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Processes influencing chemical biomagnification and trophic magnification factors in aquatic ecosystems: Implications for chemical hazard and risk assessment

Donald Mackay [a], Alena K.D. Celsie [a,*], Jon A. Arnot [b,c], David E. Powell [d]

[a] Chemical Properties Research Group, Department of Chemistry, Trent University, Peterborough, ON, K9L OG2, Canada
[b] ARC Arnot Research and Consulting Inc., 36 Sproat Avenue, Toronto, ON, M4M 1W4, Canada
[c] Department of Physical and Environmental Sciences, University of Toronto Scarborough, 1265 Military Trail, Toronto, ON, M1C 1A4, Canada
[d] Dow Corning Corporation, Health and Environmental Sciences, Auburn, MI 48611, USA

HIGHLIGHTS

- TMFs are highly dependent on a substance's K_{OW} value.
- Biotransformation can greatly reduce TMFs.
- Increased sediment-to-water ratios can influence TMFs.
- Food web omnivory has only a small effect on TMFs.
- Spatial variability in water concentrations can have a profound effect on TMFs.

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ABSTRACT

Bioconcentration factors (BCFs) and bioaccumulation factors (BAFs) are widely used in scientific and regulatory programs to assess chemical hazards. There is increasing interest in also using biomagnification factors (BMFs) and trophic magnification factors (TMFs) for this purpose, especially for highly hydrophobic substances that may reach high concentrations in predatory species that occupy high trophic level positions in ecosystems. Measurements of TMFs in specific ecosystems can provide invaluable confirmation that biomagnification or biodilution has occurred across food webs, but their use in a regulatory context can be controversial because of uncertainties related to the reliability of measurements and their regulatory interpretation. The objective of this study is to explore some of the recognized uncertainties and dependencies in field BMFs and TMFs. This is accomplished by compiling a set of three simple food web models (pelagic, demersal and combined pelagic–demersal) consisting of up to seven species to simulate field BMFs and TMFs and to explore their dependences on hydrophobicity (expressed as log K_{OW}), rates of biotransformation and growth, sediment-water fugacity ratios, and extent of food web omnivory and issues that arise when chemical concentration gradients exist in aquatic ecosystems. It is shown that empirical TMFs can be highly sensitive to these factors, thus the use of TMFs in a regulatory context must recognize these sensitivities. It is suggested that simple but realistic evaluative food web models could be used to extend BCF and BAF assessments to include BMFs and TMFs, thus providing a tool to address bioaccumulation hazard and the potential risk of exposures to elevated chemical concentrations in organisms at high trophic levels.

1. Introduction

There is scientific and regulatory interest in understanding and quantifying the fate, bioaccumulation, exposure and potential for adverse effects of chemicals released to the environment. Trophic biomagnification across a food chain or food web can considerably

* Corresponding author. Trent University, 1600 West Bank Drive, Peterborough, ON, K9J 7B8, Canada.
E-mail addresses: dmackay@trentu.ca (D. Mackay), alenacelsie@trentu.ca (A.K.D. Celsie), jon@arnotresearch.com (J.A. Arnot), david.powell@dowcorning.com (D.E. Powell).

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increase chemical concentrations, hence exposure and potential risk, at higher trophic levels compared to concentrations at lower trophic levels (Czub and McLachlan, 2004; Czub et al., 2008; Kelly et al., 2007). There is thus an incentive to understand and include these magnification processes in both hazard and risk assessment. Bioaccumulation assessments seek to identify chemicals with high potential for bioaccumulation and employ several metrics and criteria as reviewed by several authors, notably Borga et al. (2012a,b), Gobas et al. (2009), Burkhard et al. (2013), and others. Uncertainty is inherent whether the bioaccumulation data are measured from laboratory tests, through field monitoring campaigns, or calculated using models. Mass balance models provide mechanistic insights into bioaccumulation processes (Thomann et al., 1992; Arnot and Gobas, 2006; Kelly et al., 2007; Barber, 2003; Barber, 2008; Walters et al., 2011; Kim et al., 2016). Food web mass balance bioaccumulation models also highlight the basic relationships between various chemical and biological properties and ecological properties and processes and the metrics used to assess bioaccumulation and exposure (Mackay et al., 2013). Reliable measurements and models foster confidence in scientific knowledge and in applying various sources of information for decision-making.

Standard test protocols have been developed for determining bioconcentration factors (BCFs) and biomagnification factors (BMFs) under well-defined laboratory conditions (OECD, 2012). In these tests the organism is only exposed to a chemical either from the water (BCF) or from the diet (BMF). In the environment, organisms are exposed to chemical from their surrounding environment (e.g., water) and from their diet. Although insightful, the BCF is not necessarily ecologically relevant for hydrophobic chemicals because dietary exposure, and hence the potential for biomagnification, is not included (Qiao et al., 2000; Thomann et al., 1992). The bioaccumulation factor (BAF) includes all exposure routes under environmental conditions and is often determined from monitoring data (Arnot and Gobas, 2006). Biomagnification and trophic magnification are conveniently expressed in terms of fugacity increases from prey to predator or throughout the food web as advocated by Gobas et al. (2009), Burkhard et al. (2013) and others. Lipid normalised concentration can also be used instead of fugacity if it is assumed that the two quantities are proportional. For each organism the log fugacity (or log of the lipid normalized concentration) is plotted as a function of trophic position or trophic level (TL) and the trophic magnification factor (TMF) is deduced from the slope, i.e. TMF is $10^{(\text{slope})}$ or $10^{(\Delta\log f/\Delta TL)}$ (Mackay et al., 2013). The TMF is thus a metric of the "average BMF" of the chemical in the sampled ecosystem. Field metrics may be accepted as lines of evidence for bioaccumulation assessment; however, considerable variability is expected in fugacities (and concentrations) and hence BAFs, BMFs and TMFs. Recently, Conder et al. (2012), Starrfelt et al. (2013), Burkhard et al. *(2013)*, Franklin (2016), McLeod et al. (2014), and Kim et al. (2016) have discussed uncertainties inherent in the use of TMFs. Mass balance TMF models have been developed, applied and evaluated, e.g., (Walters et al., 2011). Kim et al. (2016) compiled a "multi-box" model similar to that developed here but addressing the effect of spatial differences in water and organism concentrations. They also conducted an uncertainty and sensitivity analysis.

The objective of this study is to explore some of the recognized uncertainties and dependencies in field BMFs and TMFs with a view to ensuring that BMFs and TMFs are applied rigorously in both scientific and regulatory contexts. To accomplish this we apply simple, well-accepted evaluative mass balance models to illustrate factors that influence biomagnification (specifically BMFs and TMFs), including a chemical's octanol–water partition coefficient (K_{OW}), biotransformation rates, the sediment/water fugacity ratio of the chemical, food web branching (or more properly termed omnivory) and spatial variability in water concentrations. The equations used here and the parameterisations are deliberately simplistic and thus have less fidelity to real systems, but this simplicity is justified by the objective of clearly identifying the key factors that influence TMFs. This model is only intended to be applied to neutral, relatively hydrophobic organic chemicals and not to ionogenic chemicals. There is no intention in this study to define the absolute uncertainty in reported TMFs.

2. Methods

2.1. Trophic position and magnification

Trophic level (TL) or position occupied by an organism can be estimated from the biological enrichment of ^{15}N by organisms during each digestive event. Applying an enrichment factor of typically 3.4‰ per trophic level step enables the TL to be estimated. The enrichment factor is subject to variability, especially at lower TLs. The TL is essentially the number of trophic level steps or transfers (n) that the food has experienced as it is consumed and transferred from the base of the food web (TL = 1 or TL_1) to increasingly higher trophic levels (TL = n or TL_n).

When written in terms of fugacity (f) biomagnification across a food web may be described as:

$$\log f_{y2} - \log f_{y1} = (TL_{x2} - TL_{x1}) \cdot \log TMF \quad (1)$$

The term $TL_{x2}-TL_{x1}$ is the trophic level separation between two species on a linear food chain or the length of the food web under consideration, which may be represented as ΔTL (i.e. $\Delta TL = TL_{x2}-TL_{x1}$). In the situation where ΔTL = 1, Eq. (1) reduces to TMF = f_{y2}/f_{y1}, which by definition is a BMF. The simplest case is a linear food chain in which omnivorous feeding does not occur and each predator species (TL = x) consumes only the prey species (TL = x−1) that occupies the trophic position that is one step below that of the predator. Thus if the ratio of predator to prey lipid normalised concentrations or fugacities (i.e., the BMF) is equal for each increase in TL, then for a linear food chain of n species f_n/f_1 equals $TMF^{(n-1)}$ where f_1 is the fugacity in the organism that occupies TL = 1 and f_n is the fugacity in the organism that occupies TL = n. A plot of log f versus TL for a linear ideal food chain thus has a slope of log TMF (=log BMF) and an intercept at TL_1 of log f_1. Similarly, a plot of log f versus TL for a food web has a slope of log TMF and an intercept at TL_1 of log f_1. Essentially a BMF is the slope between two points (and calculated as the ratio of concentrations because ΔTL = 1) while a TMF is a slope involving all points.

2.2. Evaluative TMF model development

To advance understanding of food web bioaccumulation it is desirable to analyse both monitoring observations and predictions or simulations from mass balance models. First, we introduce the concept of an 'ideal' food web, using the word 'ideal' in the same sense as used in the Ideal Gas Law. That law is a relatively simple mathematical expression of the behaviour of atoms or molecules in a dilute gaseous state that explains the effects of pressure, temperature, density and related transport phenomena such as diffusion using a model consistent with kinetic theory. It is acknowledged that the model fails under many conditions such as high density or temperature, but it provides a sound basis for introducing correction factors such as compressibility. It explains in broad terms the dominant phenomena using intuitively satisfying assumptions or concepts. By analogy, in this case the aim is to demonstrate the factors that influence BMFs and TMFs in ideal food