Bayesian metamodel to estimate risk for thousands of chemicals in surface water

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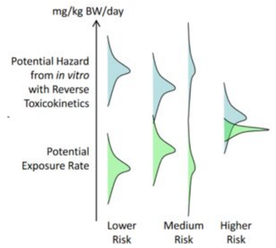
1. Introduction

Background: With thousands of chemicals in commerce and the environment, efficient tools are needed to support risk prioritization and evaluation.



Knowledge gap: Inconsistent data availability for concentrations in surface water to develop exposure estimates.

Proposed solution: Development of an open, reproducible workflow to:

1. Determine representative surface water concentrations for hundreds of organic chemicals in the United States based on already available monitoring data
2. Calibrate a metamodel to predict representative surface water concentrations for thousands of non-monitored organic chemicals
3. Prioritize organic chemicals based on the relationship between concentration ranges and predicted no-effect concentrations for freshwater standard test species

2. Method overview

$$\ln y_i = m_0 + \sum_{j=1}^{n_j} \sum_{k=1}^{n_k} m_{jk} \ln\left(l_{ji}\, p_{ki}\right)$$

Where *i* is a given chemical, *y* is the representative concentration, *j* is a source of environmental loading data, *l* is the value of that loading given the source and chemical (amount/time), *k* is an exposure model, *p* is the value of a fate prediction model (amount/amount/time), and *m* is a model weight

Each coefficient m_{jk} represents a range of weights describing how well model *k* explains observed concentration *y* given the information from loading data source *j* in 20,000 different attempted metamodels.

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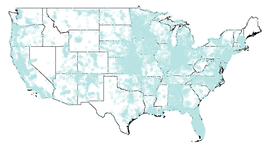
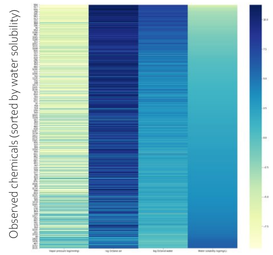
3. Surface water concentrations *y*

The Water Quality Portal provides concentrations of organic chemicals in surface water sampled from 2008 to 2018 covering broad spatial and physicochemical property ranges.





Because over 80% of samples were below varying quantification limits, representative ranges of dissolved (196 chemicals) and bulk (252 chemicals) concentrations were developed using Maximum Likelihood Estimation (MLE).

Upper right: Sampling sites of observation set represent 2114 of 2270 hydrologic subbasins. Lower left: Chemical property space (log10, calculated using OPERA 2.4) of observation set: vapor pressure (mmHg), octanol:air, octanol:water, water solubility (mg/L).

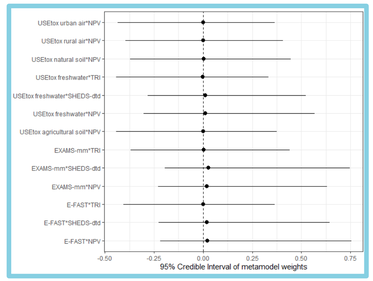
4. Environmental loading data sources *j*

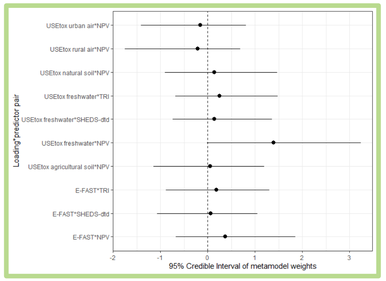
- NPV: Chemical Data Reporting under the Toxic Substances Control Act (reported to the EPA about mass imported into or produced in the U.S. by year) + Pesticides Industry Sales and Usage, 2008 – 2012 Market Estimates (2017 U.S. EPA OPP report)
- SHEDS (Stochastic Human Exposure and Dose Simulation – Down the Drain): model simulating the amount of a chemical that goes down the drain based on household usage, reduced by the percentage removed by wastewater treatment
- TRI (Toxic Release Inventory): data reported to EPA about industrial releases

5. Fate prediction models *k*

MODEL	INPUTS	OUTPUT
E-FAST	Removal from wastewater treatment (%), Estimated flow of the receiving stream	Estimation of Surface Water Exposure Concentrations in Rivers and Streams (µg/L)/(kg/day)
EXAMS metamodel	Estimated flow of the receiving stream,octanol:water,air:water	Annual average dissolved water concentration rate (mg/L)/(kg/hr)
USEtox	Molar mass, octanol:water,air:water, pKa, half-lives in air, water, soil, and sediment, organic carbon:water, vapor pressure, water solubility, fish bioaccumulation	kg bulk or dissolved chemical in freshwater at steady-state per daily kg emitted (kg/(kg/d))

6. Metamodel loading*fate coefficients (m_{jk})

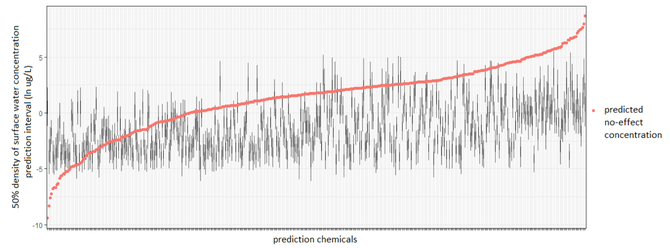




95% Credible intervals of metamodel coefficients [left: dissolved, right: bulk]

No tested loading*fate pair was predictive of observed dissolved concentrations. The most informative pair for bulk concentrations was USEtox freshwater model using loadings from NPV.

7. Prioritization based on ecotoxicity estimates



8. References

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