

Source depth of metabolites strongly influences concentration– distribution patterns in biological systems

Dr. L. Moreau¹, Dr. H. Schmidt¹, Dr. Y. Nakamura^{1*}

¹ Department of Clinical Medicine and Translational Research, Université de Paris, Paris, France

Introduction

The supporting information includes information about the data collection (Section S1), the description of the case studies (Table S1), four figures (Figure S1-S4) and additional results supporting the analysis of the main manuscript (Table S2-S3).

S1. Data sources

Data for Switzerland were retrieved from the Swiss National River Monitoring and Survey Program (NADUF, <https://www.bafu.admin.ch/bafu/en/home/topics/water/state/water--monitoring-networks/national-surface-water-quality-monitoring-programme--nawa-/national-river-monitoring-and-survey-programme--naduf-.html>, last access November 2018).

The Swedish water quality database, collected by Institute for Water and Environment (SLU, <http://info1.ma.slu.se/db.html>, last access January 2019), is containing a large number of stations, but it lacks discharge data in most stations. We matched the water quality database with the hydrological database owned by the Swedish Meteorological and Hydrological Institute (SMHI, <https://www.smhi.se/klimatdata/hydrologi/vattenwebb>, last access January 2019), but only a small number of stations overlapped.

We downloaded the data for USA from the Water Quality Portal (WQP, <https://www.waterqualitydata.us/>, last access November 2018) sponsored by the United States Geological Survey (USGS), the Environmental Protection Agency (EPA), and the National Water Quality Monitoring Council (NWQMC).

We collected the data of the Australian catchments in the region of Queensland from the Water Monitoring Information Portal (WMIP, <https://water-monitoring.information.qld.gov.au>, last access February 2019) of Queensland Government.

All the other data (Victoria in Australia, Brazil, Canada, Germany, Spain and Cameroon) are included in the GLORICH database. For documentation and further information on this database the reader can refer to the original publications (Hartmann et al., 2014; Hartmann et al., 2019).

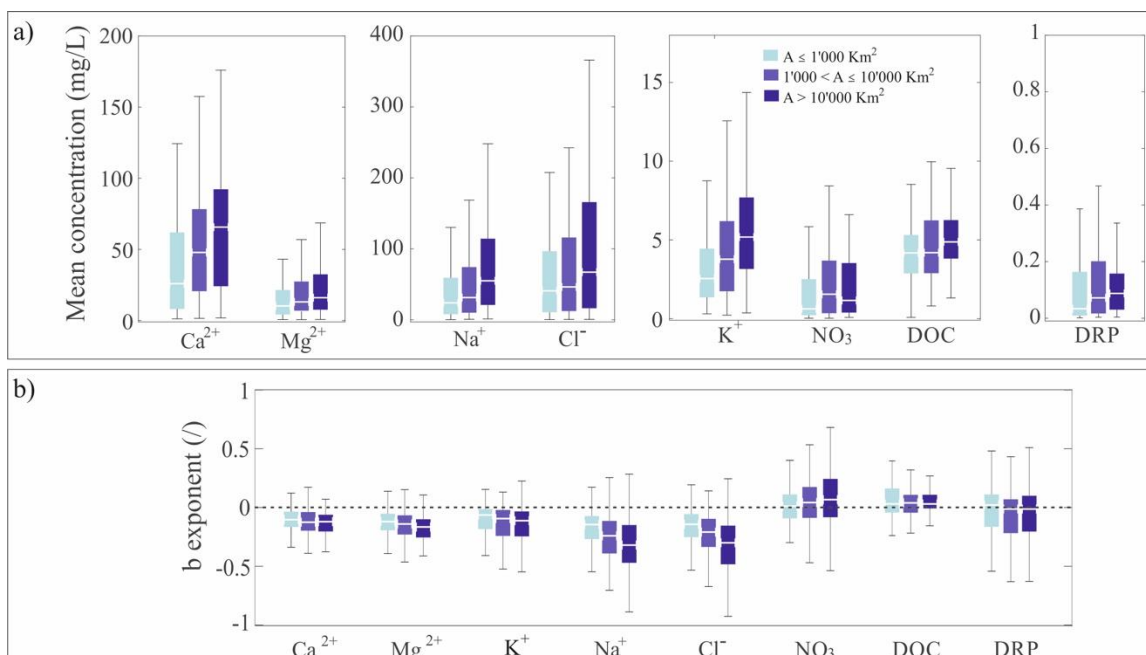


Figure S1. a) Boxplot of the mean observed concentrations across the catchments classified by catchment size (A), i.e. light blue for $A \leq 1'000 \text{ Km}^2$ (176 catchments), blue for $1'000 < A \leq 10'000 \text{ Km}^2$ (201 catchments), dark blue for $A > 10'000 \text{ Km}^2$ (172 catchments). b) Boxplot of the b-exponent of the C-Q relation of each solute in each catchment grouped by the same catchment area classes consistently with the upper panel.

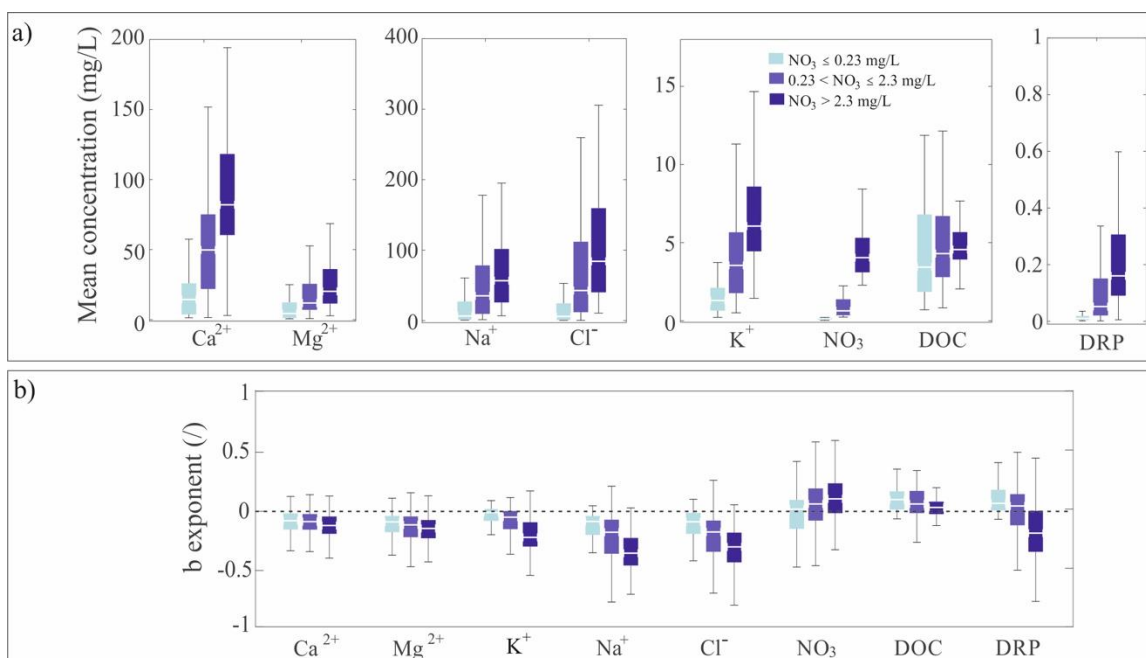


Figure S2. a) Boxplot of the mean observed concentrations across the catchments classified by mean NO₃ concentration (the threshold values refer to N-NO₃), i.e. light blue for $\text{NO}_3 \leq 0.23$

mg/L (91 catchments), blue for $0.23 < \text{NO}_3 \leq 2.3$ mg/L (242 catchments), dark blue for $\text{NO}_3 > 2.3$ mg/L (172 catchments). Values of NO_3 lower than 0.23 mg/L typically correspond to natural catchments (Madison and Brunett, 1984; Zobrist, 2010). The threshold of 2.3 mg/L is the NO_3 concentration in most countries in drinking water (WHO, 2011) and values of NO_3 above the threshold indicate an impact of anthropogenic activities in the catchments. b) Boxplot of the b-exponent of the C-Q relation of each solute in each catchment group as defined in the upper panel.

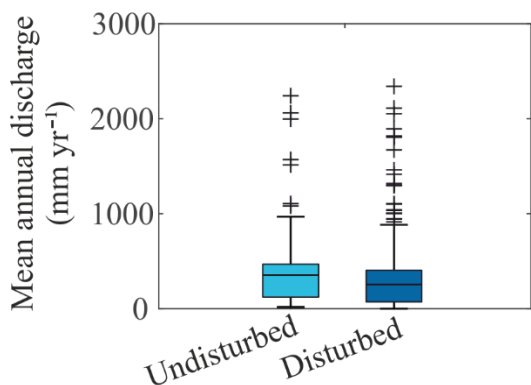


Figure S3. Mean annual discharge of undisturbed (light blue) and disturbed (blue) catchments.

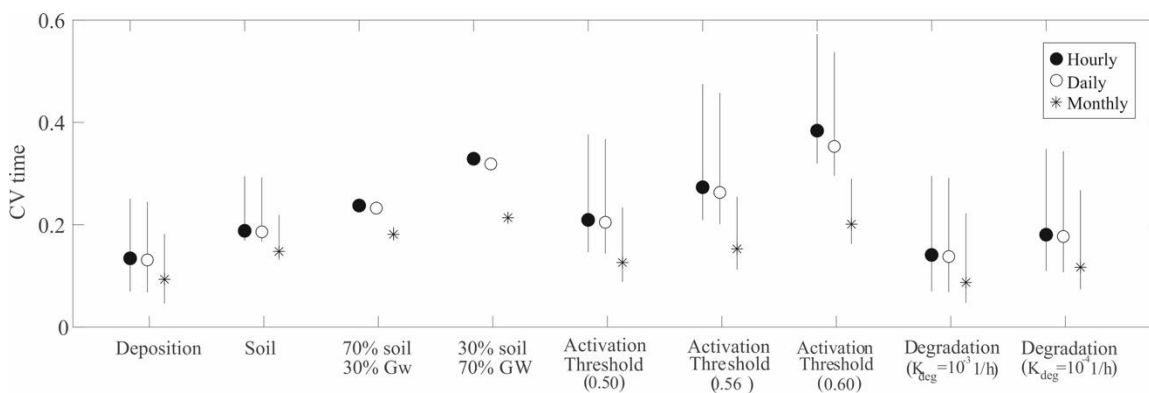


Figure S4. CV-time of the simulations divided by type of numerical experimental (see Main Text). The black dot represents the median CV-time of the results aggregated at the hourly scale, the white dot the median CV-time of the results aggregated at the daily scale and the star the median CV-time of the results aggregated at the monthly scale. The uncertainty bars span between the 25th and the 75th percentile computed with stochastic simulations randomizing the time of input injection.

See attached Excel file.

Table S1. Catchments description. The information is retrieved from the databases mentioned in session S1.

Table S2. P-values of the two-sample t-test between two classes in which the sites are classified based on (a) discharge, (b) catchment area, and (c) mean NO3 concentration. Colored cells are characterized by p-values lower than 0.05, meaning that the data in the two classes have significantly different mean.

a) Classification based on discharge			
	Class 1 and 2	Class 1 and 3	Class 2 and 3
Ca	0.314	0.000	0.001
Mg	0.555	0.000	0.000
Na	0.002	0.000	0.001
Cl	0.395	0.000	0.001
K	0.962	0.000	0.001
NO3	0.000	0.961	0.000
DOC	0.045	0.000	0.000
DRP	0.017	0.019	0.327

b) Classification based on area			
	Class 1 and 2	Class 1 and 3	Class 2 and 3
Ca	0.001	0.000	0.0317
Mg	0.223	0.084	0.725
Na	0.106	0.017	0.929
Cl	0.109	0.000	0.042
K	0.195	0.006	0.190
NO3	0.004	0.054	0.297
DOC	0.752	0.870	0.493
DRP	0.377	0.909	0.190

c) Classification based on NO3			
	Class 1 and 2	Class 1 and 3	Class 2 and 3
Ca	0.000	0.000	0.034
Mg	0.000	0.000	0.429
Na	0.001	0.000	0.520
Cl	0.001	0.001	0.962
K	0.001	0.000	0.971
NO3	0.000	0.000	0.000
DOC	0.142	0.829	0.860
DRP	0.000	0.000	0.861

Table S3 Percentage of b exponents significantly different from zero using the Student’s t test with level of significance $\alpha=0.05$ and simply applying a threshold of 0.1 or of 0.2, without using any statistical test.

	Ca	Mg	K	Na	Cl	NO3	DOC	DRP
Student's t test	99.6	100.0	99.8	100.0	99.7	99.6	66.1	98.9
Threshold = 0.1	57.1	66.1	46.0	74.5	74.4	58.6	23.8	58.6
Threshold = 0.2	21.0	30.4	29.2	53.0	50.6	36.2	7.5	35.1

References

Hartmann, Jens, Nils Moosdorf, Ronny Lauerwald, Matthias Hinderer, and A. Joshua West. (2014). “Global Chemical Weathering and Associated P-Release — The Role of Lithology, Temperature and Soil Properties.” *Chemical Geology* 363 (January): 145–63. doi:10.1016/j.chemgeo.2013.10.025.

Hartmann, Jens; Lauerwald, Ronny; Moosdorf, Nils (2019): GLORICH - Global river chemistry database. PANGAEA, <https://doi.org/10.1594/PANGAEA.902360>, Supplement to: Hartmann, J et al. (2014): A Brief Overview of the GLObal RIVer Chemistry Database, GLORICH. *Procedia Earth and Planetary Science*, 10, 23-27, <https://doi.org/10.1016/j.proeps.2014.08.005>

Madison, R. J., and Brunett, J. O. (1985). Overview of the occurrence of nitrate in groundwater of the United States. In *National Water Summary 198: Hydrological events, selected water-quality trends, and ground-water resources*, USGS Water Supply Paper 2275, 93-105. Washington, D.C.: U.S. Government Printing Office

WHO. 2011. “Nitrate and Nitrite in Drinking-Water Background Document for Development of WHO Guidelines for Drinking-Water Quality.” https://www.who.int/water_sanitation_health/dwq/chemicals/nitratenitrite2ndadd.pdf.

Zobrist, J.: *Water chemistry of Swiss Alpine rivers*, in *Alpine Waters*, edited by: Bundi, U., Springer, Berlin, 731 Heidelberg, 95–118, 2010