

A METABOLISM-BASED BIOMAGNIFICATION MODEL FOR THE PREDICTION OF CONCENTRATIONS AND EFFECTS OF DIOXINS IN HIGH TROPHIC LEVELS

Milagros Vega, María Victoria Pablos, José María Navas, José Vicente Tarazona

Laboratory for Ecotoxicology, Department of Environment, INIA, Carretera de la Coruña, km 7, 28040-Madrid, Spain.

Introduction

Toxic concentrations of some substances can be reached in predators even if the concentration in the environment remains below the threshold level for direct toxicity¹. Biomagnification of hydrophobic chemicals is a major risk for higher predators within the food webs leading to increased food chain accumulation. Models describing biomagnification processes are available to estimate tissue concentrations of (non-ionic) organic chemicals in food webs. These models show good correlation with field measures² and are being used in scientific and regulatory applications.

In the Environmental Risk Assessment (ERA) of pollutants, their chemical properties and/or bioconcentration factors (BCFs) are taken into account. However, prediction of biomagnification accounting only physico-chemicals properties is very difficult (e.g. the esteric/volumetric properties of the molecules can preclude the uptaking to the organism). In addition, the metabolism of chemicals can vary enormously between taxonomic groups (e.g. some chemicals could be easily metabolised in vertebrates but not in invertebrates, reaching particularly high concentration in some invertebrate species, that can be highly toxic for vertebrates).

This work describes an approach to a biomagnification model, which is based on estimations of Predicted Environmental Concentrations (PECs) of chemicals in sediments, water and biota³. The proposed model estimates the expected final concentration of persistent organic pollutants (POPs) in organisms from different environmental compartments. The ecological model design takes into account the pollutant-environment-organism interactions, such as relevant exposure routes and real toxicokinetic information (i.e. uptake, metabolism and elimination rates of chemicals).

Methods and Materials

Two main routes are considered relevant for the incorporation and bioconcentration of POPs in organisms: a) uptake from the surrounding compartments (PEC_{water} and PEC_{sediment}), and b) uptake through the diet (PEC_{food}). Parameters considered for modeling biomagnification properties are: contribution of different exposure routes (water, sediment, and food) through different trophic levels (primary producers and several consumers) and real toxicokinetic information such as uptake, metabolism and elimination rates of the chemical within the different trophic groups. Figure 1 presents a general scheme showing basic interactions and pathways through biotic and abiotic reservoirs. Considering this rationale, the PEC in a higher trophic level ($PEC_{\text{organisms}}$) will be the sum of the concentrations incorporated through each relevant exposure route, so that the Bioconcentration Factors (BCF), the Biota-Food Accumulation Factors (BFAF) and the Biota Sediment Accumulation Factor (BSAF) must be considered:

$$PEC_{\text{organism}} = [(PEC_{\text{water}})(BCF)] + [(PEC_{\text{food}})(BFAF)] + [(PEC_{\text{sediment}})(BSAF)]$$

RISK ASSESSMENT

These initial estimations can be refined involving toxicokinetic parameters in the systems: $BCF = k_1 / k_2$ where k_1 is the uptake rate and k_2 the depuration rate.

Following the same rationale: $BFAF_{\text{organisms, food}} = F * a / k_2$ (Where, F is the Feeding rate (ingestion/consumption rate) and a the absorption efficiency for the chemical.)

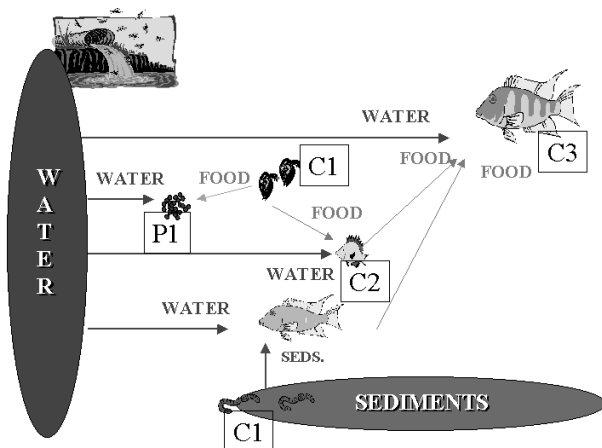


Figure 1. General diagram showing the interactions, trophic levels and chemical reservoirs taken into account to exemplify the model within a simple trophic chain. P1: Primary Producer; C1: Primary Consumers; C2: Secondary Consumers and C3: Tertiary Consumers.

A hypothetical marine trophic chain has been designed consisting in: a) Primary producers, b) Primary consumers: both, water and sediment dwelling organisms feeding on primary producers c) Secondary consumers: small fish and benthic flatfish. d) Tertiary consumers: fish eating secondary consumer fish, e) Top-predators: ictivorous marine organisms (including fish, birds and mammals). f) Filtering mammals: mammals consuming primary producers and primary consumer organisms. According to this scheme, calculations of the PECs in the different levels of the food chain are shown in Table 1.

Table 1. Generic ERA for marine organisms associated to the bioaccumulation and biomagnification of the substance through the food chain. 1P: Primary producers; 1C: Primary consumers; 2C: Secondary consumers; 3C: Tertiary consumers; TP: Top predators; FM: Filtering mammals.

PEC in different trophic levels	PECorganisms (contribution from water + food + sediment)
$PEC_{1P} =$	$PEC_{\text{water}} \times BCF_{1P}$
$PEC_{1C} =$	$[PEC_w \times BCF_{1C}] + [PEC_{1P} \times BFAF_{1C}] + PEC_s \times BSAF_{1C}$
$PEC_{2C} =$	$[PEC_w \times BCF_{2C}] + [PEC_{1C} \times BFAF_{2C}]$
$PEC_{3C} =$	$[PEC_w \times BCF_{2C}] + [PEC_{2C} \times BFAF_{2C}]$
$PEC_{TP} =$	$[PEC_w \times BCF_{TP}] + [PEC_{3C} \times BFAF_{TP}]$
$PEC_{FM} =$	$[PEC_{1P} \times 0.25] + [PEC_{1C} \times 0.75]$

The EUSES program (199xx) has been used to estimate the organic carbon/water-partitioning

coefficient, Koc. Values for the different parameters used in the model are presented in Table 2.

Table 2. Parameters used to run the model.

Trophic level	F (feeding rate)	α (%) (absorption efficiency)	BCF	Half-life (h)
1P (Primary Producers)	-	-	6 ⁴	-
1C (Primary Consumers)	6 ⁵	50	6025 ⁶	20,62 ¹²
2C (Secondary Consumers)	0,1 ⁷	40 *	6025 ⁶	495 ⁸
3C (Tertiary Consumers)	0,15 ⁷	40 *	6025 ⁶	495 ⁸
TP_fish feeding fish (ff)	0,0142 ⁷	40 *	6025 ⁶	495 ⁸
TP_birds feeding fish	0,2 ⁷	60 -90 ⁹		50.808 ¹⁰
TP_mammals feeding fish & mammals	0,1 ⁷	60 -90 ⁹		50.808 ¹⁰
TP_mammals feeding fish	0,05 ⁷	60 -90 ⁹		50.808 ¹⁰
FM (filtering mammals)	0,045 ⁷	60 -90 ⁹		50.808 ¹⁰

TP: Top Predator. Superscripts correspond references. *: estimated from Opperhuizen et al., 1986.

Results and Discussion

After the estimation of Koc of $1.4 \cdot 10^4$, the ratio PECwater/PECsediment was 1/14.000. Figure 2 shows the logarithmic concentrations estimated by the model for each trophic level, according to the initial PECs (PECwater and PECsediments) considered.

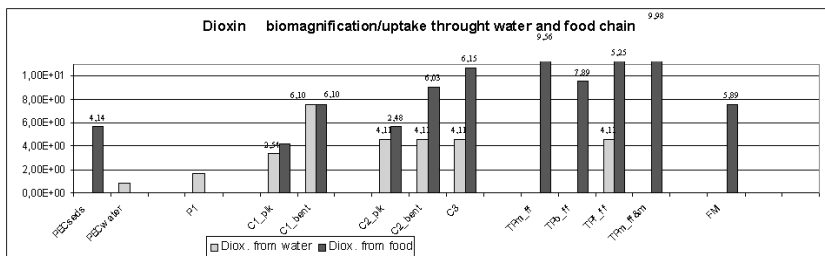


Figure 2. Logarithmic concentrations of 2,3,7,8-tetrachloro-dibenzo-*p*-dioxin (TCDD) estimated by the model.

Bioaccumulation and biomagnification of some compounds such as polychlorinated dibenzo-*p*-dioxins (PCDDs) and dibenzofurans (PCDFs) cannot be predicted from their physicochemical properties like aqueous solubility or octanol/water partition coefficient^{11, 12}. PCDDs can, for instance, reach relatively high concentrations in invertebrates without exert any toxic effect. This phenomenon

RISK ASSESSMENT

may be relevant for the transfer of contaminants through aquatic food webs to potentially sensitive vertebrates species. Differences in sensitivity between fish and invertebrates are thought to be due to differences between taxonomic groups related with the responsiveness to PCDDs mediated by the aryl hydrocarbon receptor (AhR)^{13 14}.

The model presented in this work can also be used in combination with toxicokinetic data of particular pollutants to perform some additional estimations. For example, the content of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) in avian eggs could be calculated taking into account a 33% of the TCDD body burden transferred to the eggs¹⁵. In the same way, the bioaccumulation factor observed in the trout ovary for TCDD (values ranging from 0.21 to 1.08)¹⁶ can be used as the maximal concentration to which are exposed the oocytes before the spawning, so that from these data the TCDD concentration in the eggs could be inferred.

It must also be indicated, that the results presented here have been obtained through a deterministic approach, i.e. the values used in the calculations represented the worst of all possible cases. In the future, it is hoped to use a probabilistic approach, which takes into account not only the inherent variability of all the parameters used in the model, but also other environmental variables that can also influence the organism exposure to a pollutant (i.e. time of permanence of different species in a polluted environment; pollutant distribution in different kinds of food available for omnivorous species, etc...).

References

1. Nendza M, Herbst T, Kussatz C and Gies A. (1997) *Chemosphere* 35, 1875
2. Burkhard LP. (1998) *Environ Toxicol Chem.* 17, 383
3. Carbonell G, Ramos C, Pablos MV, Ortiz JA and Tarazona JV. (2000). *Sci Total Environ.* 247, 143
4. Yockim RS, Isensee AR and Jones E. (1978) *Chemosphere* 7, 215
5. Meador JP, Stein JE, Reichert WL and Varanasi U. (1995). *Rev Environ Contam Toxicol.* 143,79.
6. Branson DR, Takahashi IT and Parker WM. (1985) *Environ Toxicol Chem* 4, 7
7. Sea World Information. <http://www.seaworld.org>
8. Sijm DTHM, Wever H and Poerhhuizen A. (1993) *Environ Toxicol Chem* 12,1895
9. Scientific Criteria Document for Standard Development. (1985) N° 4-84. Hazardous Contaminants Coordination Branch. Ontario Ministry of the Environment.
10. Nygren M, Rappe C and Lindstrom G. (1986) in: Chlorinated Dioxins and Dibenzofurans in Perspective (Rape, C., Choudhary, G., and Keith, L. Edrs) pp17-34. Chelsen, Mich. Lewis.
11. Opperhuizen A, Wagenaar WJ, van der Wielen FWM, van der Berg M, Olie K and Gobas PAPC. (1986). *Chemosphere* 15, 2049.
12. West CW, Ankley GT, Nichols JW, Elonen GE and Nessa DE (1997). *Environ Toxicol Chem.* 16, 1287.
13. Poland A and Glover E (1980). *Mol Pharmacol.* 17, 86
14. Hahn ME, Poland A, Glover E and Stegeman JJ. (1994). *Arch Biochem Biophys* 310, 218
15. Hoffman DJ, Pice CP and Kubiak TJ.(1999) in: Environmental Contaminants in Wild Life. Interpreting Tissue Concentrations. (Nelson, W.B., Heinz, G.H. and Redman-Noirmand, A.W. Edrs.) SETAC ISBN 1-56670-071-X
16. Schell JD, Campbell D and Lowe E. (1993) *Environ Toxicol Chem.* 12, 2077