Applying the RAIDAR model for ecological risk assessment: A case study for 10 organic flame retardants

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Introduction

- Measured concentrations in environmental media are limited for the majority of commercial chemicals, including organic flame retardants (OFRs) [1]; chemical emission rates are also uncertain
- Some OFRs are currently being evaluated to determine if they pose unacceptable risks to humans and the environment
- To assess risks, it is important to accurately characterize exposure, consequently, exposure data gaps can hinder application of risk-based methods for chemical prioritization, screening and comprehensive assessments
- RAIDAR is a regional-scale, evaluative, fugacity-based, multimedia mass balance model that combines exposure and effect information for screening-level risk estimation (**Figure 1**) [2]
- Estimating exposure concentrations of OFRs and other organic pollutants requires information on the amount of chemical emitted to the environment and its mode-of-entry (MOE).
- Emission data, however, are often highly uncertain, resulting in challenges for performing the exposure assessment.
- Using a complementary approach, in which monitoring data are combined with model estimates, it is possible to use "inverse modelling" as a tool to strengthen the exposure assessment.

Objectives

- Use a case study of 10 diverse OFRs to illustrate how monitoring data and mass balance models can be combined for screening-level exposure assessment (**Table 1**)
- Use existing measured air concentrations to guide emission rate estimates ("inverse modelling")
- Evaluate the model with available monitoring data in other media
- Using a tiered approach (**Figure 4**), conduct a comparative screening-level assessment for 10 OFRs

Methods

Compile and evaluate available monitoring data for the 10 OFRs sampled in temperate North America

(**Figure 2**)

Collect and evaluate chemical property and transformation half-life data for RAIDAR simulations for the 10 OFRs

(**Table 2**)

Apply inverse modelling to calculate concentrations

→ Estimate exposure

→ Include uncertainty analysis

→ Screening-level assessment

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Results and Discussion

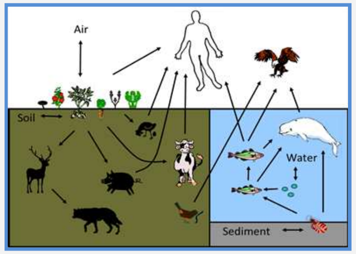

Figure 1: Conceptual overview of the RAIDAR model

Chemical name	Abbr.	Median air concentration, pg/m³
2,4,6-Tribromophenyl allyl ether	ATE	0.70
Decabromodiphenyl ethane	DBDPE	6.8
Tris(1-chloro-2-propanyl) phosphate	TCPP	250
Tris(1,3-dichloro-2-propyl) phosphate	TDCPP	56
Bis(2-ethylhexyl) 3,4,5,6-tetrabromophthalate	TBPH	2.5
2-Ethylhexyl-2,3,4,5 tetrabromobenzoate	TBB	1.7
Dechlorane Plus	DP	1.6
2-Ethylhexyl phosphate	TEHP	8.6
Tris(2-butoxyethyl) phosphate	TBEP	77
1,2-Bis(2,4,6-tribromophenoxy)ethane	BTBPE	0.43

Table 1: 10 OFRs in case study

Model Input Parameter	Range of values
Molar mass, M (g/mol)	126.1 to 1366.9
Log K_{AW} (dimensionless)	-12.71 to -0.10
Log K_{OW} (dimensionless)	-0.85 to 12.95
Log liquid or sub-cooled liquid vapor pressure (/Pa)	-15.57 to 1.56
HL- Air (h)	1.2 to 4 700
HL – Water (h)	66 to 87 300
HL – Soil (h)	130 to 175 000
HL – Sediment (h)	590 to 786 000
Biotransformation HL – Vertebrates (h)	1 to 59 000
Calibrated Regional-Scale Emission Rate, E_A (kg/h)	0.0035 to 11.6

Table 2: Summary of RAIDAR input parameters for 10 OFRS

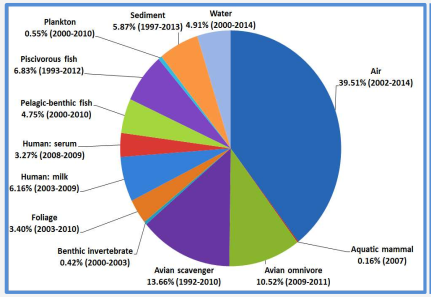

Figure 2: Summary of 3,120 measured concentrations of 10 OFRs in temperate North America (NA), (sampling years)

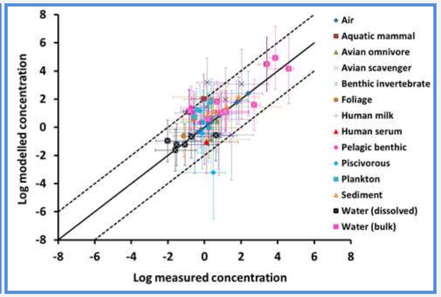

Figure 3: Model evaluation; error bars = 97.5%-ile predicted and minima and maxima reported measured concentrations

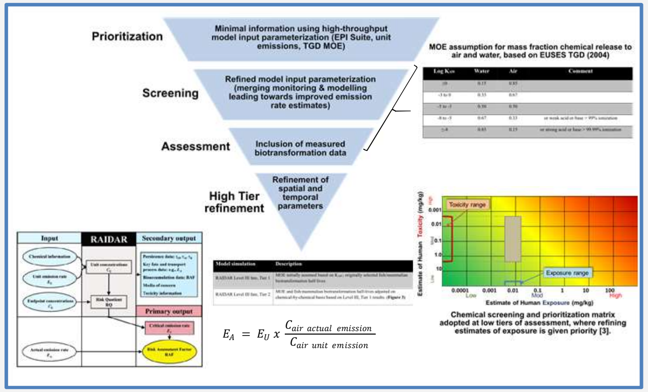

Figure 4: Tiered approach adopted in deriving estimates of exposure using RAIDAR for 10 OFRs

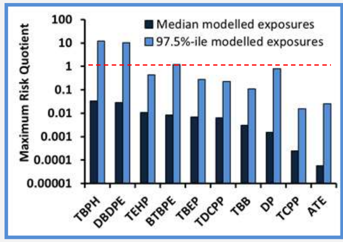

Figure 5: Maximum risk quotients from all model compartments for each OFR

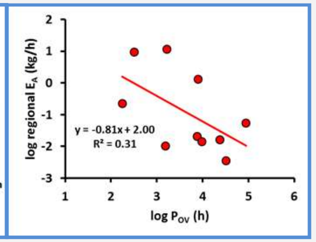

Figure 6: Comparison of est. emission rates (E_A) and overall chemical persistence (P_{OV})

- Case study chemicals comprise a diverse range of chemical properties
- Available monitoring data show high variability
- Inverse modelling provides exposure calculations that are in reasonable agreement with monitoring data across North America
- Uncertainty in exposure calculations approximates measured variability
- Relatively low range of risk quotients may be partially explained by the inverse relationship between emission rates and chemical persistence
- Model predictions can help guide future monitoring research, particularly for OFRs showing relatively high risk quotients
- Model uncertainty can be addressed by further measurements

References
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