CRC 1253 CATCHMENTS AS REACTORS

CAMPOS

Universität Stuttgart

Characterization of the catchment regime by applying optimal design of experiments

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Introduction

Knowing how the contaminant compound is released and digested by the catchment is crucial since it can help to manage water pollution.

The way a catchment releases a compound defines the chemical regime of the catchment regarding this compound:

- *dilution-type*: catchment could have a constant contaminant release subject to dilution by rainfall
- *chemostatic-type*: presents a washout of pollutants at a constant concentration

Commonly, catchment regimes are described by a simple regression slope of log-concentrations (logC) versus log-discharges (logQ) and the slope value of these plots defines the chemical regime of the catchment.

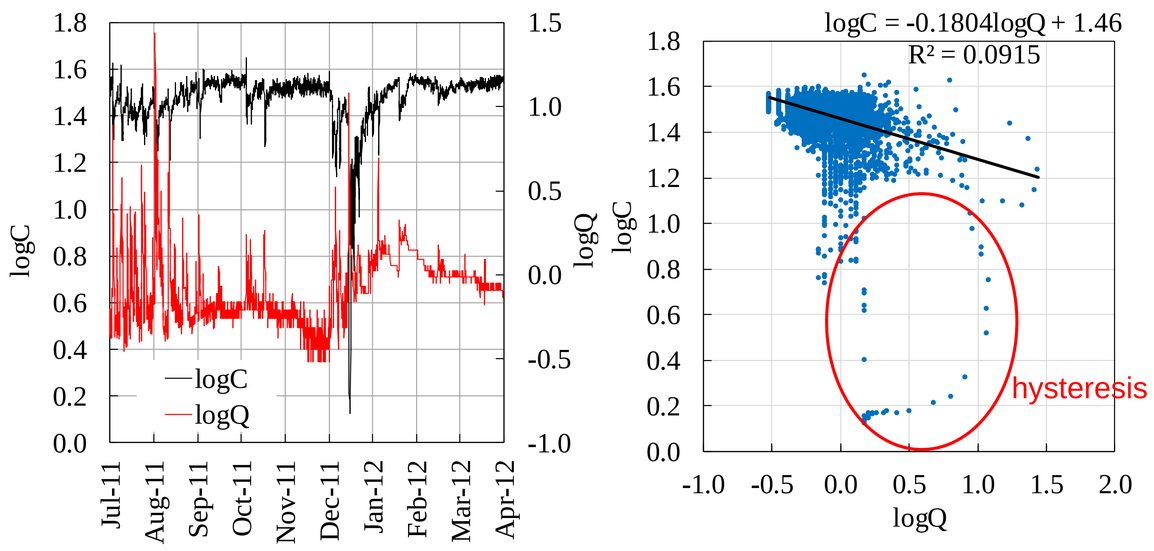
However, the assumption of standard regression is too simple, since these plots show temporal hysteresis that defies regression assumptions.

Therefore, we propose:
1) How to model this situation beyond simple regression
2) How to get the required data with least effort

Methods

Catchment and Data

Catchment of the Ammer River south-west of Germany.
Hourly data from 07/01/2011 to 03/31/2012 [1].



Proposed model

$$C_t = \frac{k_t}{Q_t{}^{\alpha}}$$

C: concentration
$-\alpha$: chemostatic strength [α=0 chemostatic-type; α=1 dilution-type]
Q: discharge rate
k: apparent release rate, autoregressive AR(1)

AR(1) can be characterized by defining: t_{ch} (characteristic time), mean and variance of k, m_k and v_k, respectively.

Then with only four parameters α, m_k, v_k, and t_{ch}, we can represent concentrations versus time in a very intuitive way [2].

Methods (cont.)

Retrospective Optimal Design of Experiments

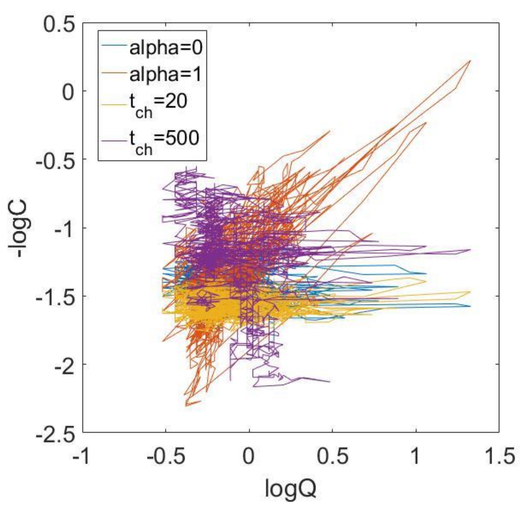
$$d_{opt} = \arg \min_{d \in \mathbf{D}} \emptyset_\alpha(d)$$

$$\emptyset_\alpha(d) = \left(\alpha_{full} - \alpha_{post,d}\right)^2 \propto \emptyset_\alpha\{p(\alpha|\boldsymbol{y}_d)\}$$

A total of 25 sampling strategies based on:
- Time and flow discharge frequency
- Event based (high Q, low Q, combinations of high and low Q)
- Random samples
- From three to 10 samples

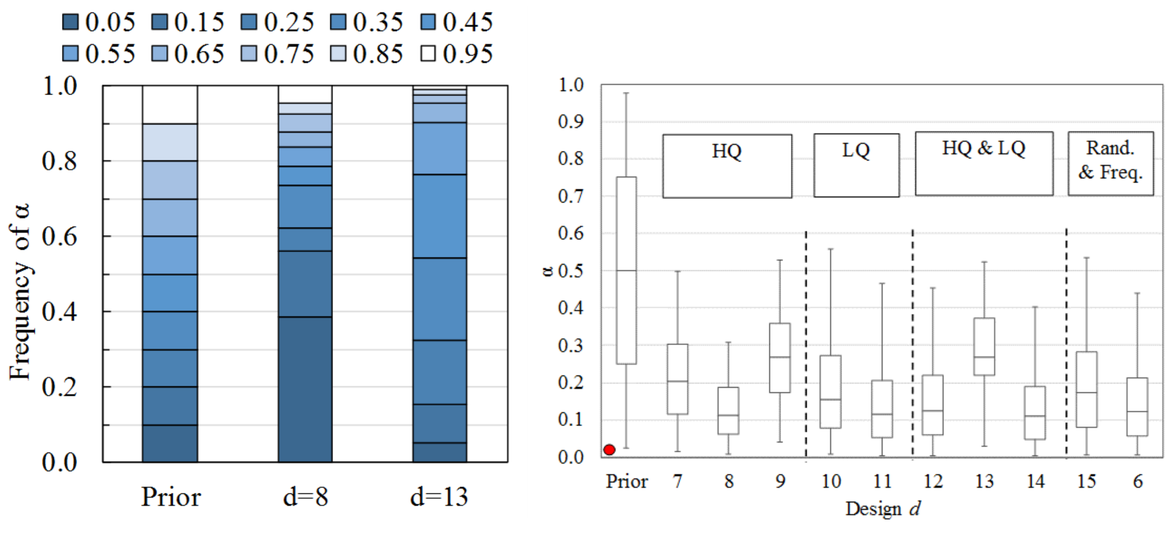
Results

Simulations and characterization with extensive time data



Parameter (unit)	Inferred value
α_{full} (/)	0.011
$t_{ch\,full}$ (h)	112.4
$m_{k\,full}$ $\left(\frac{mg}{l}\left(\frac{m^3}{h}\right)^{\alpha}\right)$	30.6
$\sqrt{v_{k\,full}}$ $\left(\frac{mg}{l}\left(\frac{m^3}{h}\right)^{\alpha}\right)$	2.8

Characterization with sparse data (sampling strategies)



Summary

- Our model is more robust and performs better that simple regression.
- We observed that only a few samples are necessary to produce a large reduction of α bias independently of the sampling strategy.
- To decrease the uncertainty of α prediction stronger sampling strategies have to be implemented, e.g. samples taken when a peak event occurs

References

[1] Schwientek, Osenbrück, Fleischer (2013), Environ. Earth Sci., 69(2), 381–393.

[2] Mehne & Nowak (2017), Journal of Energy Storage, 12, 288–296.

Acknowledgement: This work was supported by the Collaborative Research Center 1253 CAMPOS (P8: Conceptual Uncertainty, Model Legitimacy, and Optimization of Data Acquisition Strategies), funded by the German Research Foundation (DFG, Grant Agreement SFB 1253/1 2017). **Contact:** ana.gonzalez@iws.uni-stuttgart.de

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