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

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Background

Air
Water
Rocks
Energy
Biodiversity

EARTH SYSTEM

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

Proper time for hydrologic system

Tectonic system
Hydrologic system

Understanding processes in a proper spatial and temporal scale

Modelling

Resource management and impact assessment

SWAT
Soil & Water Assessment Tool

Background

SWAT
Soil & Water Assessment Tool

"(…) 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

↑ CO_2 sequestration in soils and surface water

↑ Salinity of water

SWAT + WHAM (Garneau, 2014)

Complex equations

Need for a simpler approach

Empirical equations

Hydrogeochemical model

Hypothesis and Objective

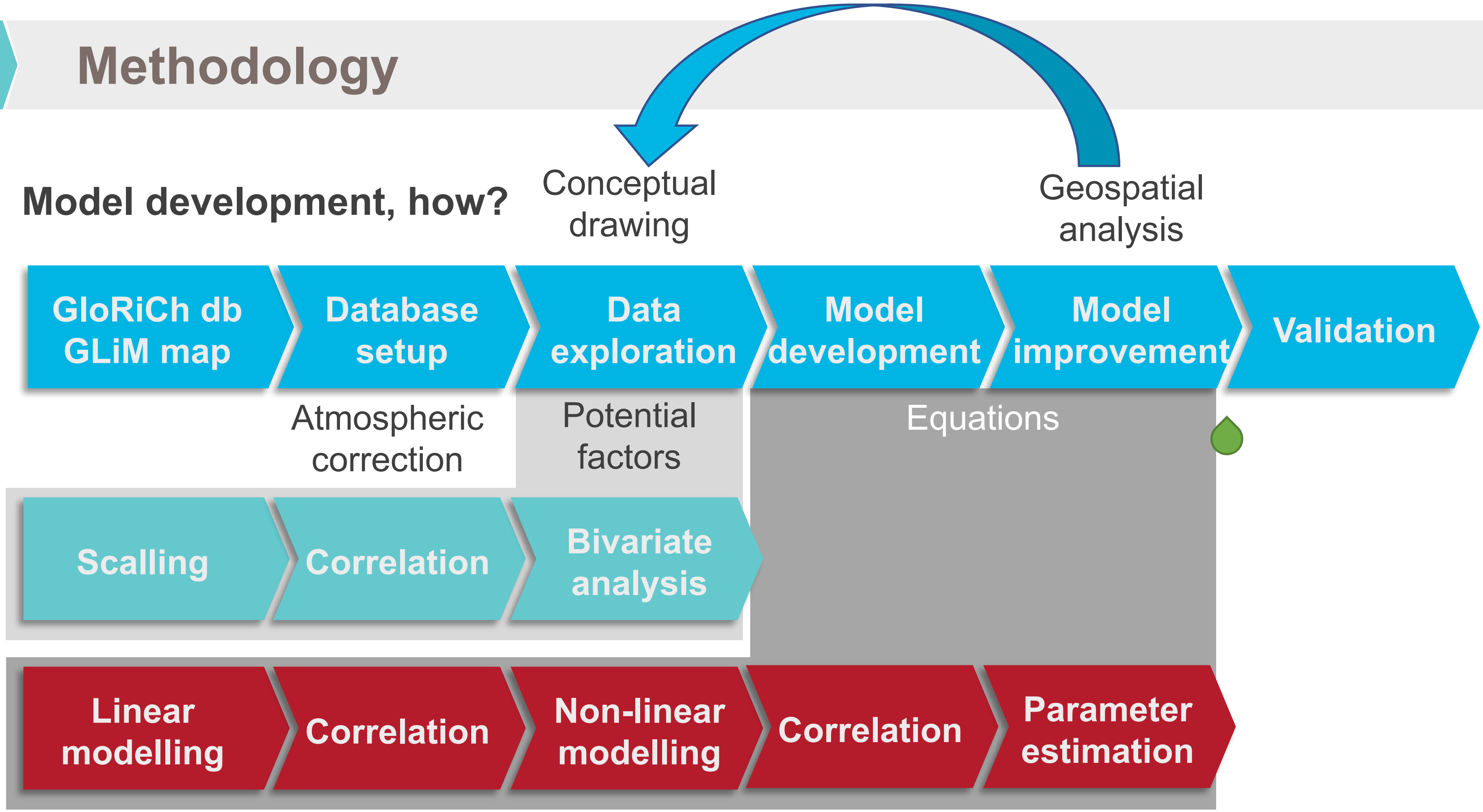
H1. Rocks classified in different lithological groups, according to their sensibility to chemical weathering, may be used to describe the composition of water in river streams, as each class is expected to drain a certain composition of water.

H2. Land 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.

Objective. Obtain several equations, with “simple” parameters, that allow for the assessment of water major ion chemical composition.

Methodology

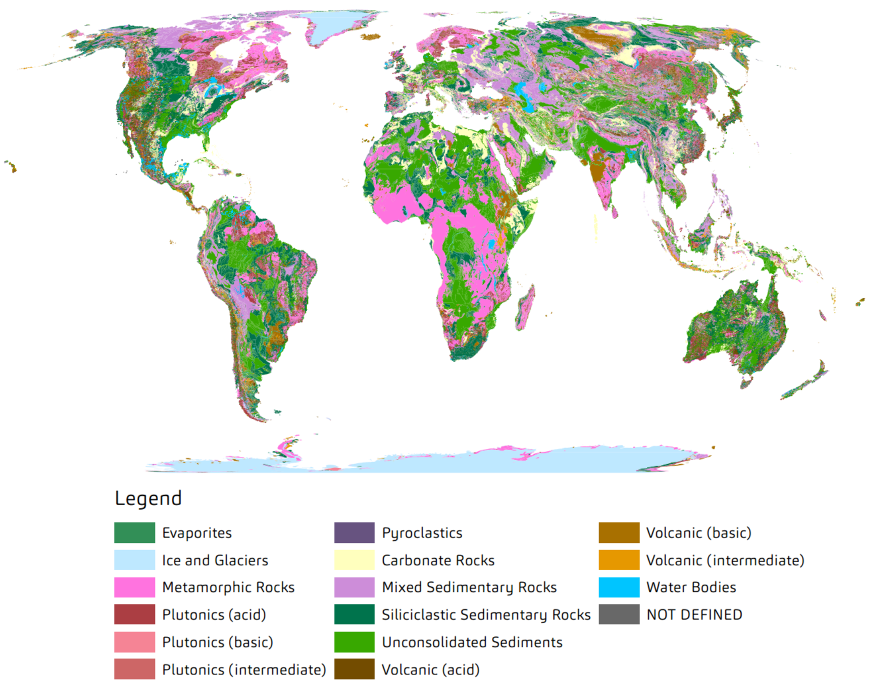
Model development, how?

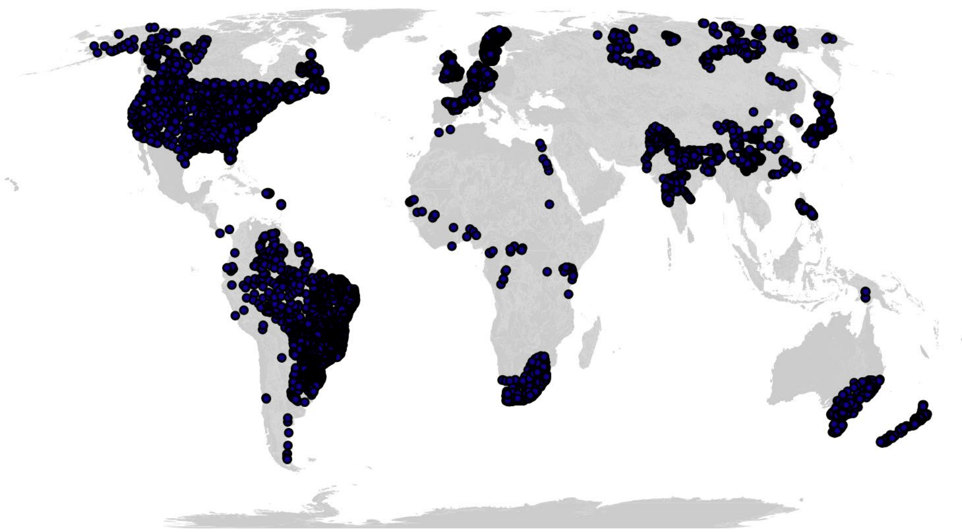


Correlation: Significant correlations according to Pearson's coefficient.
Validation: Cross Validation with 10 folds on the database.

Database description

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





Hartmann, J., and N. Moosdorf (2012), The new global lithological map database GLiM: A representation ofrock properties at the Earth surface, Geochem. Geophys. Geosyst., 13, Q12004, doi:10.1029/2012GC004370.

Hartmann, J., Lauerwald, R. and Moosdorf, N. (2014), A brief overview of the GLObal River Chemistry Database GLORICH, Procedia Earth and Planetary Science, doi:10.1016/j.proeps.2014.08.005.

Database setup

Data subset:

- Search for "natural" samples
  - Chloride concentration
    $[\mathrm{Cl}^-] < 30[\mathrm{mg} \cdot \mathrm{L}^{-1}]$
  - Samples with Ca^{2+}, Mg^{2+}, K^+, Na^+, Cl^- concentration data

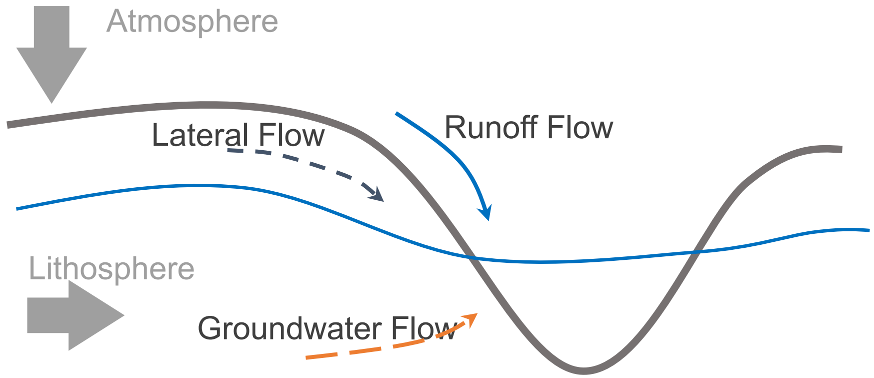
Database with 431506 samples on 5368 sampling locations

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



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

(Meybeck, 1984)

$X\left[\frac{\mathrm{mmol}}{\mathrm{L}}\right]$ Concentration of X element

$K_x[-]$ Ratio over Cl^- concentration

$\mathrm{Cl}_{\mathrm{atm}}\left[\frac{\mathrm{mmol}}{\mathrm{L}}\right]$ Atmospheric concentration of Cl^-

$P[mm]$ Precipitation

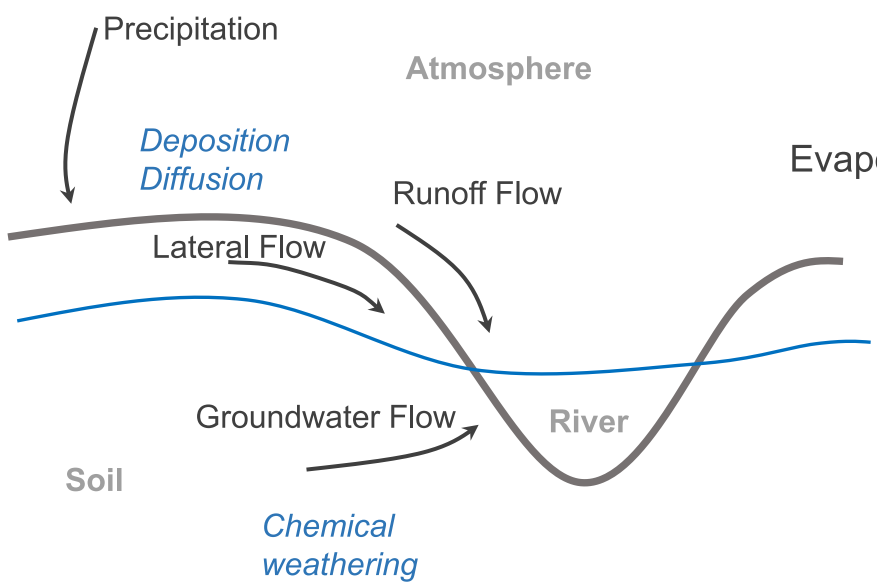
$Q[mm]$ River discharge

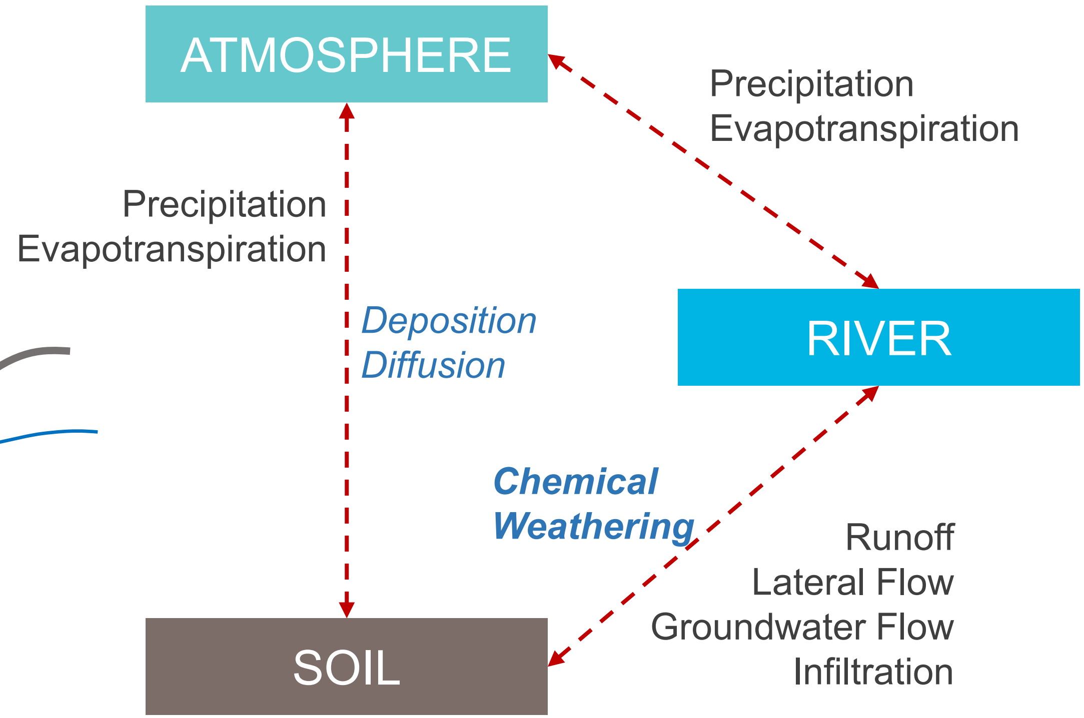
Meybeck, Michel (1984): Les fleuves et le cycle geochimique des elements. Thèse d'état. Universite Pierre et Marie Curie, Paris. Ecole Normale Superieure (ULM).

Data exploration

Conceptual draw

Conceptual model





Data exploration

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

Description	Variable	Unit	SWAT?
Annual discharge	Q	mm	Directly obtained
Sub-basin slope	Slp	%	Directly obtained
Sub-basin altitude	H	m	Directly obtained
Soil pH	Soil_Ph	(pH units)	Needs extra info
Soil Organic Carbon	SOC	$g\ C \cdot kg^{-1}$	Needs extra info
Dust deposition	D	$g\ C \cdot kg^{-1}$	Needs extra info
Vegetal Coverture	VCI	%	Needs extra info
Lithological coverture	L	%	Needs extra info
Annual precipitation	P	mm	Directly obtained

Directly obtained   Needs extra info

Number of samples considered, n = 5368

Models to test

(1) $$F_{X_{corrected}} = q \cdot C_X + cte$$

(2) $$F_{X_{corrected}} = q \cdot \sum (C_{X_i} \cdot L_i) + cte$$

(3) $$\boxed{F_{X_{corrected}} = q \cdot Slope \cdot \sum (C_{X_i} \cdot L_i) + cte}$$

Problem with the units!

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

(3.2) $$F_{X_{corrected}} = q \cdot \frac{GLC_{Forest}}{GLC_{Managed}} \cdot \exp\left(\frac{Slope}{Altitude}\right) \cdot \sum (C_{X_i} \cdot L_i) + cte$$

(4) $$F_{X_{corrected}} = q \cdot \exp\left(\frac{Slope}{Altitude}\right) \cdot Soil_{wetness} \cdot \sum (C_{X_i} \cdot L_i) + cte$$

(5) $$F_{X_{corrected}} = q \cdot Soil_{wetness} \cdot \sum (C_{X_i} \cdot L_i) + cte$$

(5.1) $$F_{X_{corrected}} = q \cdot \exp\left(\frac{Slope}{Altitude}\right) \cdot Soil_{wetness} \cdot \frac{GLC_{Forest}}{GLC_{Managed}} \sum (C_{X_i} \cdot L_i) + cte$$

Model development

Cross-validation

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

Coefficient of determination after CV (k=10)								
Model #	**1**	**2**	**3**	**31**	**32**	**4**	**5**	**51**
Ca	0.11	0.44	0.22	**0.43**	0.41	0.42	0.42	0.4
Mg	0.15	0.27	0.22	**0.27**	0.22	0.21	0.21	0.18
Na	0.18	0.17	0.08	**0.19**	0.13	0.13	0.13	0.11
K	0.23	0.31	0.25	**0.31**	0.28	0.26	0.26	0.24

$$q\left[\frac{\mathrm{L}}{\mathrm{m}^2\cdot\mathrm{y}}\right]$$

Hydrological and temporal driver

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

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

$$\exp\left(\frac{\mathrm{Slope}\ [º]}{\mathrm{Altitude}\ [\mathrm{m}]}\right)$$

Factor with hydromorphological description

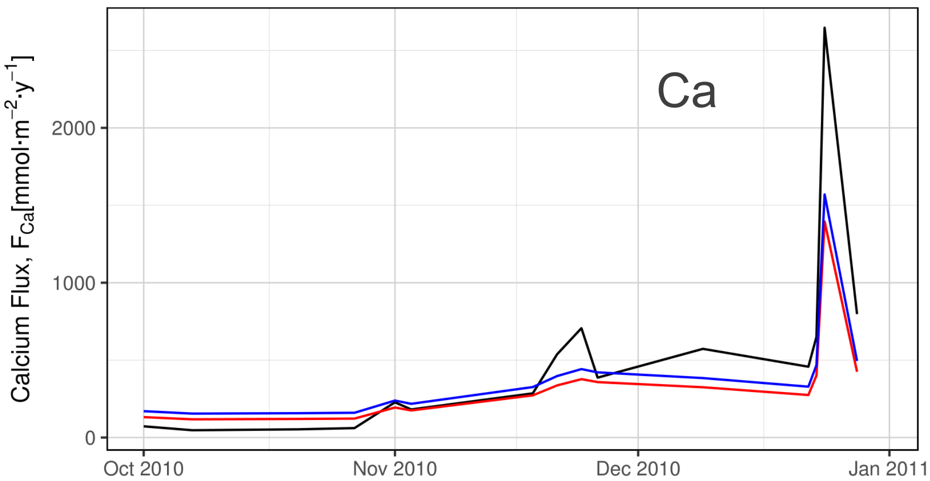
$$\mathrm{cte}\left[\frac{\mathrm{mMol}}{\mathrm{m}^2\cdot\mathrm{y}}\right]$$

This constant needs further study

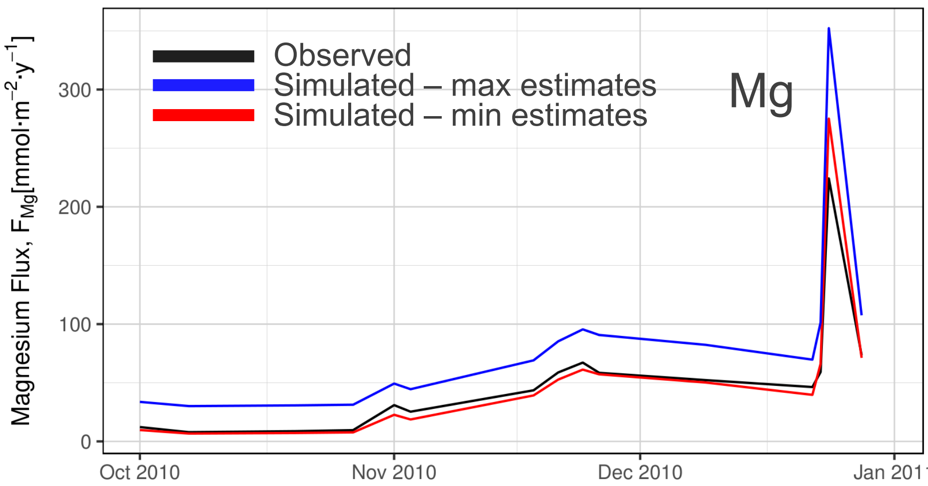
$$\boxed{\mathbf{F}_{\mathbf{X}_{\mathbf{corrected}}}\left[\frac{\mathrm{mMol}}{\mathrm{m}^2\cdot\mathrm{y}}\right]=\mathbf{q}\left[\frac{\mathrm{L}}{\mathrm{m}^2\cdot\mathrm{y}}\right]\cdot\mathbf{exp}\left(\frac{\mathbf{Slope}\ [º]}{\mathbf{Altitude}\ [\mathrm{m}]}\right)\cdot\sum\left(\mathbf{C}_{\mathbf{X_i}}\left[\frac{\mathrm{mmol}}{\mathrm{L}}\right]\cdot\mathbf{L_i}[\%]\right)+\mathbf{cte}\left[\frac{\mathrm{mMol}}{\mathrm{m}^2\cdot\mathrm{y}}\right]}$$

Model development

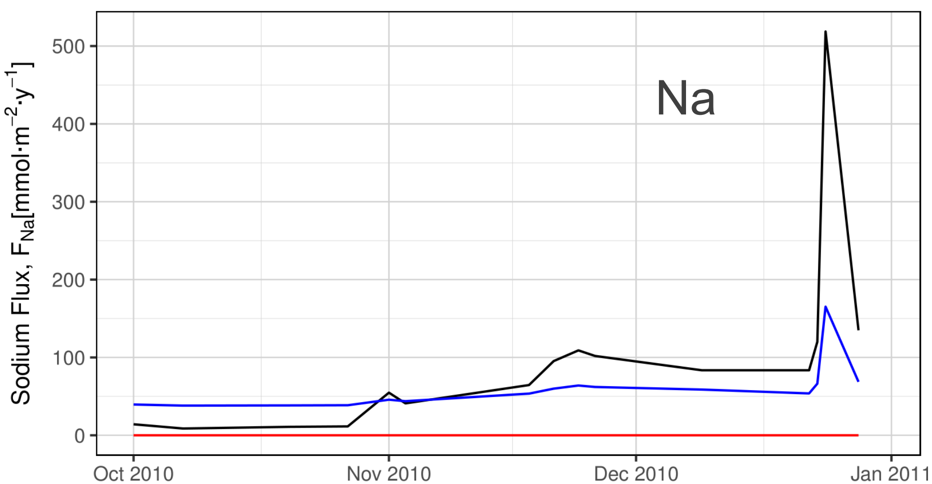
Temporal series at Alegria Catchment



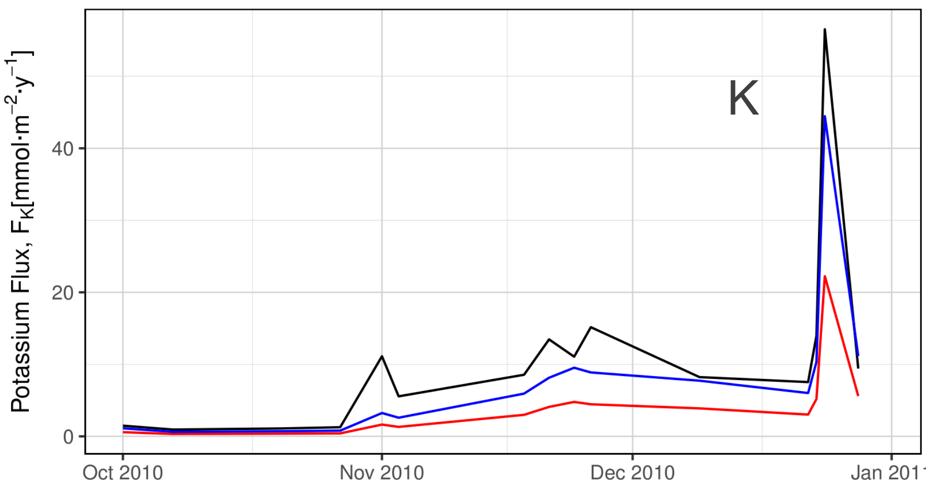
Temporal series at Alegria Catchment



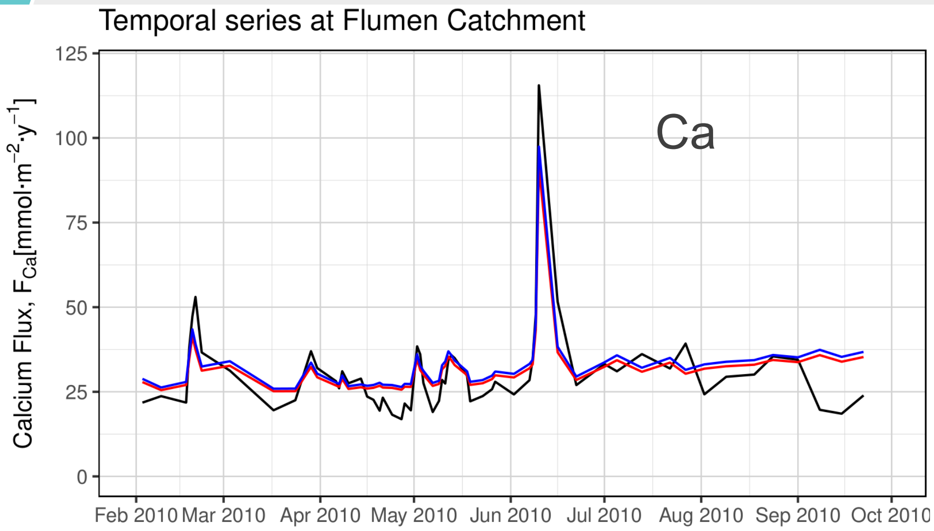
Temporal series at Alegria Catchment

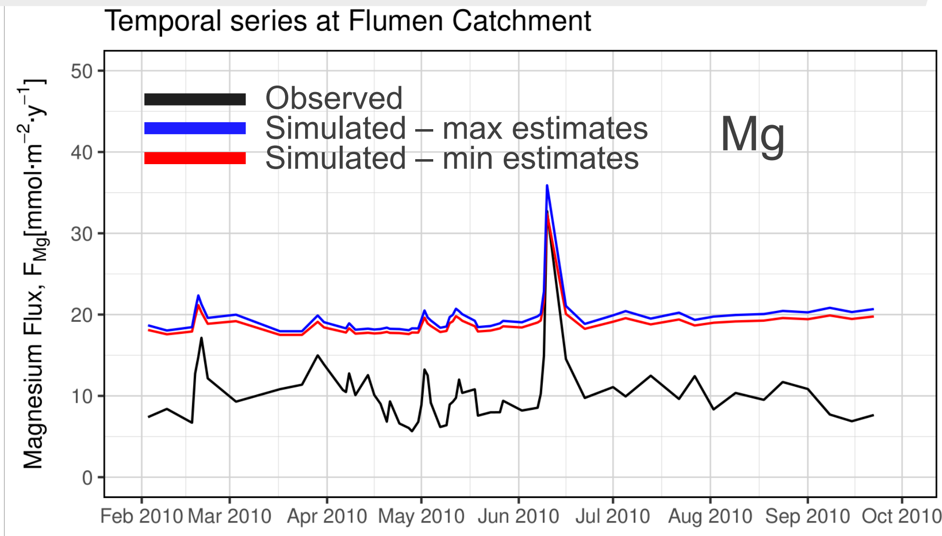


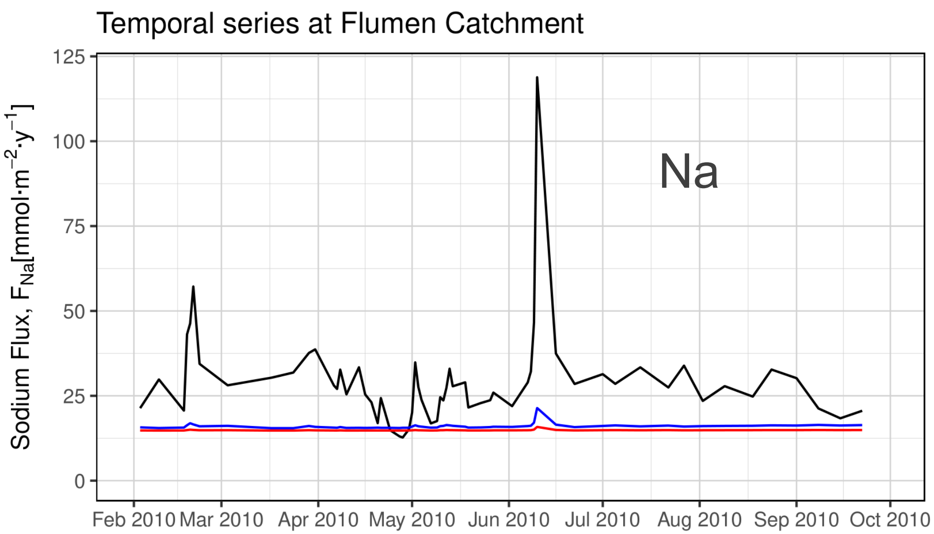
Temporal series at Alegria Catchment

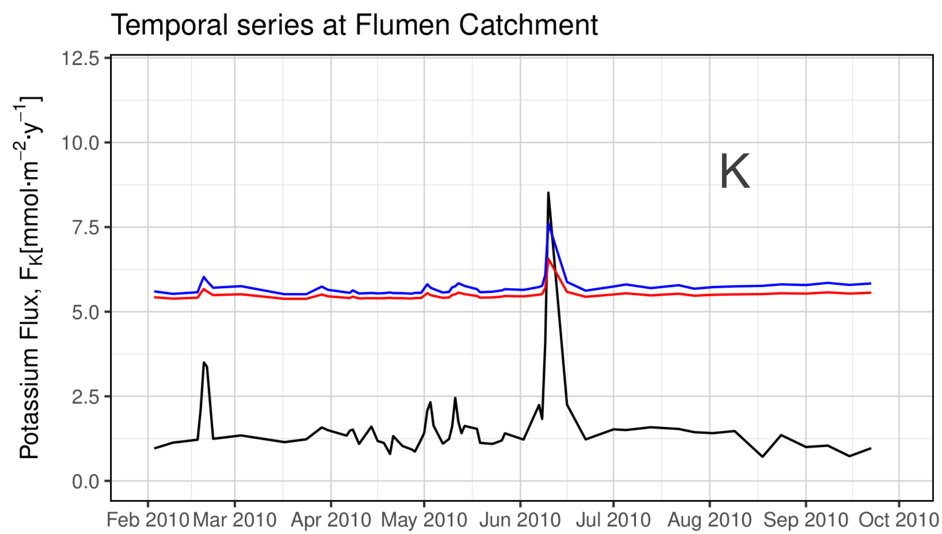


Model development









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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G-MOD

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Thank you! Merci! Dank je!

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