Developing a hydrogeochemical model for implementation in SWAT model at a global scale

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Presenter: Juan Luis Lechuga-Crespo

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Background

EARTH SYSTEM

- Air
- Water
- Rocks
- Energy
- Biodiversity

Proper time for hydrologic system

Tectonic system
Hydrologic system

Understanding processes in a proper spatial and temporal scale

Modelling

Resource management and impact assessment

Environmental hazards (Climate Change, Intensive Agriculture, etc.)

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Background

“(…) SWAT was developed to predict the impact of land management practices on water, sediment and agricultural chemical yields in large complex watersheds with varying soil, land use and management conditions over long periods of time.” (SWAT Theoretical Documentation 2009)

+ Climate Change applications

Alteration of biogeochemical cycles

↑ CO2 sequestration in soils and surface water

↑ Salinity of water

Hydrogeochemical model

SWAT + WHAM (Garneau, 2014)

Complex equations

Need for a simpler approach

Empirical equations

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Hypothesis and Objective

**H1.** Rocks classified in different lithological groups, according to their sensibility to chemical weathering, may be used to describe the composition of water in river streams, as each class is expected to drain a certain composition of water.

**H2.** Land cover, topography, and hydrology are other groups of variables which are expected to act with synergies and antagonisms regarding chemical weathering, though impacting the chemical composition found in the river streams.

**Objective.** Obtain several equations, with “simple” parameters, that allow for the assessment of water major ion chemical composition.
Correlation: Significant correlations according to Pearson’s coefficient.
Validation: Cross Validation with 10 folds on the database.
Database description

Databases
GLiM (Global Lithological Map)
GLORICH (GLObal River Chemistry database)


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Database setup

Data subset:
- Search for “natural” samples
  - Chloride concentration $[\text{Cl}^-] < 30 [\text{mg} \cdot \text{L}^{-1}]$
  - Samples with Ca$^{2+}$, Mg$^{2+}$, K$^+$, Na$^+$, Cl$^-$ concentration data

Database with 431506 samples on 5368 sampling locations

Data aggregation:
- Aggregation to a single value for sampling location

Derived variables:
- Total chemical fluxes
- River chemical flux and atmosphere chemical flux
  - Cl$^-$ acts like a tracer from atmospheric deposition

Derivation: $X_{\text{corrected}} = X - (K_x \cdot \text{Cl}_{\text{atm}}) \cdot \frac{P}{Q}$

(Meybeck, 1984)

$X \left[ \frac{\text{mmol}}{\text{L}} \right]$ Concentration of X element
$K_x [-]$ Ratio over Cl$^-$ concentration
$\text{Cl}_{\text{atm}} \left[ \frac{\text{mmol}}{\text{L}} \right]$ Atmospheric concentration of Cl$^-$
$P \left[ \frac{\text{mm}}{\text{mm}} \right]$ Precipitation
$Q \left[ \frac{\text{mm}}{\text{mm}} \right]$ River discharge

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Data exploration

Significant correlation ($p < 0.01$, Pearson) found between chemical fluxes and:

<table>
<thead>
<tr>
<th>Description</th>
<th>Variable</th>
<th>Unit</th>
<th>SWAT?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual discharge</td>
<td>Q</td>
<td>mm</td>
<td></td>
</tr>
<tr>
<td>Sub-basin slope</td>
<td>Slp</td>
<td>%</td>
<td></td>
</tr>
<tr>
<td>Sub-basin altitude</td>
<td>H</td>
<td>m</td>
<td></td>
</tr>
<tr>
<td>Soil pH</td>
<td>Soil_Ph</td>
<td>(pH units)</td>
<td></td>
</tr>
<tr>
<td>Soil Organic Carbon</td>
<td>SOC</td>
<td>g C·kg$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>Dust deposition</td>
<td>D</td>
<td>g C·kg$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>Vegetal Coverture</td>
<td>VCI</td>
<td>%</td>
<td></td>
</tr>
<tr>
<td>Lithological coverture</td>
<td>L</td>
<td>%</td>
<td></td>
</tr>
<tr>
<td>Annual precipitation</td>
<td>P</td>
<td>mm</td>
<td></td>
</tr>
</tbody>
</table>

- **Directly obtained**
- **Needs extra info**

*Number of samples considered, $n = 5368$*

Models to test

\[
F_{X_{corrected}} = q \cdot C_X + \text{cte}
\]

(1)

\[
F_{X_{corrected}} = q \cdot \sum (C_{X_i} \cdot L_i) + \text{cte}
\]

(2)

\[
F_{X_{corrected}} = q \cdot \text{Slope} \cdot \sum (C_{X_i} \cdot L_i) + \text{cte}
\]

(3)

\[
F_{X_{corrected}} = q \cdot \exp \left( \frac{\text{Slope}}{\text{Altitude}} \right) \cdot \sum (C_{X_i} \cdot L_i) + \text{cte}
\]

(3.1)

\[
F_{X_{corrected}} = q \cdot \frac{\text{GLC}_{\text{Forest}}}{\text{GLC}_{\text{Managed}}} \cdot \exp \left( \frac{\text{Slope}}{\text{Altitude}} \right) \cdot \sum (C_{X_i} \cdot L_i) + \text{cte}
\]

(3.2)

\[
F_{X_{corrected}} = q \cdot \exp \left( \frac{\text{Slope}}{\text{Altitude}} \right) \cdot \text{Soil wetness} \cdot \sum (C_{X_i} \cdot L_i) + \text{cte}
\]

(4)

\[
F_{X_{corrected}} = q \cdot \text{Soil wetness} \cdot \sum (C_{X_i} \cdot L_i) + \text{cte}
\]

(5)

\[
F_{X_{corrected}} = q \cdot \exp \left( \frac{\text{Slope}}{\text{Altitude}} \right) \cdot \text{Soil wetness} \cdot \frac{\text{GLC}_{\text{Forest}}}{\text{GLC}_{\text{Managed}}} \sum (C_{X_i} \cdot L_i) + \text{cte}
\]

(5.1)

Problem with the units!
Model development

Cross-validation

Overall, best model found for the Global database. However, performance is poor for all the cases.

<table>
<thead>
<tr>
<th>Model #</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>31</th>
<th>32</th>
<th>4</th>
<th>5</th>
<th>51</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>0.11</td>
<td>0.44</td>
<td>0.22</td>
<td>0.43</td>
<td>0.41</td>
<td>0.42</td>
<td>0.42</td>
<td>0.4</td>
</tr>
<tr>
<td>Mg</td>
<td>0.15</td>
<td>0.27</td>
<td>0.22</td>
<td>0.27</td>
<td>0.22</td>
<td>0.21</td>
<td>0.21</td>
<td>0.18</td>
</tr>
<tr>
<td>Na</td>
<td>0.18</td>
<td>0.17</td>
<td>0.08</td>
<td>0.19</td>
<td>0.13</td>
<td>0.13</td>
<td>0.13</td>
<td>0.11</td>
</tr>
<tr>
<td>K</td>
<td>0.23</td>
<td>0.31</td>
<td>0.25</td>
<td>0.31</td>
<td>0.28</td>
<td>0.26</td>
<td>0.26</td>
<td>0.24</td>
</tr>
</tbody>
</table>

\[
q \left[ \frac{L}{m^2 \cdot y} \right] \quad \text{Hydrological and temporal driver}
\]

\[
\exp \left( \frac{\text{Slope} [^\circ]}{\text{Altitude} [m]} \right) \quad \text{Factor with hydromorphological description}
\]

\[
\sum \left( C_{X_i} \left[ \frac{\text{mmol}}{L} \right] \cdot L_i [%] \right)
\]

The parameters to fit here are the concentration of each draining lithology

\[
c_{te} \left[ \frac{\text{mmol}}{m^2 \cdot y} \right] \quad \text{This constant needs further study}
\]

\[
F_{X_{\text{corrected}}} \left[ \frac{\text{mmol}}{m^2 \cdot y} \right] = q \left[ \frac{L}{m^2 \cdot y} \right] \cdot \exp \left( \frac{\text{Slope} [^\circ]}{\text{Altitude} [m]} \right) \cdot \sum \left( C_{X_i} \left[ \frac{\text{mmol}}{L} \right] \cdot L_i [%] \right) + c_{te} \left[ \frac{\text{mmol}}{m^2 \cdot y} \right]
\]
Model development

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Model development

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Conclusions

**H1.** Rocks classified in different lithological groups, according to their sensibility to chemical weathering, may be used to describe the composition of water in river streams, as each class is expected to drain a certain composition of water.

**C1.** Inclusion of lithological proportions on model development improved the Pearson’s correlation coefficient, implying that the contribution to the total flux is different.

**H2.** Land coverture, topography, and hydrology are other groups of variables which are expected to act with synergies and antagonisms regarding chemical weathering, though impacting the chemical composition found in the river streams.

**C2.** The inclusion of the correction factor considering altitude and slope improved the Pearson’s correlation coefficient as well, implying that the hydromorphological characteristics of the draining basin affect the chemical fluxes.
Future work

• Assess different model configurations for each of the elements according to their particular significant correlations

• Spatially distribute the terms in the equation, so sub-basin parameters can be properly taken in account

• Once the equations are set for each element, verify them using extra catchment cases.
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Thank you! Merci! Dank je!

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