | NA | -1 | 0 |
| 213 | 1 | 0 | NA | 189 | -10 | NA | NA |
| 223 | 0 | 0 | NA | 144 | 0 | NA | NA |
| 233 | 0 | NA | NA | 118 | 1 | NA | NA |
| 241 | 0 | NA | NA | 108 | 2 | NA | NA |
| 249 | 1 | NA | NA | 85 | 4 | NA | NA |
| 267 | 62 | NA | NA | 138 | 24 | NA | NA |
| 280 | 40 | NA | NA | 32 | 1 | NA | NA |
| 301 | 1 | NA | NA | 26 | 0 | NA | NA |
| 311 | 2 | NA | NA | 21 | 0 | NA | NA |
| 335 | 0 | NA | NA | 14 | 0 | NA | NA |
| 346 | 0 | NA | NA | 16 | 0 | NA | NA |
| 357 | NA | NA | NA | NA | NA | NA | NA |
| 370 | 0 | NA | NA | 20 | 0 | NA | NA |
| 380 | NA | NA | NA | NA | NA | NA | NA |
| 393 | NA | NA | NA | NA | NA | NA | NA |
| 401 | 0 | NA | NA | 20 | 0 | NA | NA |
| 412 | NA | NA | NA | NA | NA | NA | NA |
| 432 | NA | NA | NA | NA | NA | NA | NA |
| 440 | -6 | NA | NA | 9 | -6 | NA | NA |
| 449 | 0 | NA | NA | 11 | 0 | NA | NA |
| 462 | 0 | NA | NA | 12 | 0 | NA | NA |
| 470 | NA | NA | NA | NA | NA | NA | NA |
| 476 | NA | NA | NA | NA | NA | NA | NA |
| 493 | 0 | NA | NA | 12 | 0 | NA | NA |
| 514 | NA | NA | NA | NA | NA | NA | NA |
| 521 | 0 | NA | NA | 11 | 0 | NA | NA |
| 577 | NA | NA | NA | NA | NA | NA | NA |
| 588 | 0 | NA | NA | 10 | 0 | NA | NA |
| 598 | NA | NA | NA | NA | NA | NA | NA |
| 609 | 1 | NA | NA | 11 | 0 | NA | NA |
| 632 | NA | NA | NA | NA | NA | NA | NA |
| 644 | 0 | NA | NA | 11 | 0 | NA | NA |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 647 | 0 | NA | NA | 11 | 0 | NA | NA |
| 650 | 0 | NA | NA | 10 | 0 | NA | NA |
| 652 | -22 | NA | NA | -12 | -22 | NA | NA |
| 654 | 0 | NA | NA | 10 | 0 | NA | NA |
| 657 | 1 | NA | NA | 10 | 0 | NA | NA |