

Geochemical Equilibrium Modelling of the Aqueous Speciation of Select Trace Elements in the Great Lakes

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SUPPORTING INFORMATION

Table S1. Connecting channel hydrochemistry used in simulations.

| | St Marys River [n=5] | | St Clair River [n=5] | | Detroit River [n=4] | | Niagara River [n=5] | | St. Lawrence River [n=4] | |
|------------------|-------------------------|-------|-------------------------|-------|------------------------|-------|------------------------|-------|-----------------------------|-------|
| Parameter | Average | Stdev | Average | Stdev | Average | Stdev | Average | Stdev | Average | Stdev |
| pH | 7.3 | 0.05 | 7.4 | 0.04 | 7.4 | 0.03 | 7.4 | 0.04 | 7.5 | 0.01 |
| ORP | 193 | 17 | 186 | 13 | 183 | 15 | 172 | 16 | 175 | 8 |
| ppm | | | | | | | | | | |
| Dissolved Oxygen | 8.90 | 0.3 | 6.30 | 1.04 | 6.35 | 1.06 | 5.77 | 0.45 | 5.55 | 0.35 |
| Temperature | 23.3 | 1.3 | 22.2 | 0.9 | 23.5 | 0.4 | 25.0 | 1.2 | 25.3 | 2.2 |
| Alkalinity | 41 | 6 | 86 | 8 | 96 | 12 | 133 | 5 | 133 | 2 |
| Chloride | 1.9 | 0.8 | 9.1 | 0.3 | 11.9 | 1.4 | 16.4 | 0.2 | 17.1 | 0.5 |
| Sulfate | 3.2 | 0.1 | 12.4 | 0.2 | 13.2 | 0.6 | 15.8 | 0.1 | 17.2 | 0.9 |
| Na | 1.4 | 0.1 | 4.9 | 0.1 | 3.9 | 0.1 | 8.6 | 2 | 11.6 | 1.6 |
| Mg | 2.8 | 0.1 | 7.5 | 0.8 | 7.5 | 0.5 | 8.9 | 1 | 8.5 | 1 |
| K | 0.5 | 0.04 | 1.4 | 0.1 | 0.9 | 0.1 | 1.4 | 0.01 | 2.0 | 0.2 |
| Ca | 14 | 1 | 26 | 2 | 26 | 3 | 32 | 3 | 32 | 3 |
| ppb | | | | | | | | | | |
| Phosphate | 6.0 | 0.1 | 6.6 | 0.1 | 8.6 | 0.2 | 6.9 | 0.1 | 6.6 | 0.1 |
| Li | 0.2 | 0.06 | 0.3 | 0.18 | 0.5 | 0.07 | 1.6 | 0.11 | 1.1 | 0.06 |
| Be | 0.11 | 0.2 | 0.05 | 0.09 | 0.01 | 0.01 | 0.01 | 0.01 | 0.35 | 0.24 |
| Al | 25.8 | 10.3 | 5.7 | 2.1 | 9.6 | 2.7 | 16.7 | 11.7 | 8.9 | 2.5 |
| Si | 4064 | 1309 | 1189 | 721 | 637 | 170 | 800 | 138 | n/a | n/a |
| Sc | 0.12 | 0.20 | 0.09 | 0.15 | n/a | n/a | n/a | n/a | 0.54 | 0.06 |
| Ti | 0.6 | 0.2 | 0.3 | 0.1 | 0.4 | 0.1 | 0.3 | 0.03 | 0.7 | 0.2 |
| V | 0.4 | 0.27 | 0.2 | 0.15 | 0.4 | 0.08 | 0.3 | 0.02 | 0.7 | 0.3 |
| Cr | 0.4 | 0.17 | 0.2 | 0.12 | 0.2 | 0.03 | 0.2 | 0.09 | 0.5 | 0.27 |
| Mn | 5.1 | 1.1 | 0.4 | 0.16 | 0.8 | 0.2 | 2.6 | 1.7 | 3.5 | 2.9 |
| Fe | 71 | 44 | 5 | 1 | 17 | 11 | 114 | 152 | 31 | 17 |
| Co | 0.13 | 0.22 | 0.06 | 0.13 | 0.02 | 0.003 | 0.02 | 0.004 | 0.41 | 0.27 |
| Ni | 1.3 | 0.9 | 0.3 | 0.2 | 0.4 | 0.07 | 0.8 | 0.03 | 1.3 | 0.19 |
| Cu | 2.5 | 1.5 | 0.5 | 0.17 | 0.9 | 0.26 | 1.7 | 0.86 | 1.7 | 0.22 |
| Zn | 4.8 | 1.7 | 2.4 | 1.2 | 6.6 | 2.8 | 17.6 | 8.7 | 8.0 | 0.13 |
| Ge | 0.15 | 0.2 | 0.14 | 0.18 | n/a | n/a | 0.01 | 0.01 | 0.62 | 0.05 |
| As | 0.5 | 0.2 | 0.4 | 0.2 | 0.7 | 0.09 | 1.0 | 0.02 | 1.3 | 0.3 |
| Se | 0.3 | 0.6 | 0.4 | 0.1 | n/a | n/a | 0.04 | 0.01 | 0.6 | 0.12 |
| Rb | 1.26 | 0.27 | 0.84 | 0.21 | 0.88 | 0.03 | 1.11 | 0.03 | 1.43 | 0.25 |
| Sr | 13 | 2.5 | 12 | 5.8 | 24 | 3.5 | 181 | 19 | 84 | 43 |
| Y | 0.19 | 0.18 | 0.06 | 0.12 | 0.03 | 0.016 | 0.02 | 0.004 | 0.41 | 0.27 |
| Zr | 0.12 | 0.11 | 0.12 | 0.14 | n/a | n/a | n/a | n/a | 0.37 | 0.26 |

Table S1, cont.

| | St Marys River [n=5] | | St Clair River [n=5] | | Detroit River [n=4] | | Niagara River [n=5] | | St. Lawrence River [n=4] | |
|-----------|-------------------------|-------|-------------------------|-------|------------------------|-------|------------------------|-------|-----------------------------|-------|
| Parameter | Average | Stdev | Average | Stdev | Average | Stdev | Average | Stdev | Average | Stdev |
| Mo | 0.27 | 0.26 | 0.35 | 0.26 | 0.66 | 0.09 | 1.17 | 0.04 | 1.40 | 0.3 |
| Ag | 0.013 | 0.02 | 0.07 | 0.01 | 0.003 | 0.001 | 0.002 | 0.001 | 0.43 | 0.1 |
| Cd | 0.01 | 0.02 | 0.06 | 0.03 | 0.01 | 0.003 | 0.01 | 0.001 | 0.04 | 0.06 |
| In | 0.09 | 0.01 | 0.09 | n/a | n/a | n/a | n/a | n/a | 0.01 | 0.01 |
| Sn | 0.01 | 0.024 | 0.07 | 0.03 | 0.02 | 0.004 | 0.02 | 0.004 | 0.04 | 0.01 |
| Sb | 0.5 | 0.47 | 0.7 | 0.42 | 1.3 | 0.15 | 0.2 | 0.08 | 0.6 | 0.16 |
| Cs | 0.13 | 0.11 | 0.06 | 0.13 | 0.02 | 0.01 | 0.02 | 0.001 | 0.04 | 0.01 |
| Ba | 7 | 1.9 | 4 | 4 | 9 | 0.6 | 22 | 1.4 | 16 | 13 |
| La | 0.03 | 0.01 | 0.05 | 0.01 | 0.01 | 0.003 | 0.02 | 0.02 | 0.04 | 0.02 |
| Ce | 0.01 | 0.02 | 0.03 | 0.01 | 0.02 | 0.006 | 0.03 | 0.03 | 0.01 | 0.03 |
| Pr | n/a | n/a | 0.051 | 0.02 | 0.002 | 0.001 | 0.004 | 0.002 | n/a | n/a |
| Nd | 0.03 | 0.02 | 0.06 | 0.02 | 0.01 | 0.005 | 0.02 | 0.008 | 0.04 | 0.02 |
| Sm | 0.01 | 0.02 | 0.005 | 0.01 | 0.04 | 0.04 | 0.002 | 0.001 | 0.01 | 0.004 |
| Eu | 0.01 | 0.01 | 0.02 | 0.01 | 0.01 | 0.007 | 0.001 | n/a | 0.06 | 0.001 |
| Gd | 0.01 | 0.01 | 0.004 | 0.01 | 0.02 | 0.02 | 0.004 | 0.001 | 0.04 | 0.005 |
| Tb | 0.001 | 0.002 | 0.01 | 0.01 | 0.001 | 0.001 | n/a | n/a | 0.003 | 0.001 |
| Dy | 0.005 | 0.002 | 0.005 | 0.002 | 0.004 | 0.003 | 0.002 | 0.001 | 0.004 | 0.003 |
| Ho | 0.002 | 0.002 | 0.004 | n/a | 0.001 | n/a | n/a | n/a | 0.001 | n/a |
| Er | 0.001 | 0.001 | 0.001 | n/a | 0.002 | 0.001 | 0.001 | n/a | n/a | n/a |
| Tm | 0.001 | 0.001 | 0.005 | 0.001 | n/a | n/a | n/a | n/a | n/a | n/a |
| Yb | 0.003 | 0.002 | 0.01 | 0.01 | 0.001 | n/a | 0.002 | n/a | 0.004 | 0.002 |
| Lu | n/a | n/a | 0.002 | 0.002 | n/a | n/a | n/a | n/a | n/a | n/a |
| Hf | 0.01 | 0.02 | 0.002 | n/a | n/a | n/a | n/a | n/a | 0.05 | n/a |
| Ta | 0.03 | 0.03 | 0.02 | 0.01 | n/a | n/a | n/a | n/a | 0.01 | n/a |
| W | 0.02 | 0.02 | 0.01 | 0.01 | 0.01 | 0.001 | 0.04 | 0.01 | 0.04 | 0.02 |
| Pb | 0.22 | 0.04 | 0.12 | 0.16 | 0.12 | 0.04 | 0.15 | 0.03 | 0.45 | 0.18 |
| Tl | 0.01 | 0.07 | 0.01 | 0.01 | 0.005 | 0.001 | 0.01 | 0.001 | 0.03 | 0.06 |
| Bi | 0.11 | 0.04 | 0.05 | 0.02 | 0.002 | n/a | 0.002 | 0.001 | 0.35 | 0.001 |
| Th | 0.12 | 0.02 | 0.16 | 0.16 | n/a | n/a | n/a | n/a | 0.05 | 0.04 |
| U | 0.26 | 0.14 | 0.24 | 0.11 | 0.22 | 0.16 | 0.32 | 0.08 | 0.64 | 0.28 |

Table S2. Extrapolated parameters used in simulations (relative to 2021 data).

| Lake | Connecting Channel | 2050 | 2100 |
|--------------------|---------------------------|--------------------------------|-------------|
| | | <i>Alkalinity [ppb]</i> | |
| Superior | St Mary's | +580 | +1,580 |
| Huron | St Clair, Detroit | +1,131 | +3,081 |
| East Erie, Ontario | Niagara, St. Lawrence | +4,321 | +11,771 |
| | | <i>Phosphate [ppb]</i> | |
| Superior | St. Mary's | 5 | |
| Huron | St. Clair, Detroit | 5 | |
| East Erie, Ontario | Niagara, St. Lawrence | 10 | |
| | | <i>Chloride [ppb]</i> | |
| Superior | St. Mary's | +186 | +506 |
| Huron | St. Clair, Detroit | +1,183 | +3,223 |
| East Erie, Ontario | Niagara, St. Lawrence | +4,503 | +12,269 |