WHICH BIOACCUMULATION MODEL PARAMETERS MATTER THE MOST? SENSITIVITY ANALYSIS OF A MODEL APPLICATION FOR GRENLAND FJORDS AQUATIC FOOD WEB, NORWAY

Saloranta TM

Norwegian Institute for Water Research (NIVA), Gaustadalléen 21, N-0349 Oslo, Norway

Abstract

The Extended FAST global sensitivity analysis method is used to analyse the influence of 17 different rate constant bioaccumulation model parameters in a model application of the aquatic food web in the Grenland fjords, southern Norway. This fjord system has some of the highest concentrations of dioxins in sediments of any fjord in Norway. Parameter sensitivity indices are presented for the dioxin concentration and benthic/pelagic dioxin contamination influence of four different key species in the food web (crab, flounder, large cod and trout). The metabolic transformation and feeding related parameters are found to be the most influential for the fish species, while the equilibrium partitioning related parameters are the most influential for crab.

Introduction

The Grenland fjords, situated in the southern Norway, have some of the highest concentrations of polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs) in sediments of any fjord system in Norway. The main load of PCDD/Fs has come from a magnesium plant on Herøya in the innermost fjord basin Frierfjorden in the period 1951-2002. Since the 1960s dietary health advisories have been in place and since the 1980s commercialisation bans on all seafood caught within the Frierfjorden area, as well as health advisories on selected commercial species such as cod and crab in the outer fjord areas. Saloranta et al.[1] simulated the bioaccumulation of PCDD/Fs in the food web of Frierfjorden, consisting of 12 organisms or organism groups. They used, among others, the rate constant model formulation and parameterisation of Gobas[2]. In the following, we analyse 17 parameters of this model application with the Extended Fourier Amplitude Sensitivity Test (Extended FAST) sensitivity analysis method in order to find out which model parameters are the most influential for the whole-body concentration and the water/sediment pore water origin of PCDD/Fs in crab, flounder, large cod (>30 cm) and trout.

Materials and Methods

Our bioaccumulation model application for simulating the intake and bioaccumulation of PCDD/Fs in the Frierfjorden food web[1, 2] includes 11 (more or less) general and five application-specific parameters, in addition to the food web matrix. The purpose of these parameters are described in more details in Saloranta et al.[1] and Gobas[2]. The sensitivity of the model results to 17 model parameters, both general and application-specific (Table 1) is analysed by the Extended FAST sensitivity analysis method [3]. In this method the model is run numerous times, choosing at each run a new set of parameter values from wave-like varying parameter series extensively covering the whole multidimensional parameter space (within given parameter value ranges, see Table 1), and the model output is monitored. The contributions of the different parameters on a particular model output (variance) can then be identified based on the discrete Fourier transformation of the model output. The resulting sensitivity indices (Fig. 1) reflect both the parameters' role in the model code and the variation ranges estimated for the parameter values. The selected ranges, given in Table 1, are based on Gobas[2] and the author's expert judgement. The number of model runs in the sensitivity analysis was ~50 000. In the sensitivity analysis of Saloranta et al.[1] parameters related to the calculation of the bioavailable concentration in the aquatic environment were found to be the most influential for PCDD/F concentration in all studied food web organisms. In this paper our focus is entirely on the parameters of the bioaccumulation model, as the bioavailable concentration in the aquatic environment is assumed to be known.

We analysed parameter sensitivity for two different type of model output variables and for four food web organisms[1]: 1) crab, living directly on the contaminated bottom; 2) flounder, feeding on benthic invertebrates living on or having contact with the contaminated bottom; 3) large cod, feeding both on other fish and benthic invertebrates; 4) trout, having a diet of assumedly uncontaminated non-marine species in addition to pelagic fish and benthic invertebrates. The first analysed output variable (denoted by C_b) is the steady state whole-body concentration of PCDD/Fs in the four organisms [ng/kg wet weight], given a normalised constant bioavailable concentration in the aquatic environment, i.e. the sum of the 17 simulated PCDD/F congeners dissolved in water (C_w) and/or sediment pore water (C_s) is assumed equal to 1.0 ng/L. All concentrations in this paper are expressed in toxic equivalents[4] (TEQ), and the relative contributions of the different congeners to the total PCDD/F in the environment is assumed similar to that observed in the Frierfjorden water column[1]. The second analysed output variable (denoted by β) is the fraction of the PCDD/Fs in an organism which is caused by C_s when C_s and C_w are taken to be equal. As our model code is linear in its formulation[1], the conversion from abiotic to biotic concentrations can be written in a steady state as $C_b = K_{BCF}(\beta C_s + (1-\beta)C_w)$, where K_{BCF} is the bioconcentration (or bioaccumulation) factor[2] [L/kg wet weight] for a given organism (i.e. the whole-body concentration of PCDD/Fs in the organisms divided by the dissolved concentration in the environment). The variable β thus reflects the potential importance of sediment vs. water column for the PCDD/F concentration in an organism (the actual importance is, of course, also dependent on the concentration difference between C_s and C_w).

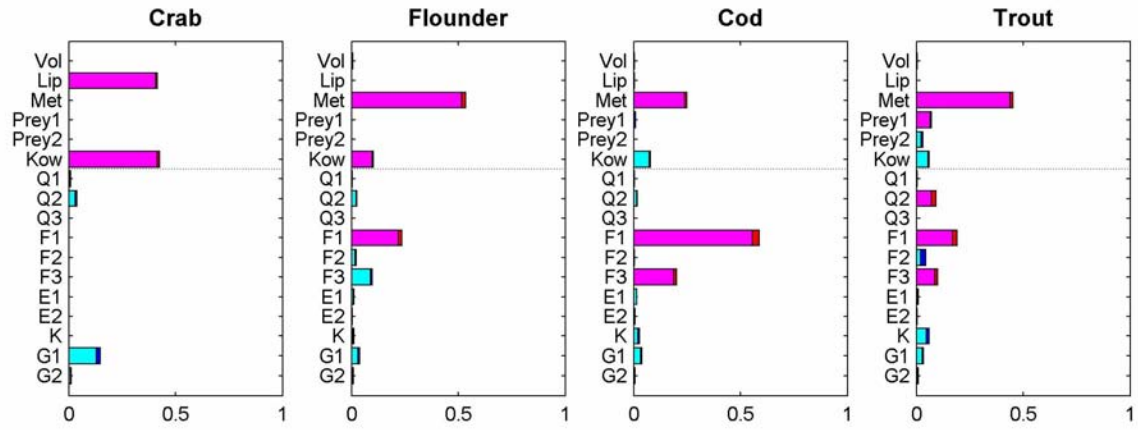
Table 1. The 17 bioaccumulation model parameters included in the sensitivity analysis and their estimated value ranges. The six first parameters (Vol to Kow) are application-specific and the rest are more or less general. Nominal parameter values[2] for the latter group are given in parentheses in the last column.

Parameter	Description	Value range (nominal value)
Vol	Body volume	0.5–2 (scaling of nominal values[2])
Lip	Lipid fraction	0.5–2 (scaling of nominal values[2])
Met	Metabolic transformation rate	0.2–5 (scaling of nominal values[2])
Prey1	Fraction of the main prey in diet	0.2–0.8
Prey2	Scaling for the fraction of the second most important prey in diet	0.2–0.8 (scaling of 1-*Prey1*)
Kow	Octanol-water partitioning coefficient	0.5–2 (scaling of nominal values)
Q1	Gill uptake: coefficient in water phase transport rate equation	60–100 (88.3)
Q2	Gill uptake: exponent (allometric) in water phase transport rate equation	0.4–0.8 (0.6)
Q3	Gill uptake: ratio of lipid to water phase transport rates	0.003–0.03 (0.01)
F1	Constant in feeding rate equation	0.007–0.07 (0.022)
F2	Exponent (allometric) in feeding rate equation	0.65–1.05 (0.85)
F3	Constant for temperature dependency in feeding rate equation	0.02–0.2 (0.06)
E1	Constant in dietary uptake equation	1.7–2.9 (2.3)
E2	Constant in dietary uptake equation	2.3×10^{-8}–8.3×10^{-8} (5.3×10^{-8})
K	Ratio of faecal egestion to ingestion rates	1/8–1/3 (1/4)
G1	Constant in growth rate equation	1.7×10^{-4}–15.0×10^{-4} (5.0×10^{-4})
G2	Exponent (allometric) in growth rate equation	-0.3 – -0.1 (-0.2)

Results and Discussion

The sensitivity indices (Fig. 1) resulting from the sensitivity analysis showed that the model output variable $\log_{10}(C_b)$ in crab was most sensitive to lipid fraction (*Lip*) and the octanol-water partitioning coefficient (*Kow*), while in large cod, flounder and trout $\log_{10}(C_b)$ was most sensitive to the metabolic transformation rate (*Met*) and to the constant *F1* in the feeding rate equation. This seem reasonable as equilibrium partitioning with the environment applies for crab in the model code (in addition to the effect of growth dilution), while for fish the diet constitutes the major PCDD/F input. Moreover, the larger uncertainty around the values of *Met* contributes to the high sensitivity indices, together with its important role as one of the six simulated PCDD/F rates in the model code. In addition to these most sensitive parameters, also the constant *G1* in the growth rate equation was found somewhat influential for crab, the constant *F3* in the feeding rate equation and *Kow* were found somewhat influential for flounder and large cod, while *F3*, the allometric exponent *Q2* in the gill uptake water phase transport rate equation, and the fraction of non-marine prey in the diet of trout (*Prey1*) were found somewhat influential for trout here. The rest of the analysed parameters (i.e. most of them) showed even less or no significant influence on the output variable $\log_{10}(C_b)$.

(a) $\log_{10}(C_b)$



(b) β

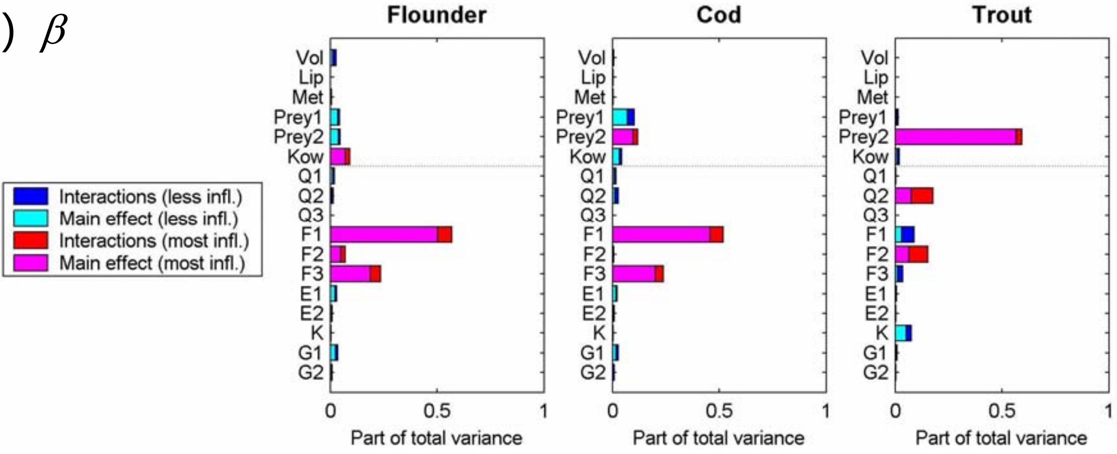


Figure 1. Sensitivity indices for the 17 parameters analysed in the Extended FAST sensitivity analysis for model output variables $\log_{10}(C_b)$ and β (see text) for crab, flounder, large cod (>30 cm) and trout. Parameter abbreviations are explained in Table 1. "Main effect" denotes the particular parameter's effect alone, and "Interactions" its effect due to higher order interactions with other parameters. All the parameters with the lowest main effect sensitivity indices, contributing together with less than 20 % of the total sum of all main effect indices, are denoted with blue colour. No sensitivity indices are shown for β for crab since this output variable is a constant in the model not affected by the analysed parameters.

No sensitivity indices were calculated for the model output variable β for crab, since β is defined as constant in the model for crab (equal to parameter f_{sed} in Saloranta et al.[2]). For the fish species, Fig. 1 shows that β for both flounder and large cod was most sensitive to the constants *F1* and *F3* in the feeding rate equation, while for trout the most sensitive parameter here was the scaling coefficient *Prey2* for the fraction of the second most important prey (clupeids) in its diet. As already pointed out above, the PCDD/F input via diet is important for the fish, and thus the magnitude of the feeding rate and the composition of diet (i.e. its relation to the contaminated bottom) turn out to be important for the simulated value of β. Since the coefficient *Prey1* for the fraction of non-marine prey in the diet of trout does not affect β, which is related to the benthic/pelagic PCDD/F source, it is quite evident that the coefficient *Prey2* stands out in the sensitivity analysis. This coefficient governs the benthic/pelagic portion of trout's diet via scaling the fraction of the purely pelagic clupeids. Since all prey organisms of flounder and large cod have either direct or indirect (via their prey) contact with the contaminated sediments, the feeding rate parameters become more influential for β than the diet fraction coefficients. Parameters found to be of secondary importance were the allometric exponent *F2* in the feeding rate equation and *Kow* for flounder, the two diet fraction coefficients *Prey1* (fraction of small cod (<30 cm)) and *Prey2* (fraction of shrimps) for large cod, and the allometric exponents *Q2* and *F2* for trout. The rest of the analysed parameters (i.e. most of them) showed again even less or no significant influence on the output variable β.

Fig. 2 shows distributions of different values of the model output variables $\log_{10}(C_b)$ and β that result in the simulations in the sensitivity analysis when parameter values are sampled from the given parameter ranges (Table 1). In these distributions 95 % of the $\log_{10}(C_b)$ values are in the range 4.2–5.0 in crab, 4.0–5.3 in flounder, and 4.0–5.7 in large cod and trout. As the normalised constant bioavailable PCDD/F concentration in the aquatic environment is 1.0 ng/L, the above ranges of $\log_{10}(C_b)$ are equal to the corresponding ranges for the log-transformed bioconcentration factor $\log_{10}(K_{BCF})$. Similar distributions for β in Fig. 2 show the constant value of 0.64 for crab[2], as well as somewhat lower median values for flounder, even lower for large cod, and lowest for trout, reflecting the differences in the benthic/pelagic PCDD/F source for these fish species. In these distributions 95 % of the simulated β values are within an interval of 0.22–0.26 units for the three fish species.

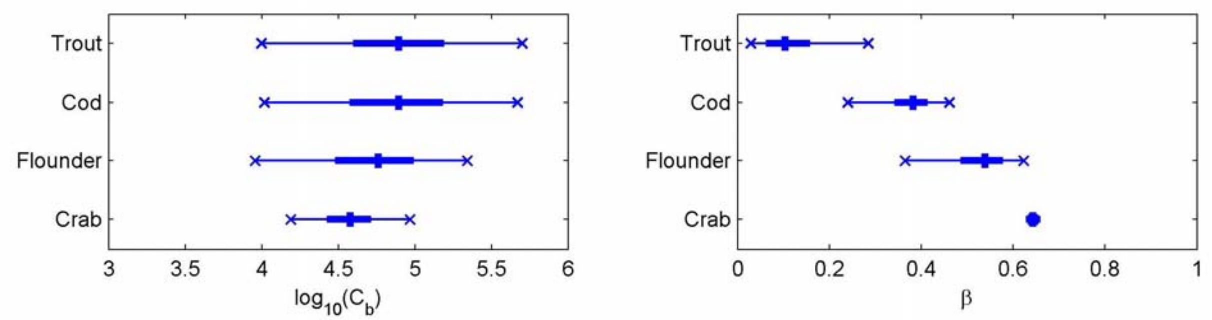


Figure 2. Distribution of the values of the model output variables $\log_{10}(C_b)$ and β (see text) that resulted in the 50 000 model simulations in the sensitivity analysis (Fig. 1) using the parameter ranges given in Table 1. The marker in the middle denotes median, the thicker lines the 25–75th percentile value range, and the thin lines (with end marker "×") the 2.5–97.5th percentile value range.

Acknowledgements
This study was funded by the Norwegian Institute for Water Research (NIVA) and the Research Council of Norway (contract 172708/S30).

References

1. Saloranta TM, Andersen T, Næs K. *Environ. Toxicol. Chem.* 2006; 25:253.
2. Gobas FAPC. *Ecol. Model.* 1993; 69:1.
3. Saltelli A, Chan K, Scott EM. *Sensitivity analysis*, Wiley, New York, 2000.
4. Van der Berg M, Birnbaum L, Bosveld ATC, Brunström B, Cook P, Feeley M, Giesy JP, Hanberg A, Hasegawa R, Kennedy SW, Kubiak T, Larsen JC, van Leeuwen FXR, Liem AKD, Nolt C, Peterson RE, Poellinger L, Safe S, Schrenk D, Tillitt D, Tysklind M, Younes M, Wærn F, Zacharewski T. *Environ. Health Perspect.* 1998; 106:775.