Development and evaluation of consensus metamodel for estimating national concentrations of organic chemicals in surface water

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Introduction

USEPA’s risk prioritization framework\(^1\) for the thousands of chemicals to which people could possibly be exposed

Hazard: High-throughput assays, such as ToxCast and Tox21

Toxicokinetics: assays and generalizable PBPK models, such as Ref6\(^2\)

Exposure: one example is SEEM (Systematic Evaluation of Empirical Models), a consensus framework to integrate, evaluate, and calibrate existing exposure predictors to monitoring data through Bayesian linear regression\(^3\)

This version of SEEM, ECOSSEEM, describes screening-level estimates of average concentrations of organic chemicals (and their likelihoods) in surface water, based on openly-available fate and transport models and chemical data evaluated against monitoring data. Extending that relationship to other chemicals can serve as a possible data stream for chemical prioritization.

Method overview

A model may not be equally correlated to the data across chemicals.

Prior: domain knowledge represented by the fate and transport model or other exposure predictor

Posterior: credible interval of model parameters based on the relationship between monitoring data and the prior

Posterior = Likelihood + Prior

Normalization

Representation of Bayes theorem.

Metamodel inputs

Hazard

No single predictor was more accurate than using the overall mean as an estimate.

Results

Exposure prediction evaluation

- USEtox\(^4\)
- RAIRDAR\(^5\)
- EXAMS\(^6\)
- NPV/CDR\(^7\)

Of the tested predictors, National Production Volume is most likely to describe median observed water concentrations. When regressing on physchem properties, all coefficients include 0.

Future work

Apply Bayesian maximum entropy approach to estimate likely concentrations in non-sampling areas. Values from the entire estimation grid will describe an average and variance for the whole country over the time period.

References

1) USEPA’s risk prioritization framework\(^1\) for the thousands of chemicals to which people could possibly be exposed

2) ToxCast and Tox21

3) PBPK models, such as Ref6

4) USEtox\(^4\)

5) RAIRDAR\(^5\)

6) EXAMS\(^6\)

7) NPV/CDR\(^7\)