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Evaluating the roles of biotransformation, spatial concentration differences, organism home range, and field sampling design on trophic magnification factors

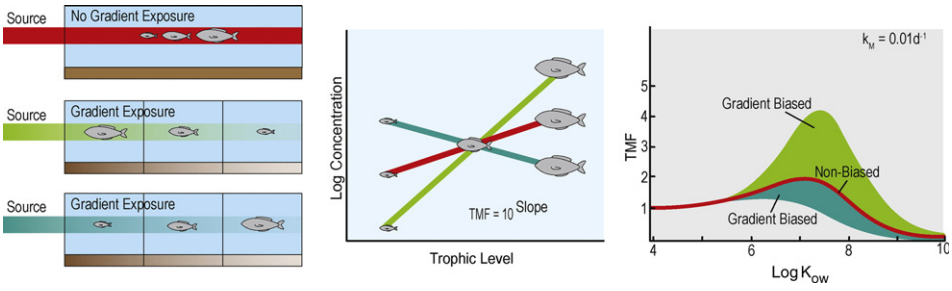
Jaeshin Kim [a], Frank A.P.C. Gobas [b], Jon A. Arnot [c,d], David E. Powell [a,*], Rita M. Seston [a], Kent B. Woodburn [a]

[a] Health and Environmental Sciences, Dow Corning Corporation, 2200 W. Salzburg Road, Auburn, MI 48611, USA
[b] School of Resource & Environmental Management, Simon Fraser University, Burnaby, British Columbia V5A 1S6, Canada
[c] ARC Arnot Research and Consulting Inc., 36 Sproat Avenue, Toronto, Ontario M4M 1W4, Canada
[d] Department of Physical and Environmental Sciences, University of Toronto Scarborough, 1265 Military Trail, Toronto, Ontario M1C 1A4, Canada

HIGHLIGHTS

- A new model was developed to evaluate bioaccumulation in aquatic food webs.
- Model parameters having the greatest influence on bioaccumulation were evaluated.
- Model results in excellent agreement with field results for a well-studied ecosystem.
- Spatial concentration differences may bias interpretation of bioaccumulation.
- Model is useful for a priori design and a posteriori evaluation of field studies.

GRAPHICAL ABSTRACT



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ABSTRACT

Trophic magnification factors (TMFs) are field-based measurements of the bioaccumulation behavior of chemicals in food-webs. TMFs can provide valuable insights into the bioaccumulation behavior of chemicals. However, bioaccumulation metrics such as TMF may be subject to considerable uncertainty as a consequence of systematic bias and the influence of confounding variables. This study seeks to investigate the role of systematic bias resulting from spatially-variable concentrations in water and sediments and biotransformation rates on the determination of TMF. For this purpose, a multibox food-web bioaccumulation model was developed to account for spatial concentration differences and movement of organisms on chemical concentrations in aquatic biota and TMFs. Model calculated and reported field TMFs showed good agreement for persistent polychlorinated biphenyl (PCB) congeners and biotransformable phthalate esters (PEs) in a marine aquatic food-web. Model testing showed no systematic bias and good precision in the estimation of the TMF for PCB congeners but an apparent underestimation of model calculated TMFs, relative to reported field TMFs, for PEs. A model sensitivity analysis showed that sampling designs that ignore the presence of concentration gradients may cause systematically biased and misleading TMF values. The model demonstrates that field TMFs are most sensitive to concentration gradients and species migration patterns for substances that are subject to a low degree of biomagnification or trophic dilution. The model is useful in anticipating the effect of spatial concentration gradients on the determination of the TMF; guiding species collection strategies in TMF studies; and interpretation of the results of field bioaccumulation studies in study locations where spatial differences in chemical concentration exist.

* Corresponding author.

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1. Introduction

Globally, chemicals are routinely evaluated for their bioaccumulation potential (European Chemicals Agency, 2008; European Parliament and the Council of the European Union, 2006; Government of Canada, 1999; Government of Canada, 2000; UNEP, 2001). Several metrics for assessment of chemical bioaccumulation in aquatic organisms and food webs can be considered, including the octanol-water partition coefficient (K_{OW}), bioconcentration factor (BCF), bioaccumulation factor (BAF), biomagnification factor (BMF), and trophic magnification factor (TMF) (Burkhard et al., 2012; Gobas et al., 2009; Weisbrod et al., 2009). The BCF is often preferred over K_{OW} (considered a surrogate for lipid-water partitioning in aquatic biota) because the BCF considers absorption and biotransformation processes in addition to simple organism-water partitioning. However, the BCF is determined under laboratory conditions and does not include dietary exposures and hence excludes the potential for biomagnification (Connolly and Pedersen, 1988; Gobas et al., 1999). In the environment, the diet is often the dominant exposure pathway for very hydrophobic chemicals (Connolly and Pedersen, 1988; Qiao et al., 2000), and the need to consider bioaccumulation metrics that include dietary exposures is generally well recognized (Abelkop et al., 2013; Gottardo et al., 2014; Moermond et al., 2012). Field-derived BAFs, BMFs and TMFs are environmentally relevant because they include all routes of chemical exposure and ecosystem processes. It is notable that TMF and BMF, which were proposed as the most relevant metrics for the identification and categorization of bioaccumulative chemicals, based on a threshold TMF or BMF > 1.0 (Gobas et al., 2009), are explicitly included in weight-of-evidence assessments of bioaccumulation under REACH (ECHA, 2011; ECHA, 2014). Similarly, it has been proposed that the greatest weight-of-evidence ought to be given to high quality field studies when assessing the potential for bioaccumulation and biomagnification (Bridges and Solomon, unpublished manuscript). However, interpretation of field data is susceptible to systematic bias because of uncertainty due to spatial heterogeneity and temporal variability in environmental concentrations (Burkhard, 2003), uncertainty in trophic interactions, species migration and organism home range (Borgå et al., 2012), limited statistical power (Conder et al., 2012), and other ecosystem-specific factors such as sediment-water disequilibrium conditions (Gobas and MacLean, 2003). In some cases, the between-study and within-study variability in exposure conditions is so great that the field data may be questionable and its usefulness severely limited unless experimental designs are implemented that control or account for such variation (Cressie, 1993; Gilbert, 1987). Starrfelt et al. (2013) used Bayesian inference to reduce uncertainty and increase precision of field TMFs. However, this approach does not decrease variability or systematic bias of the TMF that may occur, for example, as a result of spatial differences in sediment-water concentration distributions.

Field TMFs of well-studied hydrophobic chemicals that are known to biomagnify in aquatic food webs, such as several polychlorinated biphenyl (PCB) congeners and other legacy contaminants, are regularly determined with relatively high precision for individual study areas and hence are often used as reference chemicals (e.g., PCB-153 and PCB-180) for trophic magnification studies. However, several studies have reported that TMFs are highly variable when compared across study areas, which has been attributed to uncertainty in the determination of TMF, especially for legacy contaminants and emerging chemicals that have been identified as being very bioaccumulative. For example, Franklin (2015) highlighted the variability and uncertainty in field BMFs and TMFs for per- and poly-fluoroalkyl substances (PFASs) from various ecosystems. Published field TMFs for the most intensively studied PFASs ranged from 0.58 to 13 (n = 10 studies) for perfluorooctanoic acid (PFOA) and from 1.0 (TMF not statistically significant; $p > 0.05$) to 20 (n = 12 studies) for perfluorooctane sulfonic acid (PFOS). The variability and uncertainty were hypothetically attributed to such factors as non-achievement of steady state, differences in feeding ecology, biotransformation, seasonal and annual growth rates, gender, reproductive off-loading, and failure to co-locate prey and predators, among others. Franklin (2015) thus concluded that given the possible confounding factors in field studies, it was preferable to base regulatory decisions on tests conducted under strictly monitored laboratory conditions with selected species and use field observations as only one component of a broader weight of evidence evaluation.

Similar to that observed for PFAS, review of published field TMFs for the most intensely studied polychlorinated biphenyls in aquatic poikilothermic food webs ranged from 0.48 to 15 (n = 49 studies) for PCB-153 and from 0.56 to 17 (n = 43 studies) for PCB-180 (D. E. Powell, unpublished results). Review of published and reported field TMFs for the most intensely studied cyclic volatile methylsiloxanes (cVMS) ranged from 0.54 to 1.5 (n = 20 studies) for octamethylcyclotetrasiloxane (D4), from 0.25 to 3.2 (n = 21 studies) for decamethylcyclopentasiloxane (D5) (Gobas et al., 2015), and from 0.32 to 2.7 (n = 20 studies) for dodecamethylcyclohexasiloxane (D6); Table S1 of the of the Supplemental information, SI. For a subset of the cVMS (n = 11 study areas) and the PCB congeners (n = 6 study areas), differences between field TMFs do not appear to be explained by systematic differences between the study areas—i.e., between environment (marine vs. freshwater), type of food web (pelagic vs. demersal), length of the sampled food webs, or species composition of the sampled food webs (Table S1 of the SI). Rather, the TMF contradictions between study areas may be related to differences in food web dynamics and variable conditions of exposure. Similarly, Guildford et al. (2008) concluded that the variability associated with field TMFs for PCBs in salmonid food webs was influenced by habitat use and lake characteristics.

The contradictions in reported field TMFs between study areas emphasizes the importance of identifying the apparent causes of variability, including whether the different findings are due to different ecosystems investigated, sampled food web species, insufficient understanding of food web dynamics (i.e., predator prey relationships and trophic level structure), or other differences in food web characteristics, study methodology, and experimental design. For example, it is typically assumed when calculating a field TMF that all individuals and species in the sampled food web are exposed to the same conditions across the study area such that the confounding factors of non-uniform patterns of organism movement and variable conditions of exposure may therefore be ignored (Borgå et al., 2012). Consequently, the location from where samples are taken may not be considered important even for environments where spatial concentration differences are inevitably present. Spatial concentration differences of a chemical in the water and sediment are expected to exist due to the presence of point source(s) of the chemical, as may occur, for example, from a wastewater treatment facility or a production facility. However, spatial concentration differences may also occur across thermoclines, pycnoclines, and other physical interfaces in areas that are remote from point sources, which is where most TMF studies have thus far been conducted. Sediment focusing and advective transport of sediment bound contaminants from high energy erosional areas to low energy depositional areas may also cause spatial concentration differences to exist in areas that do not receive point source emissions. Also, sediment-water fugacity ratios can vary among locations as a result of temporal changes of contamination levels and differences in the degree of carbon utilization among locations (Gobas and MacLean, 2003).

It is recognized that, while the use of environmentally-relevant bioaccumulation metrics is highly desirable, the current variability in data generated from field studies may hinder widespread use of field derived bioaccumulation data for regulatory assessment. Improved quality and scientific understanding of field bioaccumulation metrics, such as the TMF, and the factors that affect these metrics are thus needed to reduce variability and foster confidence in using this type of data for decision-making (Burkhard et al., 2013). A better recognition of the factors controlling field derived bioaccumulation metrics may also provide