MODELLING OF BIOACCUMULATION OF POLYBROMINATED DIPHENYL ETHERS IN FOOD WEBS

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Introduction

Brominated flame retardants (BFRs), especially polybrominated diphenyl ethers (PBDEs) and hexabromocyclo-dodecane (HBCD) are found globally in the environment, in wildlife and in human tissues. This indicates that certain BFRs are resistant to biodegradation and biotransformation. Given the fact that many BFRs are fairly lipophilic, this combination of substance properties gives BFRs the potential to bioaccumulate in food webs. As part of the EU-funded FIRE program, bioaccumulation of BFRs in aquatic ecosystems was studied in temperate and arctic food webs. The data generated in these studies were used for modeling of food web transfer of BFRs. As part of the FIRE program, a food web model was developed that describes transfer of BFRs in foodwebs[1].

The model was calibrated and validated on field measurements of PCBs in aquatic food webs. The biotransformation of PCBs by primary producers and cold-blooded organisms is generally very low, and therefore the model calibrated on field bioaccumulation of PCBs can be considered as a worst case prediction of bioaccumulation. This then functions as the base-line model against which field data for other compounds can be compared. From experiments with teleosts, it is clear that PBDE congeners can be biotransformed[2], indicating that the bioaccumulation potential differs between different PBDE congeners. The bioaccumulation model was therefore expanded with a biotransformation model. Based on observed differences for the structurally similar PCBs, the following properties were taken into account that determined biotransformation potential in pinnipeds and cetaceans in previous studies[3]: number of brominated *ortho* positions, presence of adjacent ortho bromines (22' or 66'), the presence of *meta-para* vicinal hydrogen atoms, the presence of *ortho-meta* vicinal hydrogen atoms. The importance of these factors was determined by calibrating the baseline model on PBDE field data and simulating the importance of each factor influencing biotransformation by model optimization on the data.

Materials and Methods

Food web accumulation was modeled using a matrix-type food web model as described previously [1]. Uptake of substances is included as passive diffusion over respiratory and digestive tract membranes. Loss processes are included as clearance (passive elimination), biotransformation, reproductive loss and growth dilution (pseudo elimination). Uptake and loss processes are driven by the partitioning of BFRs over phases: water, lipid, proteins and structural tissues[4].The model was described as a one-compartment model and solved for steady-state.

Several types of input are needed: a) Readily available physico-chemical properties of the chemical e.g. octanol-water partitioning coefficient (Kow), molecular weight, vapour pressure; b) Characteristics of the environment such as concentrations of BFRs in sediment or water, organic carbon content of water and sediment; c) Characteristics of the species that form the foodweb, such as diet, lipid content, weight etc. The model estimates relevant properties of all three different categories to permit the use of defaults as much as possible[1]. The importance of PBDE properties for biotransformation potential was estimated by calibrating the model on the data in an iterative approach. The model was fitted to the data based on least squares optimization of residuals.

Results and Discussion

The further development of the SimpleWeb model encompassed including rules for biotransformation. The difference in biotransformation potential, depending on the molecular structure of the PBDE congeners/isomers, were calibrated on the field data collected in the FIRE project. Especially the BFR data from the North Sea, the Wadden Sea and the Scheldt estuary were used to focus on the transfer of PBDEs from invertebrates to relevant species for the risk assessment such as fish and fish-eating birds (terns). With this procedure, (relative) structure-transformation rules could be quantified into field-relevant biotransformation rates for inclusion in the

SimpleWeb model. Especially the presence of brominated ortho positions and the presence of *meta-para* or *ortho-meta* vicinal hydrogen atoms influenced the fit of the model to the data.

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