Applying the RAIDAR model and the chemical activity approach for ecological risk assessment: A case study for select organic flame retardants

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Introduction

- Measured concentrations in environmental media are limited for the majority of commercial chemicals [1]
- Exposure data gaps hinder application of risk-based methods for chemical prioritization, screening and comprehensive assessments
- The chemical activity (*a*) approach is a proposed integrating concept for chemical hazard, exposure and risk assessment [2,3]
- Chemical emission rates are uncertain
- Chemical activity (*a*; unitless) is fugacity (f; Pa) divided by the liquid or (for solids) sub-cooled liquid vapor pressure (P_L; Pa)
- RAIDAR is a fugacity-based multimedia mass balance model that combines exposure and effect information for screening-level risk estimation → provides output in terms of chemical concentrations, fugacities and activities (**Figure 1**) [4]
- Some organic flame retardants (OFRs) are currently being evaluated to determine if they pose unacceptable risks to humans and the environment

Objectives

- Illustrate how monitoring data, mass balance models and chemical activity can be applied for screening-level risk assessment
- Obtain and critically evaluate monitoring and biomonitoring data and chemical property information required for RAIDAR simulations
- Use existing measured air concentrations to guide emission rate estimates for 10 OFRs ("inverse modelling")
- Demonstrate how RAIDAR can quantify risks by comparing exposures and effects expressed in terms of chemical activity
- Conduct a comparative risk assessment for the 10 OFRs (**Table 1:** brominated, chlorinated and organophosphate) assuming baseline toxicity mode of action as a case study

Methods

Compile and evaluate available monitoring data for the 10 OFRs sampled in temperate North America (**Figure 2**)

Collect and evaluate chemical property, transformation half-life data for RAIDAR simulations for the 10 OFRs (**Table 2**)

Apply inverse modelling to calculate concentrations and activities

→ Estimate risk

→ Include uncertainty analysis

→ Comparative risk assessment

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Results and Discussion

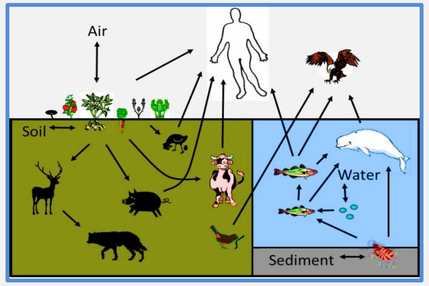

Figure 1: Conceptual overview of the RAIDAR model

Chemical name	Abbr.	Measured air concentration (median), 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
HL- Air (h)	1.15 to 4.70 x 10^{+03}
HL – Water (h)	6.58 x 10^{+01} to 8.73 x 10^{+04}
HL – Soil (h)	1.32 x 10^{+02} to 1.75 x 10^{+05}
HL – Sediment (h)	5.93 x 10^{+02} to 7.86 x 10^{+05}
Biotransformation HL – Vertebrates (h)	1 to 5.9 x 10^{+04}
Regional emission rate, E_A (kilotonne/y)*	3.09 x 10^{-05} to 1.02 x 10^{-01}

Table 2: Summary of RAIDAR input parameters for 10 OFRS

- **Figure 2:** Summary of 2600 measured concentrations of 10 OFRs in temperate North America
- **Figure 3:** Comparison of RAIDAR predicted and measured concentrations (model evaluation)
- **Figure 4:** RAIDAR chemical activity calculations for Dechlorane Plus (DP) in representative multimedia compartments compared to assumed baseline toxicity range
- **Figure 5:** Comparative risk assessment of 10 OFRs
- **Figure 6:** Comparison of emission rates (E_A) and overall persistence (P_{OV}) for 10 OFRs

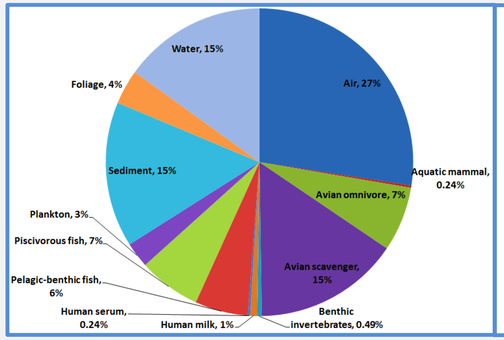

Figure 2: Summary of monitoring and biomonitoring data for 10 OFRs in temperate North America (NA)

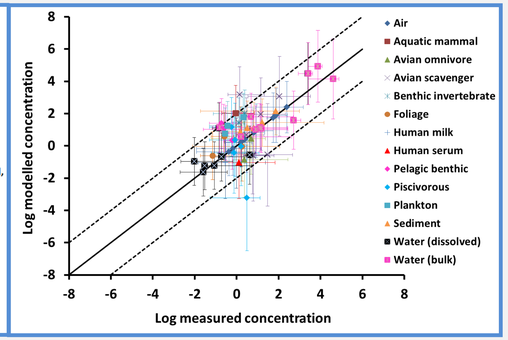

Figure 3: Model evaluation; error bars = 97.5%-ile predicted and minima and maxima reported measured

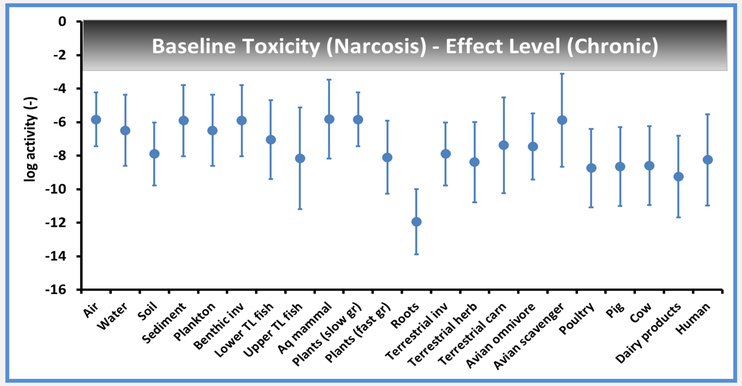

Figure 4: RAIDAR chemical activity calculations for Dechlorane Plus; error bars = 97.5%-iles

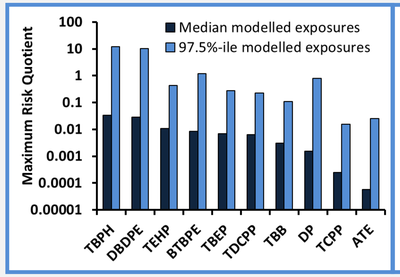

Figure 5: Maximum risk quotients from all model compartments for each OFR

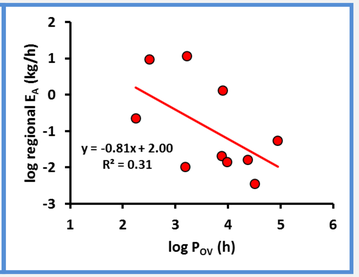

Figure 6: Comparison of emission rates (E_A) and overall chemical persistence (P_{OV})

- Integrated modelling provides exposure calculations that are in good agreement with available monitoring data across North America
- Uncertainty in exposure calculations approximates measured variability
- Some OFRs may be approaching chemical activities in the environment associated with toxicity
- Relatively low range of risk quotients may be partially explained by the inverse relationship between emission rates and chemical persistence
- Current model predictions can help guide future monitoring research, particularly for OFRs showing relatively high risk potential
- Continue model evaluations for model refinement and also address uncertainty in model output by measuring key chemical properties
- Conduct region-specific simulations for refined exposure estimates

References
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