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

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# Metamodel inputs

Observed surface water concentrations (In ug/L)

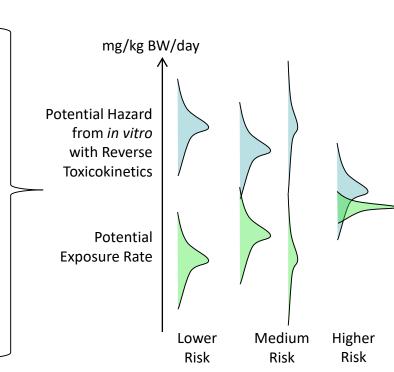
USEPA's risk prioritization framework<sup>1</sup> for the thousands of chemicals to which people could possibly be exposed

Toxicokinetics: assays and generalizable PBPK models, such as httk<sup>2</sup>

Hazard: high-throughput assays,

such as ToxCast and Tox21

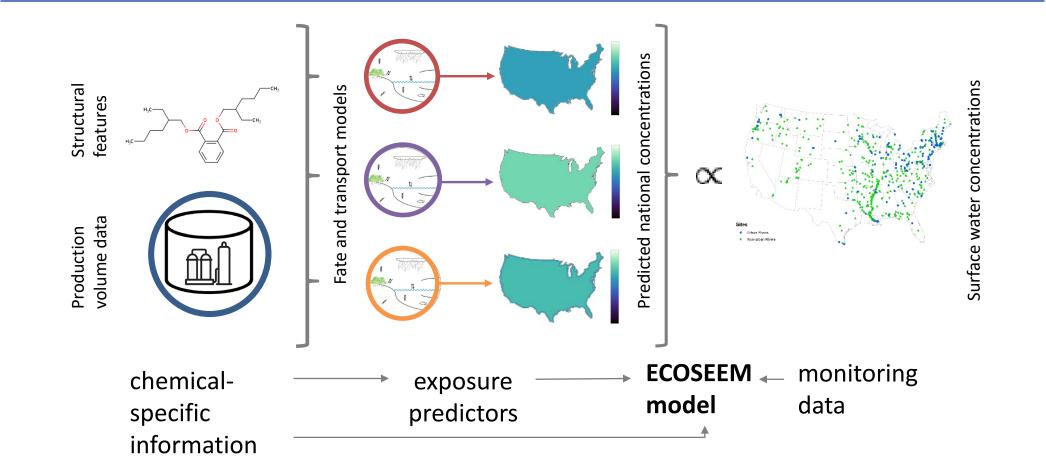
Exposure: one example is **SEEM** (Systematic Evaluation of Empirical Models), a consensus framework to integrate, evaluate, and calibrate existing **exposure predictors** to **monitoring data** through Bayesian linear regression<sup>3</sup>



This version of SEEM, **ECOSEEM**, 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

Introduction



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

 $Posterior = \frac{Likelihood*Prior}{Normalization}$ 

Representation of Bayes theorem

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

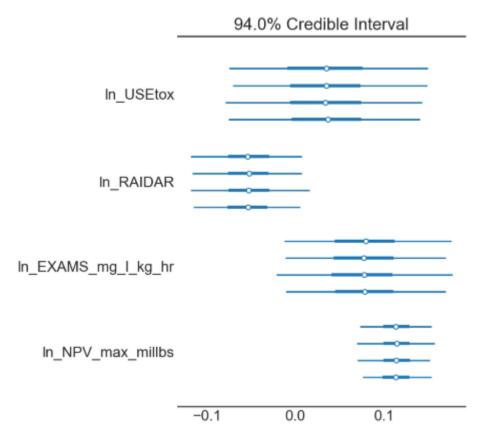
**Monitoring data** Download all surface water sampling results (includes USGS, EPA, state) in 1998 to 2018 from National Water Quality Monitoring Council<sup>4</sup> for **any organic chemical**: ~ **1700** (remove some sample types, unit types, activity types; normalize units) Aggregate chemicals by unique identity: ~1400 Restrict to within domain of applicability of all models: ~1200 Remove chemicals unrelated to production volume: ~900 Subset with enough **detects** (uncensored values) to develop a potential above 80% acceptance: 225 **Exposure predictors & chemical-specific information** r = 0.08r = 0.50| 0.75 | r = 0.35r = 0.09r = -0.25

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

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#### Results

#### Exposure prediction evaluation



Predictor	Inputs	Outputs
USEtox <sup>5</sup>	physchem properties from TEST <sup>8</sup> , OPERA <sup>9</sup> , EPI Suite <sup>10</sup>	Mass in the environment (freshwater compartment) for 1 kg/day emitted (kg per kg/d)
RAIDAR <sup>6</sup>	physchem properties from TEST, OPERA	Amount in water (kg per kg/hr emission rate)
EXAMS <sup>7</sup>	physchem properties from OPERA; water system flow rate	Annual average dissolved water concentration rate (mg/L per kg/hr)
NPV/CDR <sup>11</sup>	reports by producers and importers	lb/yr produced

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



Develop hierarchical model to aggregate concentrations at a watershed level

Figures adapted from Woody Setzer

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

## References

1) Wood MD, Plourde K, Larkin S, Egeghy PP, Williams AJ, Zemba V, Linkov I, Vallero DA. Advances on a Decision Analytic Approach to Exposure-Based Chemical Prioritization. Risk Anal. 2018 May 11. doi:10.1111/risa.13001. 2) Pearce RG, Setzer RW, Strope CL, Wambaugh JF, Sipes NS. httk: R Package for High-Throughput Toxicokinetics. J Stat Softw. 2017 Jul 17;79(4):1-26. doi: 10.18637/jss.v079.i04. 3) Wambaugh, J.F. et al. High-Throughput Models for Exposure-Based Chemical Prioritization in the ExpoCast Project. Environmental Science & Technology 2013 47 (15), 8479-8488 doi:10.1021/es400482g 4) Read EK et al. Water quality data for national-scale aquatic research: The Water Quality Portal. Water Resour. Res. 53, 1735−1745, doi:10.1002/2016WR019993 5) Rosenbaum, R.K., Bachmann, T.M., Gold, L.S. et al. USEtox—the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. Int J Life Cycle Assess (2008) 13: 532. doi:10.1007/s11367-008-0038-4 6) Arnot, J.A., Mackay, D., Webster, E., Southwood, J. M. 2006. A screening level risk assessment model for chemical fate and effects in the environment. Environ. Sci. Technol. 40 (7): 2316 - 2323. 7) Barber, M.C., Isaacs, K.K., Tebes-Stevens. C. Developing and applying metamodels of high resolution process-based simulations for high throughput exposure assessment of organic chemicals in riverine ecosystems. 2017. Science of the Total Environment, 605-606 (15 December): 471-481. 8) Martin, T.M., Harten, P., Venkatapathy, R., Das, S., Young, D.M. (2008). "A Hierarchical Clustering Methodology for the Estimation of Toxicity." Toxicology Mechanisms and Methods, 18, 2: 251–266. 9) Mansouri et al. OPERA models for predicting physicochemical properties and environmental fate endpoints. J Cheminform (2018) 10:10 doi:10.1186/s13321-018-0263-1 10) US EPA. 2019. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. United States Environmental Protection Agency, Washington, DC, USA. 11) US EPA 2

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