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Stochastic modelling of trace contaminants in wet-weather discharges

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Highlights

- Large dataset shows at high variability of event mean concentrations of trace contaminants
- Lognormal distribution visual fitting to describe event mean concentrations
- Stochastic model could be useful to predict contaminant loads and concentrations

Introduction

Urban wet-weather discharges (combined sewer overflows, CSO, and stormwater outlets from separate sewers, SWO) contain various trace contaminants which can pose a threat to receiving waters (e.g. Launay et al., 2016; Mutzner et al., 2020; Wicke et al., 2021b). The deterministic model prediction of trace contaminants loads and concentrations in wet-weather discharges is challenging due to the inherent high spatiotemporal variability (e.g. Mutzner et al., 2020; Rippy et al., 2017; Wicke et al., 2021a). The observed high spatiotemporal variability is attributed to locally varying factors such as substance use behaviors, land use, and rainfall intensities, however to date no reliable correlation based on such local factors could be identified. Stochastic model predictions based on available data have been previously used successfully to predict TSS concentration in wet-weather discharges (Rossi et al., 2005). In this study, we aim to predict the loads and concentrations of selected trace contaminants based on a large field monitoring data collection (> 60 sites, (Mutzner et al., in prep.) and integrate this information in a stochastic model. The results will be directly useful for regulators and utilities as a first predictor of the influence of trace contaminants in urban wet-weather discharges on receiving waters.

Methodology

Collected field monitoring data on trace contaminants in urban wet-weather discharges

We selected data sets for trace contaminants in urban wet-weather discharges (CSO and SWO) fulfilling the criteria that sampling was done by composite sampling, meaning the collection of several samples per event, resulting in an event mean concentration (EMC). The authors were contacted for the raw data resulting in 63 sites, 506 monitored events and more than 42’000 observations (Table 1). Details on sampling, chemical analysis and sample preparation are explained in the publications corresponding to the data and in (Mutzner et al., in prep.).

Table 1. List of datasets with location, number of sites, events, medium type, sampling strategy and reference for campaign details.

#	Country	# sites	# events/site[a]	Type[b]	Sampling	Reference
1	Germany	5	18 to 41	SWO	Vol-prop. C-WS	(Wicke et al., 2021b)
2	US	21	1 to 4	SWO	Flow-prop C-WS	(Masoner et al., 2019)
3	Switzerland	22	1 to 7	CSO	Time-prop PS & C-WS	(Mutzner et al., 2020)
4	US	2	11 & 13	SWO	Vol-prop C-WS	(Burant et al., 2018)
5	France	2	19 & 22	SWO	Flow-prop C-WS & time-prop manual WS	(Gasperi et al., 2014)
6	France	1	11	SWO	Flow-prop C-WS	(Garnier, 2020; Gasperi et al., 2014; Sébastian et al., 2015)
7	Australia	9	5 to 21	SWO	Flow-prop C-WS	(Rippy et al., 2017)
8	Denmark	2	27 & 28	CSO, SWO	C-WS	Danish EPA (Miljøstyrelsen, 2017, 2006)

[a]Total number of events sampled per site, single substances were often analysed for fewer events, [b]SWO: stormwater outlets, CSO: combined sewer overflows, [c]C-WS: Composite water sampling with automated sampler, PS: Passive sampling

Statistical data analysis

The data was transformed to consider the different limit of quantifications (LOQ) or detection (LOD) in the data sets. Contaminant concentrations <LOQ were treated as censored values and estimated using

regression on order statistics (ROS). All calculations were done in R (R Core Team, 2020). ROS was done if there were more than 3 observations per site and less than 80% left-censored data (<LOQ). The data was analyzed for distributions of EMCs over all sites for selected trace contaminants with high occurrence (>50 % of all sites at least once >LOQ). In a next step, we will upgrade an existing deterministic substance flow model (Mutzner et al., 2016) which is based on a simple hydrological model (Rauch et al., 2002) and include a stochastic pollutographs predictor.

Results and discussion

The majority of the analysed observations are <LOQ, or less than 3 observations per site are available. Thus around 30% (13’800 out of >42’000 observations) can be used for further statistical analysis. The ROS analysis based on an assumed log-normal distribution visually shows good correlations for the entire set of EMCs (Figure 1). Thus, lognormal distributions will be used to estimate the concentrations in urban wet-weather discharges.

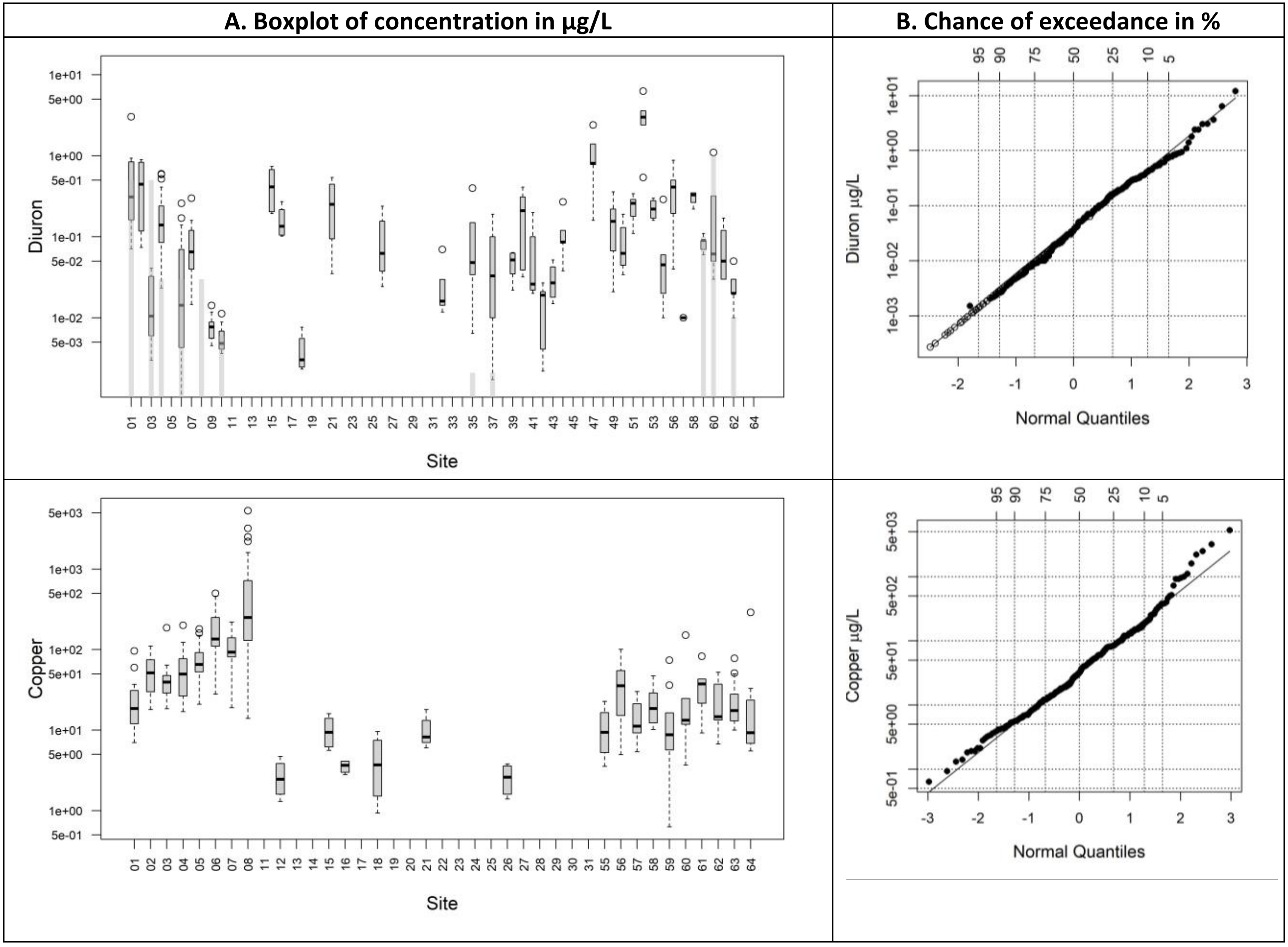

Figure 1. A. Concentrations of exemplary trace contaminants event mean concentrations (EMCs) per site. Only sites shown were contaminants was measured. Light grey area indicated part of the boxplot with censored data (<LOQ) for which a ROS estimate of the concentration was done. Boxes represent the first and third quartile (Q1 and Q3), whiskers’ lengths are max 1.5 x (Q3-Q1). The grey zone shows the maximum limit of quantification of the data. **B.** Quantiles shown for assumed log-normal distribution, each point on the graph is a EMC measurement – black point: EMCs > LOQ, empty white point: EMC estimated with ROS <LOQ (Diuron).

The sampled contaminant concentrations are highly variable, with the coefficient of variation (CV) of the EMC ranging from 0.2 to 1.2 (80%-interquantile range, median: 0.6). These high CV are associated with the inherent variability due to behavioral use patterns, sources and urban land use. However, part of the observed variability might also be due to limited data quality, although we tried to reduce this factor by using data sets with experimental reliable procedures (sampling and chemical analysis). In comparison, for traditional pollutants and TSS, CVs range from 1.1 to 3.3 in stormwater outlets (Lee et al., 2007). The CVs of the EMCs also hint at distinct differences between chemical classes, as heavy metals, household and industrial related pollutants have lower CVs than pesticides and PAHs. Thus, we will consider this difference in CV per chemical class in the stochastic predictor by selecting a representative trace contaminant per chemical class.

Conclusions and future work

- High variability of event mean concentrations observed despite large data set collected
- Clear hints that deterministic model prediction is challenging and potential of stochastic prediction assuming lognormal distribution for trace contaminants shown.
- Preliminary work presented that will be finalized for presentation at UDM conference, assessing the potential of using a stochastic model to predict trace contaminants in urban wet-weather discharges.

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