Exploring the use of multimedia fate and bioaccumulation models to calculate trophic magnification factors (TMFs)

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Introduction:

- Globally, tens of thousands of chemicals are legislated for persistence (P), bioaccumulation (B), and toxicity (T) assessment, e.g. [1]; however, few measured data are available, e.g. [2].
- The Trophic Magnification Factor (TMF) is the average factor by which the (lipid) normalized chemical concentration in biota of a food web increases per trophic level. The TMF is determined from the slope derived by linear regression of logarithmically transformed (lipid) normalized chemical concentration in biota and trophic position of the sampled biota [3].
- The TMF is a proposed metric for assessing "B" and assumes "steady state" conditions:

  TMF > 1, then "B"; TMF < 1 then "not B" [3].
- Fugacity (*f*; Pa) is a chemical quantity and a thermodynamic equilibrium criterion.
- Biomagnification in an aquatic food web was originally determined using fugacity [4].
- Lipid normalized concentration in biota ≈ fugacity.

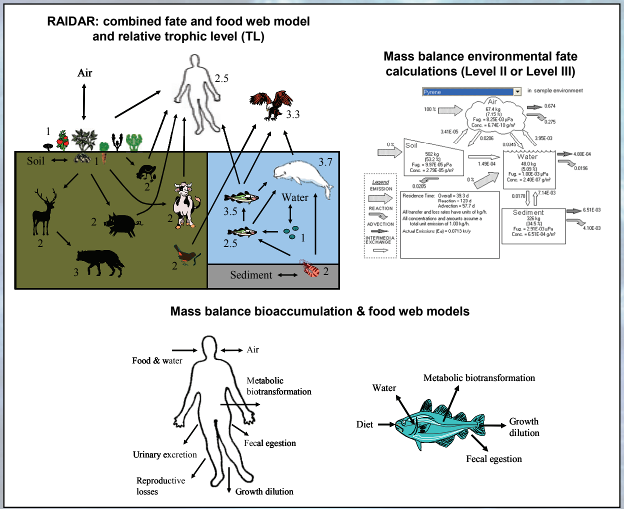
Objectives:

- Use a multimedia mass balance fugacity model to calculate TMFs from chemical properties.
- Explore differences in selected food web components, the influence of chemical mode-of-entry to the environment and disequilibrium conditions in the environment on calculated TMFs.
- Compare screening-level TMFs calculated by the model with measured TMF data.

Methods:

- Risk Assessment IDentification And Ranking (RAIDAR) model (**Figure 1**; [5]):
  - combines fate and food web mass balance fugacity calculations at steady state;
  - provides either Level II (equilibrium in air, water, soil and sediment) or Level III (disequilibrium in air, water, soil and sediment) environmental fate calculations;
  - includes a wide range of representative species residing in air, water, soil and sediment;
  - includes biomagnification and biotransformation processes in vertebrate species, biotransformation half-lives were obtained from *in vivo* estimates or QSAR predictions [6].
- RAIDAR revised to calculate TMFs and various Level II and III simulations were conducted for:
  - 740 hypothetical neutral organic chemicals with diverse partitioning properties (**Figure 2**);
  - Chemicals with measured TMF data, as selected from the Lab-Field Bioaccumulation Workshop sponsored by SETAC, US EPA and ILSI-HESI (**Table 1**).

Figure 1: Schematic of RAIDAR mass balance model concepts [5].



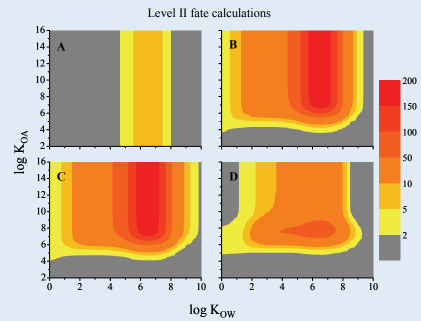


Figure 2: Maximum fugacity ratios (*f*organism / *f*environment) calculated in representative RAIDAR species for 740 hypothetical chemicals. A: Piscivorous fish; B: Marine mammal; C: Wolf; D: Adult human – mixed diet.

Table 1: Chemical properties (half-life: *HL* is normalized to a 10 g fish) [7].

Chemical	Log K_{OW}	Log K_{OA}	Biotransformation *HL* (days)	Qualitative rate
Pyrene	5.19	8.73	2.1	moderate
Hexachlorobenzene (HCB)	5.61	7.12	272.9	very slow
Di(2-ethylhexyl) phthalate (DEHP)	7.56	13.01	2.8	moderate
PBDE-47	6.39	10.44	39.5	slow
PBDE-153	7.08	11.89	102.6	very slow
PBDE-209	8.68	15.29	14.5	slow
PCB-52	5.95	8.22	132.0	very slow
PCB-153	6.86	9.45	352.4	very slow
PCB-209	8.27	10.95	731.1	very slow

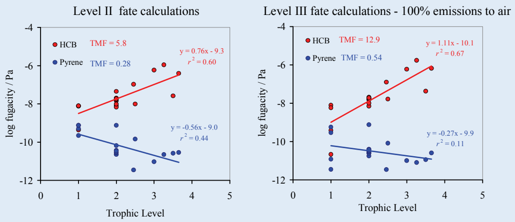


Figure 3: Modelled fugacities (Pa) and TMFs calculated using all RAIDAR organisms for HCB and pyrene.

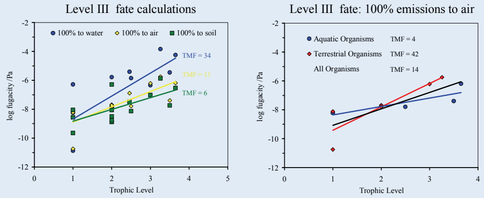


Figure 4: Influence of mode-of-entry to the environment on TMF (left) and differences in TMF as a function of organisms sampled (right) for HCB.

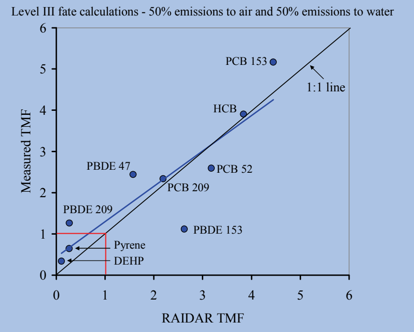


Figure 5: Comparison of modeled and measured (average) TMFs. The measurements are predominantly from aquatic based food webs [7] and thus the modeled TMFs are from plankton to marine mammals. The red line reflects the TMF "B" criterion.

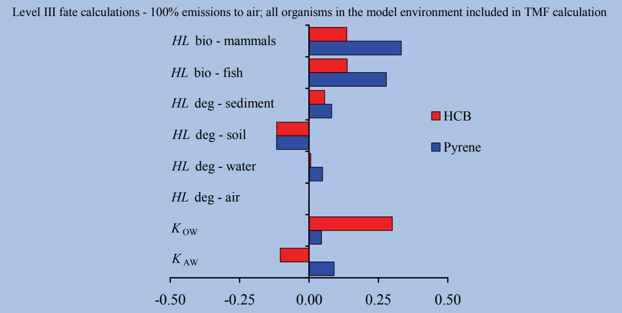


Figure 6: Sensitivity of chemical properties (input parameters) on modeled TMFs.

Results and summary discussion:

- TMFs can be calculated using multimedia mass balance models for a wide range of neutral organic chemicals (**Figure 2**), and thus models may be useful for screening-level TMF assessments.
- Chemical disequilibrium in the physical environment influences TMFs and the fugacities in air, water, soil and sediment for the same chemical can span several orders of magnitude (**Figure 3**).
- Chemical mode-of-entry to the environment influences TMFs (**Figure 4**).
- The organisms and food webs selected for measurement influence the TMFs (**Figure 4**).
- Modeled TMFs are in reasonable agreement with measured TMFs (**Figure 5**).
- Biotransformation half-lives are sensitive parameters, particularly when TMF < 1 (**Figure 6**).
- Future work will include (i) further revisions to the model, (ii) more model evaluations for more diverse chemicals, and (iii) further simulations and "hypothesis generation" to better understand the environmental, biological and chemical properties that influence the TMF.

References:

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