National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

Environmental risk limits for hexachlorobenzene and hexachlorobutadiene in water

Using bioaccumulation data to convert biota standards into water risk limits

RIVM letter report 601714015/2011
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Colofon

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This investigation has been performed by order and for the account of Directorate-General for Environmental Protection, Sustainable Production Directorate, within the framework of the project 'Chemische aspecten van KRW en RPS'

Abstract

Environmental risk limits for hexachlorobenzene and hexachlorobutadiene in water

RIVM has derived environmental risk limits (ERLs) for hexachlorobenzene and hexachlorobutadiene (HCB and HCBD) in water. HCB and HCBD are classified as priority hazardous substances under the European Water Framework Directive. ERLs are proposed for HCB and HCBD in the water column using the data from previous European evaluations combined with a new evaluation of the bioaccumulation data.

Within the WFD, quality standards for chronic exposure in surface water are derived based on three protection goals: direct ecotoxicity to aquatic organisms, exposure of humans through consumption of fishery products, and exposure of predatory birds and mammals through feeding on other animals/prey. Because of the high bioconcentration potential of HCB and HCBD, the latter two are most critical and determine the final quality standard.

The European Commission has set maximum concentrations in biota for HCB and HCBD based on these two critical protection goals, but in the Netherlands regulators have a preference for quality standards based on water concentrations. The Commission offers this possibility, provided that the water quality standards ensure the same level of protection. The reasons and basis for using this approach, and the scientific underpinning of the alternative standards for water should then be notified to the Commission and other Member States. The present report provides the scientific basis for such a notification.

Keywords:
hexachlorobenzene, hexachlorobutadiene, environmental risk limits, human health, secondary poisoning

Rapport in het kort

Milieurisicogrenzen voor hexachloorbenzeen en hexachloorbutadieen in water

Het RIVM heeft milieurisicogrenzen bepaald voor hexachloorbenzeen (HCB) en hexachloorbutadieen (HCBD) in water. HCB en HCBD worden binnen de Europese Kaderrichtlijn Water (KRW) geclassificeerd als prioritair gevaarlijke stoffen. De milieurisicogrenzen voor HCB en HCBD in water zijn afgeleid met gebruik van de gegevens uit eerder Europese evaluaties, gecombineerd met een nieuwe evaluatie van gegevens over opname in biota.

Bij het afleiden van chronische milieurisicogrenzen voor water volgens de Kaderrichtlijn Water (KRW) worden drie beschermingsdoelen in beschouwing genomen: directe ecotoxiciteit voor waterorganismen, blootstelling van mensen via het eten van vis of schaaldieren en blootstelling van vogels en zoogdieren via het eten van dieren/prooi (doorvergiftiging). Door de hoge mate van bioconcentratie van HCB en HCBD zijn deze laatste twee routes het meest kritisch om de uiteindelijke milieurisicogrens te bepalen.

De Europese Commissie heeft maximale concentraties in biota voor HCB en HCBD afgeleid, maar in Nederland bestaat bij de betrokken ministeries een voorkeur voor milieurisicogrenzen gebaseerd op waterconcentraties. De Commissie staat deze mogelijkheid toe, mits de risicogrenzen in water hetzelfde beschermingsniveau garanderen. De redenering achter en basis voor het gebruik van deze methode en de wetenschappelijke onderbouwing van de milieurisicogrenzen voor water moeten dan genotificeerd worden aan de Commissie en andere lidstaten. Het huidige rapport biedt de wetenschappelijke basis voor deze notificatie.

Trefwoorden:
hexachloorbenzeen, hexachloorbutadieen, milieurisicogrenzen, humane blootstelling, doorvergiftiging

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Summary

Within the WFD, quality standards for chronic exposure in surface water are derived based on three protection goals: direct ecotoxicity to aquatic organisms, exposure of humans through consumption of fishery products, and exposure of predatory birds and mammals through secondary poisoning. Because of the high bioconcentration potential of HCB and HCBD, the latter two are most critical and determine the final quality standard.

The European Commission has set maximum concentrations in biota for HCB and HCBD based on these two critical protection goals, but in the Netherlands a preference exists for quality standards based on water concentrations. The Commission offers this possibility, provided that the water quality standards ensure the same level of protection. The reasons and basis for using this approach, and the scientific underpinning of the alternative standards for water should then be notified to the Commission and other Member States. The present report provides the scientific basis for such a notification.

ERLs were determined for HCB and HCBD in the water column using the data from previous European evaluations combined with a new evaluation of the biomagnification and bioconcentration data. In this report the resulting ERLs are reported. Please note that the new values correspond to the dissolved concentration in water, while the values from the substance data sheet refer to total concentrations in water.

Hexachlorobenzene (HCB)
In the substance data sheet for HCB (EC, 2005a), a $QS_{biota,\ hh}$ of 9.74 µg/kg and a $QS_{biota,\ secpois}$ of 16.7 µg/kg are derived. However, compliance checking by means of monitoring in water has advantages over biota sampling in terms of reproducibility, costs and uniformity of sampling. Thus, BAF, BMF and BCF values were evaluated to assess whether they can be used to recalculate biota standards into water standards. This introduces uncertainties regarding the height of the BAF used and the resulting ERL value is thus more uncertain than the value for biota. Therefore, expression of ERLs on the basis of concentrations in biota seems most appropriate. However, this implies that the biota that are monitored in order to check compliance to these WFD requirements, should correspond to the same trophic level as the level the EQS refers to. This also introduces a lot of uncertainties, because HCB concentrations in biota can be highly variable and may depend on the age and trophic level of the fish species sampled, and there is no guidance on this point yet.

A tiered approach is suggested in which the critical water standard of 0.044 ng/L is used in the first instance. If this standard is exceeded in the field, case by case biota can be sampled and compared to the biota standard for compliance checking.

For HCB, using the $QS_{freshwater,\ hh}$ and $QS_{freshwater,secpois}$ values from the substance data sheet is the least preferred option from a scientific point of view, since the BAF value used for these calculations is not correct.

Table 1 Environmental risk limits for hexachlorobenzene in water. Values in µg/L.

ERL[a]	Hexachlorobenzene	
	This report[b]	Substance data sheet[c]
$MPC_{freshwater, eco}$		0.013
$MPC_{saltwater, eco}$		0.013
$MPC_{freshwater, hh}$	0.000044	0.00023
$MPC_{saltwater, hh}$	0.000044	0.00023
$MPC_{freshwater, secpois}$	0.000076	0.0004
$MPC_{saltwater, secpois}$	0.000025	0.0004

[a] MPC = Maximum Permissible Concentration. The subscript 'eco' refers to direct ecotoxicity; the subscript 'secpois' refers to secondary poisoning, the subscript 'hh' refers to consumption of fish and shellfish by humans.
[b] Dissolved concentrations
[c] Total concentrations

Hexachlorobutadiene (HCBD)

From Table 2, it is clear that the proposed values for HCBD were lower by a factor of 1.2 to 4 for secondary poisoning and a factor of 1.3 to 30 for human consumption of fishery products, depending on the choice of BCF in the substance data sheet. It is however clear, that the ERLs for human consumption of fishery products and secondary poisoning are much lower than the ERL based on direct ecotoxicity of 0.44 µg/L for HCBD.

Table 2 Environmental risk limits for hexachlorobutadiene in water. Values in µg/L.

ERL[a]	Hexachlorobutadiene	
	This report[b]	Substance data sheet[c]
$MPC_{freshwater, eco}$		0.44
$MPC_{saltwater, eco}$		0.44
$MPC_{freshwater, hh}$	0.00055	0.0007-0.0174
$MPC_{saltwater, hh}$	0.00055	0.0007-0.0174
$MPC_{freshwater, secpois}$	0.0025	0.003
$MPC_{saltwater, secpois}$	0.00082	0.003

[a] MPC = Maximum Permissible Concentration. The subscript 'eco' refers to direct ecotoxicity; the subscript 'secpois' refers to secondary poisoning, the subscript 'hh' refers to consumption of fish and shellfish by humans.
[b] Dissolved concentrations
[c] Total concentrations

1 Introduction

1.1 Water quality standards

The European Water Framework Directive (WFD) aims at “maintaining and improving the aquatic environment in the Community”. Member States should achieve the objective of at least a “good ecological status” and a “good chemical status” by defining and implementing the necessary measures within integrated ‘programs of measures’. For a good chemical status the WFD requires that environmental quality standards (QSs) are met. These QSs thus serve as a benchmark to decide whether or not specific measures are required.

The methodology for deriving QSs for hexachlorobenzene and hexachlorobutadiene was developed by Lepper (2005), based on the Technical guidance document (TGD) in support of the risk assessment for new and existing substances and biocides (EC, 2003). In this report, the draft new QS guidance is followed (EC, 2010). The QSs for priority (hazardous) substances are set on EU community level. For other compounds that are relevant to individual member states, standards are set on a national level. In the Netherlands, the methodology of the WFD is incorporated in the derivation of Environmental Risk Limits (ERLs) within the context of the project ‘Standard setting for other relevant substances within the WFD’, which is closely related to the project INS (‘International and national environmental quality standards for substances in the Netherlands’).

1.2 Use and release of HCB and HCBD

Hexachlorobenzene (HCB) was formerly used as a fungicide, but due to its harmful properties it has been banned globally under the Stockholm Convention[1]. It is also used for the production of fireworks, ammunition and synthetic rubber, and as an intermediate during the production of pesticides. Hexachlorobenzene is a byproduct of the production of chlorinated solvents, but this process takes place in closed systems.

Hexachlorobutadiene (HCBD) is mainly used as solvent for other chlorinated compounds. HCBD is formed as a byproduct during the production of carbon tetrachloride and tetrachloroethene. HCBD is used as a scrubber in order to remove chlorine containing contaminants from gas streams, for the manufacturing of flame resistant hydraulic fluids and lubricants, and for isolation fluids in electrotechnical practices. HCBD used to be applied as a pesticide, but this use has been stopped because of its ecotoxicity.

1.3 Biota standards for HCB and HCBD

Water quality standards for chronic exposure are based on three protection goals: direct ecotoxicity to aquatic organisms, exposure of humans through consumption of fish and fishery products (referred to as the ‘human route’), and exposure of predators through secondary poisoning. The most critical of these routes determines the final standard. For compounds that have a strong potential to bioaccumulate in fish, the human and secondary poisoning routes are often the most critical. Due to the characteristics of these compounds, concentrations increase along the food chain. Consumption of fish therefore

[1] http://chm.pops.int/Home/tabid/36/language/en-US/Default.aspx

leads to critical levels in humans or predators while at similar concentrations in water, aquatic organisms are not affected. For these compounds, concentrations in fish can be calculated that will not cause adverse effects in humans or predatory birds and mammals upon lifetime consumption.

For the priority hazardous substances hexachlorobenzene and hexachlorobutadiene, the human and secondary poisoning routes are the most critical, because of the high level of bioconcentration of these compounds. According to the preamble of Directive 2008/105/EC (EC, 2008), EU community level QSs based on surface water concentrations are sufficient for the majority of substances. However, for HCB, HCBD (and mercury), it was considered appropriate to establish QSs for biota at the EU community level, because for these substances it is "not possible to ensure protection against indirect effects and secondary poisoning at Community level by QS for surface water alone".

Therefore, maximum concentrations in biota for HCB and HCBD of 10 and 55 $\mu g/kg_{ww}$ are set in Art 3(2) of Directive 2008/105/EC, based on substance data sheets that were compiled in 2005 (EC, 2005a and 2005b). The reason for setting standards based on concentrations in biota rather than concentrations in the water column was primarily the uncertainty surrounding bioconcentration and biomagnification factors (BCFs and BMFs, see below).

1.4 Aim of this report: derivation of water-based risk limits

When quality standards are set for biota, this also means that water quality should be monitored based on measured concentrations in biota. In the Netherlands, measuring water samples is preferred above designing and maintaining a biota monitoring program. According to Directive 2008/105/EC, if member states do not apply standards for biota they shall introduce equal or stricter quality standards for water than those in the daughter directive, in order to achieve the same level of protection as the standards for biota. In that case, the Commission and other Member States should be notified of the rationale for using this approach, the alternative quality standard for water established, including the data and the methodology by which the alternative quality standard was derived, and the categories of surface water to which it would apply.

The responsible ministries in the Netherlands decided to investigate the possibility to rely on water-based quality standards for HCB and HCBD and requested RIVM to derive ERLs for water for these compounds. In the Netherlands, the term "ERL" is used for the scientific advisory values that are used as a basis for (legal) environmental quality standards (QSs). ERLs should thus be considered as preliminary values that do not have an official status until approved by the responsible authorities.

1.5 Methodology: Quality standards for bioaccumulating compounds

The methodology for the derivation of ERLs for water is described in detail in the INS-guidance (Van Vlaardingen and Verbruggen, 2007). This guidance is prepared within the context and using the methodology of the WFD. In this report, the draft new QS guidance is followed as much as possible (EC, 2010).

Chronic risk limits for water are represented by the Maximum Permissible Concentration (MPC). The risk limits for secondary poisoning of birds and mammals ($MPC_{freshwater,\ secpois}$) and human fish consumption ($MPC_{freshwater,\ hh}$) are equivalent to the $QS_{freshwater,\ hh}$ and $QS_{freshwater,\ secpois}$, respectively. A new

evaluation of biomagnification and bioconcentration data is performed and appropriate input data are selected for derivation of water-based ERLs. The QSs as derived by the Commission based on other routes (i.e. direct ecotoxicity) are not discussed.

According to the WFD-methodology, the QS for human consumption of fishery products, expressed as a concentration in fish ($QS_{biota,\ hh}$)[2], is calculated from the human-toxicological threshold (TDI), assuming a body weight of 70 kg, a daily intake of 115 g fish/day, and a maximum contribution to the TDI of 10%. The QS for predatory birds or mammals, also expressed as a concentration in fish ($QS_{biota,\ secpois}$), is derived by applying an assessment factor to the No Observed Adverse Effect Level (NOAEL) from toxicity experiments.

Starting from these biota standards (see Figure 1), corresponding water concentrations can be calculated. For this, information on the accumulation of substances by aquatic organisms from the aqueous phase (bioconcentration) and accumulation in the food chain (biomagnification) has to be taken into account. These processes are represented by a laboratory bioconcentration factor (BCF) and biomagnification factors (BMF), or the bioaccumulation factor (BAF).

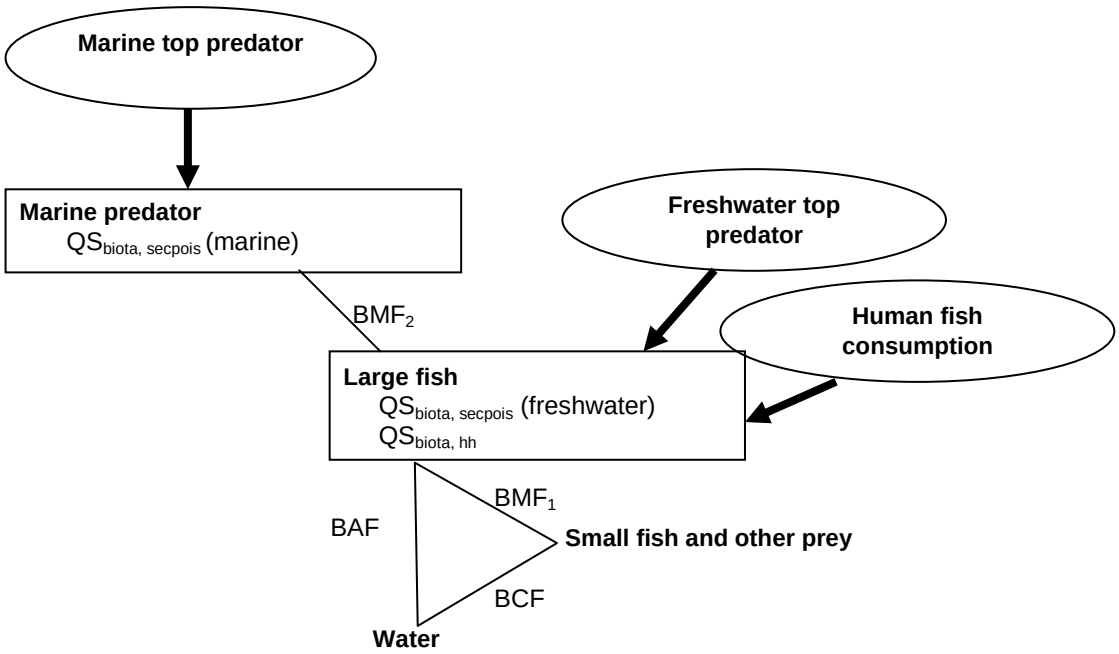

Figure 1 Scheme on how to recalculate biota standards into water concentrations. Ovals are protection goals (species to be protected); rectangles are the trophic levels on which the QSs are set to protect the upper trophic levels.

[2] For reasons of consistency, the terminology of the draft new QS guidance is used. In previous documents, other terms were used, e.g. $QS_{hh\ food,\ biota}$ and $QS_{hh\ food,\ water}$ instead of $QS_{biota,\ hh}$ and $QS_{freshwater,\ hh}$

Bioconcentration

The BCF is the ratio of the concentration in the organism (in wet weight, preferably normalised to 5% lipids (ECHA 2008) divided by the water concentration. BCF values are mostly determined in the laboratory, where the only exposure is through the water phase.

Biomagnification

The BMF is the ratio of the concentration in the predator organism divided by the concentration in the prey organism (for hydrophobic organic chemicals commonly normalised to lipid content of prey and predator). Two BMFs are distinguished. The first, BMF_1, describes the biomagnification from small fish to larger fish that in turn is eaten by predators (including humans). For the marine environment, a second BMF_2 is included to account for accumulation in bird and mammals (e.g. seals, dolphins, seabirds) that serve as food for top predators such as polar bears and killer whales. In general, biomagnification, and thus total bioaccumulation, increases with increasing bioconcentration potential.

Using the biota standards, the accompanying concentrations in water ($QS_{water,\ hh}$ and $QS_{freshwater,\ secpois}$) are calculated by dividing the $QS_{biota,\ hh}$ and $QS_{biota,\ secpois}$ by the product of BCF and BMF_1 for freshwater and BCF, BMF_1 and BMF_2 for marine waters. For example, for the QSs for secondary poisoning:

$$QS_{freshwater,secpois} = \frac{QS_{biota,secpois}}{BCF \times BMF_1}$$

$$QS_{saltwater,secpois} = \frac{QS_{biota,secpois}}{BCF \times BMF_1 \times BMF_2}$$

Bioaccumulation

The term BCF x BMF may be replaced by a bioaccumulation factor (BAF), which is the ratio of the concentration in the organisms (in wet weight, preferably normalised to 5% lipids (ECHA, 2008)) divided by the concentration in its surroundings (the water column). The BAF is often determined in the field, where the uptake routes include both uptake through the water phase and uptake through food. Thus, for example the $QS_{water,\ secpois}$ can also be calculated according to:

$$QS_{water,secpois} = \frac{QS_{biota,secpois}}{BAF}$$

1.6 Dissolved versus total concentrations

According to the newest methodology (EC, 2010), all QSs are reported as dissolved concentrations. To recalculate these into total concentrations, the methodology as described in paragraph 3.1.8 of Van Vlaardingen and Verbruggen (2007) can be used, using a valid K_{OC}.

2 Hexachlorobenzene

2.1 Data collection

Bioaccumulation data were collected by searches for public literature in Scopus (July 2009) and using data from the European substance data sheets. All other data were taken from the substance data sheets.

2.2 Physico-chemical properties

Physico-chemical properties of HCB are summarised in the table below. All data are taken from the substance datasheet (EC, 2005a). Original references are given in the table.

Table 3 Physico-chemical properties of hexachlorobenzene as reported in the substance data sheet (EC, 2005a).

Property	Value	Original reference
CAS number	118-74-1	
Molecular weight	284.8 g/mol	De Bruijn et al., 1999
Vapour pressure	1.1 – 1.45 mPa (20 ºC)	Frimmel, 2001a
	2.3 – 2.5 mPa (25 ºC)	Frimmel, 2001a and Eurochlor, 2002a
Henry's law constant	131 Pa/mol.m^3	Eurochlor, 2002a
Water solubility	5 µg/L (25 ºC)	Eurochlor, 2002a
	5 – 6 µg/L (25 ºC)	Frimmel, 2001a
Log K_{ow}	5.5 (5-6.92)	Eurochlor, 2002a
	5.31	Agences de l'eau, 1999
	5.73	De Bruijn et al., 1999
	3.93-6.53	Frimmel, 2001a

2.3 Human toxicology

The WHO has derived two different TDI values: one for non-neoplastic effects and one for neoplastic effects. For non-neoplastic effects, the lowest reported NOEL is 0.05 mg/kg_{bw}/day for hepatic effects in pigs and rats exposed orally, resulting in a TDI of 0.17 µg/kg_{bw}/day. For neoplastic effects, a tumorigenic dose is used (TD_5), which is the intake associated with a 5% excess incidence of tumours. The TD_5 value of 0.81 mg/kg_{bw}/day for tumours in the liver in female rats results in a TDI of 0.16 µg/kg_{bw}/day. This value is used in the EU-datasheet (EC, 2005a).

The lowest $NOEC_{food}$ for population-related endpoints (mortality, reproduction) is 0.5 mg/kg food for the mink *Mustela vision* and the ferret *Mustela putorius*.

2.4 Bioconcentration and biomagnification

2.4.1 Bioconcentration factors

The BCF value in a laboratory study is determined by exposing aquatic organisms to the substance dissolved in water. The BCF is calculated as the ratio between the concentration in the organisms and in the water determined at equilibrium, or by dividing the uptake rate constant by the depuration rate constant (kinetic method). The standard guideline to perform bioconcentration tests with fish is the OECD 305 guideline. A detailed table with BCF values can be found in Appendix A. Table 4 summarises all valid data for fish, with a column with non-normalised BCFs and a column with BCFs normalised to 5% lipids for those studies where lipid contents of the fish were reported.

Besides studies with exposure through the water phase, laboratory BCF-studies with dietary exposure are also reported. In these studies, fish were exposed to HCB through spiked food during the uptake phase, and then transferred to clean water with uncontaminated food for the depuration phase. The BCF is then also calculated using the kinetic method, i.e., with an uptake rate and a depuration rate constant. The uptake rate constant for aqueous exposure is based on fish weight, according to the REACH guidance (REACH guidance chapter R7C; ECHA, 2008). The depuration rate constant is measured during the experiment.

The overall BCF is derived by first calculating the geometric mean for one species, and then taking the mean of these geometric means-per-species. Both the non-lipid-normalised and the lipid-normalised geometric mean BCF are 12800 L/kg. Lipid normalisation reduces the variability that is caused by differences in characteristics of the fish used in the experiments. Therefore, the lipid-normalised geometric mean value of 12800 L/kg is considered most reliable.

As a comparison, the BCF for fish can be calculated using the linear relationship developed by Veith et al. (1979): Log BCF = 0.85 × log K_{OW} -0.70. Using the log K_{ow} of 5.73, the resulting BCF is 14800 L/kg. This is in good agreement with the selected experimental value.

For invertebrates BCFs between 13200 and 75000 L/kg have been determined, for insects a BCF of 29000 L/kg is available, and for oligochaetes BCFs range between 25100 and 106800 L/kg (See appendix A). For the purpose of ERL derivation, these data serve as circumstantial evidence but are deemed to be less reliable when good data for bioconcentration in fish are available.

Besides studies with animals, there are also studies with SPME fibers available, which report K_{SPME} values of 66000 L/kg fiber material (Verbruggen et al., 2000) and 68300 L/kg fiber material (Leslie et al., 2002). This fiber material is supposed to mimic lipid tissue in biota and thus the K_{SPME} can be roughly compared to a BCF normalised to 100% lipids. For details see Appendix A. These values are not further used for ERL derivation but may serve as circumstantial evidence.

Table 4 Summary of fish bioconcentration data for HCB

Species	BCF [L/kg]	BCF 5% lipids	Remark	Reference
Gambusia affinis	3730	6016		Chaiksuksant et al., 1997
Gambusia affinis	3776	6090		Chaiksuksant et al., 1997
Gambusia affinis	3753	6053	Geomean	
Gasterosteus aculeatus	22100	40900		Egeler et al., 2001
Ictalurus punctatus	11000	7450	Dietary study	Woodburn et al., 2008
Lepomis macrochirus	21900			Veith et al., 1979
Oncorhynchus mykiss	12100			Lu and Wang, 2002
Oncorhynchus mykiss	16700	29800	Dietary study	Exxon Mobil database version 1.0
Oncorhynchus mykiss	15800	16500	Dietary study	Exxon Mobil database version 1.0
Oncorhynchus mykiss	10800	22500	Dietary study	Exxon Mobil database version 1.0
Oncorhynchus mykiss	10100	15800	Dietary study	Exxon Mobil database version 1.0
Oncorhynchus mykiss	22200	13700	Dietary study	Exxon Mobil database version 1.0
Oncorhynchus mykiss	15000	13400	Dietary study	Exxon Mobil database version 1.0
Oncorhynchus mykiss	5500			Veith et al., 1979
Oncorhynchus mykiss	19500	23800	Dietary study	Fisk et al., 1998
Oncorhynchus mykiss	13232	18578	Geomean	
Pimephales promelas	26700			Carlson and Kosian, 1987
Pimephales promelas	21400			Carlson and Kosian, 1987
Pimephales promelas	22500			Carlson and Kosian, 1987
Pimephales promelas	17700			Carlson and Kosian, 1987
Pimephales promelas	20200			Carlson and Kosian, 1987
Pimephales promelas	16600			Veith et al., 1979
Pimephales promelas	18200			Veith et al., 1979
Pimephales promelas	17800			Veith et al., 1979
Pimephales promelas	45700			Veith et al., 1979
Pimephales promelas	16200			Veith et al., 1979
Pimephales promelas	18500			Veith et al., 1979
Pimephales promelas	12200	8840		Nebeker et al., 1989
Pimephales promelas	15300	11100		Nebeker et al., 1989
Pimephales promelas	21100	15300		Nebeker et al., 1989
Pimephales promelas	12600	9130		Nebeker et al., 1989
Pimephales promelas	13300	9640		Nebeker et al., 1989
Pimephales promelas	11500	8330		Nebeker et al., 1989
Pimephales promelas	20700	15000		Nebeker et al., 1989
Pimephales promelas	93800			Schuytema et al., 1989
Pimephales promelas	19948	10743	Geomean	
Poecilia reticulata	15660	14500		Könemann and van Leeuwen, 1980
Poecilia reticulata	7664	9580	Dietary study	Clark and Mackay, 1991
Poecilia reticulata	10955	11786	Geomean	
Overall geomean	12848	12771	See text	

2.4.2 *Biomagnification factors*

The BMF is the ratio of the concentration in the predator organism divided by the concentration in the prey organism. In general, the most reliable data on biomagnification originate from trophic magnification studies. In such studies the levels of contaminants in several species in an ecosystem are measured and expressed as a function of the trophic level. The trophic level is mostly derived from stable nitrogen isotope ratios and a regression is made between contaminant concentration and trophic level. The contaminant values should preferably be normalised to the fraction in the organisms that contains the substance *e.g.* lipids in the case for lipophilic organic chemicals. This so-called trophic magnification factor (TMF) is considered to be the most reliable representation of the BMF, because it is normalised to trophic level and levels out fluctuations in biomagnification between individual species by regression over several trophic levels. Thus, where BMFs are measured for predator and prey only (and may be corrected to represent one exact trophic level), TMFs are measured over the whole foodweb and represent the biomagnification per trophic level.

In Appendix B, studies on biomagnification are summarised. An overview of all valid BMF values derived from these studies is given in Table 5. Trophic magnification factors (TMFs) are also summarised in Appendix B. An overview of all valid TMF values is given in Table 6.

Table 5 Overview of valid BMF values for HCB

Predator/prey	BMF	Remark	Reference
amphipods/prey	3.8	corrected for trophic level	Fisk et al., 2001
fish/invertebrate	4		Borgå et al., 2001
fish/invertebrate	2.4		Borgå et al., 2001
fish/oligochaetes	0.53		Egeler et al., 2001
fish/oligochaetes	1.3		Egeler et al., 2001
fish/fish	1.7		Borgå et al., 2001
fish/fish	2.1		Ruus et al., 1999
fish/fish	0.79		Russell et al., 1995
fish/prey	6.1	corrected for trophic level	Fisk et al., 2001
fish/prey	6.8	corrected for trophic level	Catalan et al., 2004
fish/food	0.35	laboratory study	Woodburn et al., 2008
bird/fish	63		Borgå et al., 2001
bird/fish	13		Borgå et al., 2001
bird/fish	5.2		Borgå et al., 2001
bird/fish	8.9		Borgå et al., 2001
bird/prey	5.0-21.6	corrected for trophic level	Fisk et al., 2001
seal/fish	2.7		Ruus et al., 1999
seal/fish	0.3		Ruus et al., 1999
seals/prey	0.2	corrected for trophic level	Fisk et al., 2001

Table 6 Overview of valid TMF values for HCB

TMF	Remark	Reference
-0.9 - 6.9	Average is 2.9. Food webs in 17 lakes	Houde et al., 2008
4.7	Invertebrates, fish, birds, seals	Hop et al., 2002
2.96	Algae, invertebrates, fish, birds	Wan et al., 2005
1.36	Zooplankton, fish, seals, whales	Hoekstra et al., 2003
4.1	Zooplankton, invertebrate, fish, birds, seal	Fisk et al., 2001
1.75	Food web without birds and benthic oriented species	Fisk et al., 2001, recalculated by Hoekstra et al., 2003
1.55	Food web without birds and benthic oriented species	Hop et al., 2002, recalculated by Hoekstra et al., 2003
<1	Polychaetes, fish, seal, bird	Ruus et al., 2002

2.4.3 Bioaccumulation factors

Bioaccumulation factors are the ratio of a compound in the organism over the concentration in water. In contrast to a measured laboratory BCF, the BAF not only includes exposure through water, but also exposure through food. Thus the BAF represents the quotient of the BCF and the BMF. Furthermore, BAFs are often determined in the field, while BCFs are mostly determined in the laboratory. For HCB, only studies with water concentrations expressed as dissolved concentrations are valid, because there is equilibrium between biota and the dissolved concentration and not the total concentration (including suspended solids). BAFs are often reported based on lipid-weights (e.g., amount of HCB per gram lipid), but for comparison with BCFs the BAF can also be normalised to 5% lipids.

A description of bioaccumulation studies is given in Appendix C. Results of valid studies are summarised in Table 7. All reported BAFs are based on lipid-weights. Recalculated BAFs normalised to 5% lipids are also included in the table.

In the European substance datasheet for HCB (EC, 2005a), a BAF of 42000 L/kg is used based on data for bream from the river Elbe. However, this value was deemed to be less reliable since it is based on muscle tissue wet weight instead of 5% lipid-normalised whole fish, and was based on total concentrations in water (incl. suspended solids) instead of dissolved concentrations. Moreover, the trophic position of the species used is low (2.31 according to Van Riel et al, 2006 and 2.94±0.37 according to fishbase.org) and the species is mainly benthivorous, which renders the value of the BAF less reliable.

Table 7 Summary of valid BAF data for HCB

Species	Trophic position		BAF [L/kg] (lipid-weight)	BAF [L/kg] (normalised to 5% lipids)	Reference
	fishbase[a]	Calc.[b]			
Crustacea					
Pontoporeia affinis			4.0×10^6	200000	Oliver and Niimi, 1988
Fish					
Alosa pseudoharengus	3.51±0.48		1.9×10^6	95000	Oliver and Niimi, 1988
Comephorus dybowskii[c]	3.44±0.57	3.86±0.08	6.7×10^6	333000	Kucklick et al., 1996
Comephorus baikalensis[c]	3.29±0.53	3.96±0.08	6.1×10^6	305000	Kucklick et al., 1996
Coregonus autumnalis migratorius[c]	3.57±0.56	3.40±0.34	1.8×10^7	8856000	Kucklick et al., 1996
Cottus cognatus	3.37±0.47		3.2×10^6	158000	Oliver and Niimi, 1988
Osmerus mordax	3.00±0.02		1.3×10^6	63000	Oliver and Niimi, 1988
Osmerus mordax	3.00±0.02		2.3×10^6	117000	Oliver and Niimi, 1988
Salmo trutta (muscle)	3.16±0.42	3.14	8.7×10^6	433000	Catalan et al., 2004
salmonids (*Oncorhynchus kisutch*, *Oncorhynchus mykiss*, *Salvelinus namaycush* and *Salmo trutta*)	4.22±0.73 4.42±0.38 4.29±0.71 3.16±0.42		2.3 × 106	115000	Oliver and Niimi, 1988

[a] Source: www.fishbase.org; accessed September 13, 2010
[b] Derived from data presented in the studies
[c] Geomean of samples from various year classes

The geometric mean of the 5% lipid-normalised BAFs is 221000 L/kg. This is based on the geometric mean of BAF values per species, in which data for salmonid species were averaged to one value. The worst-case BAF value is 885600 L/kg for the geometric mean of different age classes of *Coregonus* sp. BAF measurements show a high variation of more than one order of magnitude. Normally, BAFs correlate with trophic level or age of the fish, but for HCB this is not the case (see Figure 2). An explanation for this deviation of what is expected from theory is lacking. Even at lower trophic levels (algae, small zooplankton), accumulation of HCB already far exceeds what is expected through equilibrium partitioning. For instance the BAF for amphipods and plankton normalised to 5% lipids was 107000 L/kg in the Oliver and Niimi study (1988), which amply exceeds the laboratory BCF values for fish. This affects BAFs at higher trophic levels as well.

Although the fish do not differ much in trophic level according to fishbase.org, there are distinct differences in feeding strategies. For example, the foodchain in lake Ontario, where samples in the Oliver and Niimi study (1988) originated from, includes *Cottus cognatus* as a benthic predatory fish, *Osmerus mordax* and *Alosa pseudoharengus* as pelagic predatory fish, and salmonids as a top predator. From the Kucklick study (1996), *Coregonus* is also a salmonid which feeds on smaller fish. However, both trophic level (Figure 2) and feeding strategy do not seem to be the main determinant for the BAF for HCB. The five highest BAF values are all for *Coregonus*.

In the study by Kucklick et al (1996) only BAF values for fish could be derived, because data for invertebrates were below the limit of detection, which means that the BAF values normalized to 5% lipid weight should be below 92000 L/kg. With the trophic level for zooplankton around 2 and the trophic level of the

predatory amphipod *Macrohectopus branicii* around 2.5, an increase in BAF with a factor of at least 2 per trophic level would be deduced from these data. The same pattern was observed for PCBs, where in the group of fish no clear trend with trophic level was observed, while there was a significant relationship with trophic level if invertebrates were included.

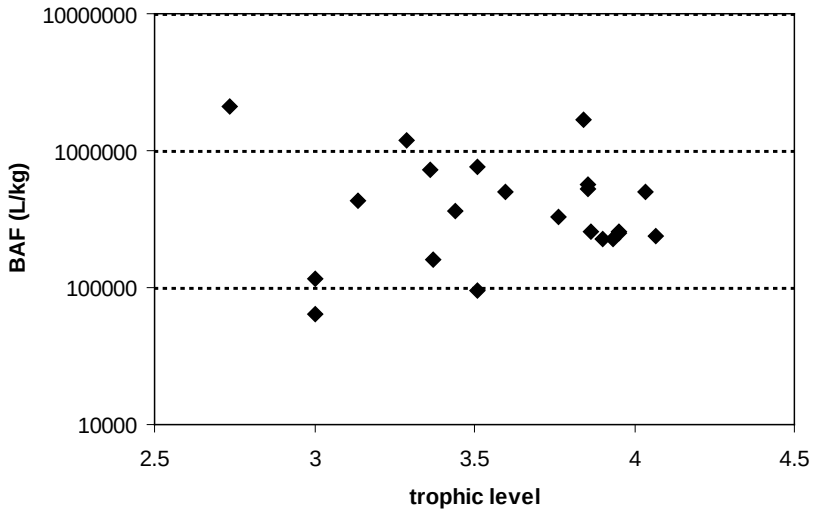

Figure 2 Influence of trophic level on BAFs (based on individual data from the references included in Table 7

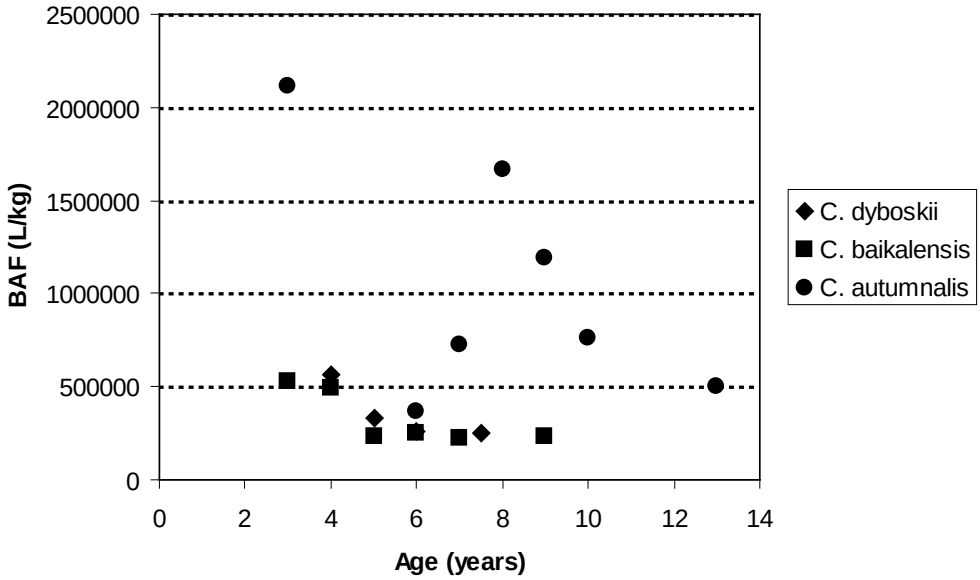

Figure 3 Influence of age on BAF values for fish (datasource: Kucklick et al., 1996)

Age of the fish could also influence the magnitude of the BAF, especially for top predators. For HCB however, the expected increase in BAF values with increasing age is not found for three fish species in the study by Kucklick et al (1996). To the contrary, the reverse is observed, although a high variation is shown (Figure 3). It should be added that the correlation between trophic level and age is also rather weak, although positively correlated.

Concludingly, all correlations are not significant and therefore, no conclusions should be drawn from these observations. Thus, the observed BAF values for fish cannot be easily explained from the age of the fish, nor from the trophic level.

Another source of uncertainty for BAF values is the uncertainty surrounding the measurements of the aqueous concentrations, which are very low in the field. Because BAFs for HCB only originate from three studies, no definite conclusions can be drawn on the influence of the height of the water concentrations on BAFs, but there does not seem to be a relationship. However, it should be stressed that the concentrations of HCB are rather consistent over the three studies in the range of 10 to 150 pg/L. This probably reflects the global distribution of this substance.

2.4.4 Conclusion on BCF, BMF and BAF

For lipophilic organic chemicals, data on bioconcentration and bioaccumulation can be normalised to the percentage lipids of the organisms. This strongly reduces variability for these substances. BCF values are available for a number of fish species. As stated above, the lipid-normalised geometric mean BCF-value of 12800 L/kg is considered most reliable.

Considering all available data, the use of a BMF value of 3 kg/kg is considered most appropriate for further calculations. This value is around the geometric mean of all BMF and TMF values, and closely resembles the average TMF of 2.9 kg/kg from by the well-performed study of Houde et al. (2008).

Lower trophic levels (plankton, amphipods) have BAF values far above what may be expected from the BCFs for fish. When comparing BCF values for fish multiplied by the BMF_1 (12800 × 3 = 38400 L/kg) to the observed BAF values for fish, there appears to be a large gap between laboratory data (38400 L/kg) and field data (range 63000 – 8856000 L/kg). The confidence in the laboratory data is high; BCFs based on dietary studies and laboratory water-only BCF values are in good agreement with each other. The explanation for the observed discrepancy between the product of BCF and BMF_1 and the observed BAF values for fish lies in the fact that already at the base of the food chain the BAF values exceed laboratory BCFs to a large extent.

It can be concluded that the methodology of BCF x BMF works only if BAF values for small fish and other aquatic species are comparable to the laboratory BCF data. For HCB, this is apparently not the case. It appears that the BAF values are almost a factor of 20 higher than the BCF values, while the increase per trophic level is only a factor of 3. This means that the number of trophic levels that should be taken into account for the biomagnification process is 2 to 3 instead of the single trophic level that is considered in the methodology for risk assessment and quality standard derivation. It is not considered appropriate to use BCF x BMF values to recalculate the biota standards into water standards, because this methodology greatly underestimates field BAFs for HCB.

The question arises if the lack of consistency results from a flaw in the methodology, or is the result of deviating behaviour of a single compound. The unexpectedly high accumulation already at the base of the food chain, which may be a determining factor for accumulation at higher trophic levels, seems to suggest that the latter is the case. Until now, for the compounds for which this methodology has been followed (for instance PFOS; Moermond and Verbruggen, 2010) no deviations from generally accepted scientific principles have been shown. The general conclusion is that the approach as outlined in section 1.5 can be followed, unless available data suggest that this approach is not valid, as is the case for HCB.

2.5 Discussion on derivation of ERLs for hexachlorobenzene in water

In the substance data sheet for HCB (EC, 2005a), a $QS_{biota,\ hh}$ of 9.74 µg/kg and a $QS_{biota,\ secpois}$ of 16.7 µg/kg are derived. According to the substance datasheet, these can be recalculated into water concentrations using a BAF of 42000 L/kg, which results in a $QS_{freshwater,\ hh}$ of 0.00023 µg/L and a $QS_{freshwater,\ secpois}$ of 0.00004 µg/L.

The value of 42000 L/kg for the BAF, is however not based on an extensive literature search. It is deemed to be less reliable, since it is based on muscle tissue wet weight instead of 5% lipid-normalised whole fish, and based refers to total concentrations in water (incl. suspended solids) instead of dissolved concentrations.

To recalculate the biota standards into water standards, there are four options. These are all discussed below. It should be noted that the option that is to be preferred from a scientific point of view, may not be the most desirable option from a policy maker's point of view.

1. Use the $QS_{biota,\ hh}$ and $QS_{biota,\ secpois}$ from the substance data sheet. This would involve the highest degree of certainty surrounding the value. However, in the Netherlands biota is not regularly monitored.
   ⇒ $MPC_{biota,\ hh}$ = 9.74 µg/kg.
   ⇒ $MPC_{biota,\ secpois}$ = 16.7 µg/kg.
2. Use the $QS_{freshwater,\ hh}$ and $QS_{freshwater,\ secpois}$ from the substance data sheet, where a BAF of 42000 L/kg is used (based on total concentrations in water). However, this BAF is deemed to be less reliable and underestimates the observed BAF values and no extensive literature search was performed.
   ⇒ $MPC_{freshwater,\ hh}$ = 0.00023µg/L = 0.23 ng/L.
   ⇒ $MPC_{freshwater,\ secpois}$ = 0.0004µg/L = 0.4 ng/L
   Since the BAFs are based on total concentrations in water, the resulting risk limits also refer to total concentrations.

3. Use the worst-case BAF of 885600 L/kg for *Coregonus migratorius autumnalis* (Kucklick, 1996). This value is a geomean of BAF values of individual fish of different ages; no age-dependency of the value could be shown but there was a large variability among the values. The BAF for *C. migratorius* is however very high and seems to be an outlier when compared to the other valid BAFs which are more than a factor of two lower.
   ⇒ $MPC_{freshwater,\ hh}$ = 0.000011 µg/L = 0.011 ng/L.
   ⇒ $MPC_{freshwater,\ secpois}$ = 0.000019 µg/L = 0.019 ng/L.
   Because the BAF values are based on dissolved concentrations, these MPC values refer to dissolved concentration as well. If a total water concentration is desired, these MPC values should be recalculated.
4. Use the geometric mean of all valid BAFs, 221000 L/kg. There are some uncertainties surrounding this value, since the variation among BAFs is high and the height of the BAF is relatively high (for comparison, the BAF calculated as BCF x BMFwould have been 38400 L/kg (see discussion in section 2.4.4).
   ⇒ $MPC_{freshwater,\ hh}$ = 0.000044 µg/L = 0.044 ng/L.
   ⇒ $MPC_{freshwater,\ secpois}$ = 0.000076 µg/L = 0.076 ng/L.
   Also in this case the BAF values and thus the resulting MPC values are based on dissolved concentrations.

Please note that the differences in MPC values among the four options are not only caused by the height of the BAF or BCF/BMF used, but are also caused by a difference in MPCs based on dissolved concentrations versus total concentrations. This difference is not easy to quantify, because it depends on the amount of suspended solids in the systems (see also section 1.6).

Regarding the final choice for the above options, option 2 is not preferred because of the less reliable BAF value used. From a scientific point of view, option 3 is also not preferred. The worst-case BAF is extremely high, and seems to be an outlier.

However, compliance checking by means of monitoring in water (option 4) has advantages over biota sampling (option 1) in terms of reproducibility, costs and uniformity of sampling. However, recalculating biota standards into water standards (option 4) introduces uncertainties regarding the height of the BAF used and the resulting ERL value is thus more uncertain than the value for biota. Therefore, expression of ERLs on the basis of concentrations in biota (option 1) seems most appropriate because it has the least numerical uncertainties regarding its ERL derivation. However, this implies that the biota that are monitored in order to check compliance to these WFD requirements, should correspond to the same trophic level as the level the EQS refers to. This also introduces a lot of uncertainties, because HCB concentrations in biota can be highly variable and may depend on the age and trophic level of the fish species sampled, and there is no guidance on this point yet.

The following “tiered approach” is suggested: Use the geometric mean BAF (option 4), leading to a critical water standard of 0.044 ng/L (dissolved concentrations). If this standard is then exceeded in the field, case by case biota can be sampled and compared to the biota standard for compliance checking.

The limit of quantification (LOQ) for HCB in water is 0.001 µg/L (Dorien ten Hulscher, personal communication), with the limit of detection, depending on the laboratory, about a factor of 10 lower. This is still significantly higher than the MPCs for the water column. This means that concentrations of HCB in the water column which are close to the $MPC_{freshwater}$ cannot be measured directly (via liquid-liquid extraction) and may have to be measured using passive sampling devices. If conventional methods are used, the MPC may already be exceeded when concentrations are still below the detection limit.

For the marine environment, biota standards are the same as the standards for biota in freshwater. However, the $MPC_{saltwater, hh}$ equals the $MPC_{freshwater, hh}$, while the $MPC_{saltwater, secpois}$ equals the $MPC_{freshwater, secpois}$ divided by the BMF (3).

3 Hexachlorobutadiene

3.1 Data selection

Bioaccumulation data were collected by searches for public literature in Scopus (July 2009) and using data from the European substance data sheets. All other data were taken from the substance data sheets.

3.2 Physico-chemical properties

Table 8 Physico-chemical properties of hexachlorobutadiene as reported in the substance data sheet (European Commission, 2005b).

Property	Value	Remarks
CAS number	87-68-3	
Molecular weight	260.8 g/mol	Eurochlor, 2002b in data sheet
Vapour pressure	20 Pa (20 ºC)	Eurochlor, 2002b in data sheet
	36 Pa (20 ºC)	Frimmel, 2001b in data sheet
Henry's law constant	1630 Pa/mol.m^3	Eurochlor, 2002b in data sheet
Water solubility	3.2 mg/L (20 ºC)	Eurochlor, 2002b in data sheet
	2-4 mg/L (25 ºC)	Frimmel, 2001b in data sheet
Log K_{ow}	4.78 – 4.9	Eurochlor, 2002b and Frimmel, 2001b in data sheet
	4.9	Agences de l'eau, 1999 in data sheet

3.3 Human toxicology

The WHO-ICPS has derived a TDI of 0.2 µg/kg_{bw}/day based on a chronic toxicity study with rats and mice with a NOAEL of 0.2 mg/kg_{bw}/day. No carcinogenic or endocrine disrupting properties are known.

3.4 Bioconcentration and biomagnification

3.4.1 Bioconcentration factors

The BCF value in a laboratory study is determined by exposing aquatic organisms to the substance dissolved in water. The BCF is calculated as the ratio between the concentration in the organisms and in the water determined at equilibrium. The standard guideline to perform bioconcentration tests with fish is the OECD 305 guideline. In Appendix A2, an overview is given of the bioconcentration data available in public literature. The only valid data are from the Japanese NITE database, with BCFs of 6608 and 7555 L/kg at exposure concentrations of 0.831 and 0.087 µg/L, respectively. Normalised to 5% lipids these BCFs are 6480 and 7410 L/kg.

Table 9 Summary of valid BCF data for HCBD

Species	BCF (L/kg ww)	BCF (normalised to 5% lipids)	Reference
Fish			
Cyprinus carpio	6608	6480	NITE database, 2009
Cyprinus carpio	7555	7410	NITE database, 2009

Using a log K_{ow} of 4.9, the BCF for fish can be calculated using the linear relationship developed by Veith et al. (1979): Log BCF = 0.85 × log K_{ow} -0.70 = 3.47. The resulting BCF is 2917 L/kg. This is substantially lower than the experimental values, indicating that for this compound this QSAR based on log K_{ow} underestimates the bioconcentration potential.

In the substance data sheet on HCBD (EC, 2005b) a number of other BCF data are reported, which are highly variable and range from below 50 to 19000 L/kg for fish. A value of 17000 L/kg is used for further calculations on secondary poisoning in the substance data sheet. However, this value originates from the study of Oliver and Niimi (1983), which we deem to be not valid because of the high loading of the fish (18 g/L) combined with a too low exposure concentration for valid aqueous concentration measurements. For the human consumption of fishery products, also a BCF of 700 for fish fillet and a BCF of 2000 for blue mussel are used, resulting in a range of values for the final $QS_{freshwater,hh}$ in the substance data sheet.

3.4.2 Biomagnification factors

The BMF is the ratio of the concentration in the predator organism divided by the concentration in the prey organism (for hydrophobic organic chemicals commonly normalised to lipid content of prey and predator).

No experimental data are available for HCBD. Kelly et al. (2007) calculated theoretical BMFs in invertebrates, fish, reptiles, amphibians, birds, non-human mammals, and humans based on the log K_{ow}. For all of these organisms, the calculated BMF was below 1, indicating no potential for biomagnification. A similar conclusion was drawn in the substance data sheet for hexachlorobutadiene (EC, 2005b). However, as stated above the log K_{ow} based QSAR underestimates the bioconcentration potential, and biomagnification might be expected to be underestimated accordingly. Field data (see below) indeed show that considerable bioaccumulation occurs. Given the data on bioconcentration, the assumption of absence of biomagnification most likely does not hold true.

3.4.3 Bioaccumulation factors

As explained in section 1.5, bioaccumulation factors are the ratio of a compound in the organism over the concentration in water. The BAF also includes exposure through food while the BCF only includes exposure through the water. For HCBD, only studies with water concentrations expressed as dissolved concentrations are valid, because there is an equilibrium between biota and the dissolved concentration and not the total concentration (including suspended solids).

A description of bioaccumulation studies from public literature is given in Appendix D. Results of valid studies are summarised in Table 10. All reported BAFs are based on lipid-weights. Recalculated BAFs normalised to 5% lipids are also included in the table.

Table 10 Summary of valid BAF data for HCBD

Species	BAF (lipid-weight)	BAF (normalised to 5% lipids)	Reference
Crustacea			
Mysis relicta	185200	9260	Oliver and Niimi, 1988
Pontoporeia affinis	5000000	250000	Oliver and Niimi, 1988
Fish			
Cottus cognatus	347200	17360	Oliver and Niimi, 1988

There is only one BAF for fish available, 17360 L/kg. No bioaccumulation factors are reported in the substance data sheet (EC, 2005b).

3.4.4 *Final choice of BCF, BMF and BAF*

Because the BCF value of 17000 L/kg from the study of Oliver and Niimi (1983) was deemed to be not valid, the 5% lipid-normalised BCF value of 7410 L/kg from the Japanese NITE database is used for further calculations. This value is chosen over the value of 6480 L/kg because it was determined at the environmentally most relevant exposure concentration. In this report, the same BCF value is used for secondary poisoning and human consumption of fishery products. In contrast, in the substance data sheet (EC, 2005b) a range of values is used for the calculation of the $QS_{freshwater,hh}$.

It is considered most appropriate to rely on the reliable laboratory BCF-value of 7410 L/kg and apply a fixed value for BMF_1 and BMF_2, instead of using the single experimental BAF. The TGD (EC, 2003) recommends to rely on experimental data for selection of the BMF. In case such data are not available, which is the case here, defaults are suggested that are related to the BCF. A BMF of 10 kg/kg is recommended for compounds with a BCF > 5000 L/kg. If the BCF-value of 7410 L/kg (normalised to 5% lipid) is selected as the most reliable value for further calculations, a BMF_1 of 3 kg/kg would also be justified. The resulting product of BCF and BMF_1 of 22230 L/kg adequately covers the BAF-value obtained for fish species in the field study of Oliver and Niimi (1988). There are no BAF-data to underpin the choice of the BMF_2. From other compounds it appears that setting the BMF_2 to the same value as the BMF_1 is sufficient to predict accumulation in top predators. This is also in line with the TGD. In conclusion, calculations are performed using a BCF of 7410 L/kg and BMF_1 and BMF_2 of 3 kg/kg.

3.5 Derivation of environmental risk limits

3.5.1 *$MPC_{freshwater, hh}$ and $MPC_{saltwater, hh}$*

In the European substance data sheet for hexachlorobutadiene, the TDI of 0.2 $\mu g/kg_{bw}$/day is used to derive the QS for human consumption of fishery products. Using this TDI, the $MPC_{biota, hh}$ is (0.1 × 0.2 × 70) / 0.115 = 12.2 µg/kg.

This $MPC_{biota, hh}$ is the concentration in biota. To calculate this value into a water concentration, the BCF and BMF should be used according to $MPC_{freshwater, hh}$ = $MPC_{biota, hh}$ / (BCF × BMF) = 12.2 / (7410 × 3) = 5.5 × 10^{-4} µg/L.

For the marine environment, the $MPC_{saltwater, hh}$ equals the $MPC_{freshwater, hh}$.

3.5.2 *$MPC_{freshwater,\ secpois}$ and $MPC_{saltwater,\ secpois}$*

The lowest NOAEL for rats and mice of 0.2 mg/kg_{bw}/day can be recalculted into a $NOEC_{food}$ using a concversion factor of 20 for rats and 8.3 for mice. This results in a $NOEC_{food}$ for rat of 0.2 × 20 = 4 mg HCBD/kg food and a $NOEC_{food}$ for mice of 0.2 × 8.3 = 1.66 mg HCBD/kg food.

The lowest $NOEC_{food}$ of 1.66 mg/kg food for mice can be recalculated in an MPC_{oral} using an assessment factor of 30 (chronic mammal study), resulting in an MPC_{oral} of 5.5 × 10^{-2} mg/kg diet. This equals the QS for predators in the European substance data sheet. Subsequently, the $MPC_{freshwater,\ secpois}$ can be calculated using a BCF of 7410 L/kg and a BMF_1 of 3 kg/kg and becomes 5.5 × 10^{-2} / (7555 × 3) = 2.5 × 10^{-6} mg/L = 2.5 × 10^{-3} µg/L.

For the marine environment, an extra biomagnification factor (BMF_2) should be used. Thus, the $MPC_{saltwater,\ secpois}$ becomes 5.5 × 10^{-2} / (7555 × 3 × 3) = 8.2 × 10^{-7} mg/L = 8.2 × 10^{-4} µg/L.

3.5.3 *Detection limits*

The limit of quantification (LOQ) for HCBD in water is 0.01 µg/L (Dorien ten Hulscher, personal communication), with the limit of detection, depending on the laboratory, about a factor of 10 lower. This is still significantly higher than the MPCs for the water column. This means that concentrations of HCBD in the water column which are close to the $MPC_{freshwater}$ cannot be measured directly (via liquid-liquid extraction) and may have to be measured using passive sampling devices. If conventional methods are used, the MPC may already be exceeded when concentrations are still below the detection limit.

4 Comparison with measurements in the Netherlands

As an indication, in this paragraph some monitoring data are compared to the ERLs determined in this report. Most of these data are from non-regular monitoring programs.

An indication for the height of HCB and HCBD concentrations in biota can be obtained from a number of papers:

- Roex and Van den Heuvel-Greve (2010) report results from routine monitoring programs in the Netherlands. Starting in 1992, a number of compounds was measured in eel and mussels at various freshwater sampling sites. The trend for HCB is that concentrations in mussels were decreasing, except for the lower river area where concentrations stayed equal. For freshwater mussels (*Dreissena polymorpha*), monitoring stopped in 2005 because concentrations were so low that analysis was deemed less relevant. For red eel (*Anguilla anguilla*), which is an organism which is relatively high in the food chain and has a high lipid content (20%), the concentration of HCB is also decreasing over the years. However, in 2008 there were still some sampling sites where the MPC_{biota} was exceeded by a maximum factor of 2. Also for the near future it is expected that concentrations in eel will exceed the MPC_{biota} at locations such as the Lek and the Hollands Diep (Roex and Van den Heuvel-Greve, 2010). Concentrations of HCBD in biota have not decreased since 1997, but these concentrations are a factor of 5-10 below the MPC_{biota}.
- Kotterman (2008) reports data for eel (also reported by Roex and Van den Heuvel Greve, 2010; see above) and roach (*Rutilus rutilus*), sampled in 2008. For roach, all concentrations of HCB and HCBD were below the MPC_{biota}.
- From 1984 and onwards, data are available for flounder at various coastal waters (Roex and Van den Heuvel-Greve, 2010). Concentrations of HCB in livers of flounder (*Platichthys flesus*) decreased from 1984 until the mid-90's, after which the decrease stopped. The concentrations in liver are about a factor of 3 below the MPC_{biota}, which means that whole-body concentrations are far below the MPC_{biota}.

At the Hollands Diep and Lek locations, where for eel the HCB concentration in biota exceeds the MPC_{biota}, the water concentration (determined using passive samplers; Smedes, 2010) also exceeds the $MPC_{freshwater}$ (determined with option 4 – the geometric mean BAF). However, the water concentrations at other locations also exceed this $MPC_{freshwater}$ with a maximum factor of 4, while the HCB concentration in fish sampled at these locations did not exceed the MPC_{biota}. For HCBD, only at one location is the water concentration slightly higher, by a factor of 1.1, than the $MPC_{freshwater}$. Biota samples did not exceed the MPC_{biota} for HCBD at any of the locations sampled.

The last paragraph indicates that a tiered approach (first compare water concentrations to the MPC, and if exceeded, sample biota and compare biota concentrations) might be applicable for the Dutch situation. If the tiered approach was applied to the data of Roex and Van den Heuvel-Greve (2010) and Smedes (2010), biota concentrations only exceed the MPC_{biota} if the $MPC_{freshwater}$

is also exceeded. In these data, there are no cases where the $MPC_{freshwater}$ would not have been exceeded in the first tier, while the MPC_{biota} is exceeded in the second tier. This means a tiered approach can be used to assess HCB and HCBD-related water quality in the Netherlands.

5 Conclusions

Hexachlorobenzene
In the substance data sheet for HCB (EC, 2005a), a $QS_{biota, hh}$ of 9.74 µg/kg and a $QS_{biota, secpois}$ of 16.7 µg/kg are derived. However, compliance checking by means of monitoring in water has advantages over biota sampling in terms of reproducibility, costs and uniformity of sampling.

Thus, BAF, BMF and BCF values were evaluated to assess whether they can be used to recalculate biota standards into water standards. This introduces uncertainties regarding the height of the BAF used and the resulting ERL value is thus more uncertain than the value for biota. Therefore, expression of ERLs on the basis of concentrations in biota seems most appropriate. However, this implies that the biota that are monitored in order to check compliance to these WFD requirements, should correspond to the same trophic level as the level the EQS refers to. This also introduces a lot of uncertainties, because HCB concentrations in biota can be highly variable and may depend on the age and trophic level of the fish species sampled, and there is no guidance on this point yet.

A tiered approach is suggested in which the critical water standard of 0.044 ng/L is used in the first instance. If this standard is exceeded in the field, case by case biota can be sampled and compared to the biota standard for compliance checking.

Using the $QS_{freshwater, hh}$ and $QS_{freshwater,secpois}$ values from the substance data sheet is the least preferred option from a scientific point of view, since the BAF value used for these calculations is not correct.

Please note that the new values correspond to the dissolved concentration in water, while the values from the substance data sheet refer to total concentrations in water.

Table 11 Environmental risk limits for hexachlorobenzene in water. Values in µg/L.

ERL[a]	**Hexachlorobenzene**	
	This report[b]	Substance data sheet[c]
$MPC_{freshwater, eco}$		0.013
$MPC_{saltwater, eco}$		0.013
$MPC_{freshwater, hh}$	0.000044	0.00023
$MPC_{saltwater, hh}$	0.000044	0.00023
$MPC_{freshwater, secpois}$	0.000076	0.0004
$MPC_{saltwater, secpois}$	0.000025	0.0004

[a] MPC = Maximum Permissible Concentration. The subscript ‘eco’ refers to direct ecotoxicity; the subscript ‘secpois’ refers to secondary poisoning, the subscript ‘hh’ refers to consumption of fish and shellfish by humans.
[b] Dissolved concentrations
[c] Total concentrations

Hexachlorobutadiene

From Table 12, it is clear that the proposed values for HCBD were lower by a factor of 1.2 to 4 for secondary poisoning and a factor of 1.3 to 30 for human consumption of fishery products, depending of the choice of BCF in the substance data sheet. It is however clear, that the ERLs for human consumption of fishery products and secondary poisoning are much lower than the ERL based on direct ecotoxicity of 0.44 µg/L for HCBD.

Please note that the new values correspond to the dissolved concentration in water, while the values from the substance data sheet refer to total concentrations in water.

Table 12 Environmental risk limits for hexachlorobutadiene in water. Values in µg/L.

ERL[a]	**Hexachlorobutadiene**	
	This report[b]	Substance data sheet[c]
$MPC_{freshwater, eco}$		0.44
$MPC_{saltwater, eco}$		0.44
$MPC_{freshwater, hh}$	0.00055	0.0007-0.0174
$MPC_{saltwater, hh}$	0.00055	0.0007-0.0174
$MPC_{freshwater, secpois}$	0.0025	0.003
$MPC_{saltwater, secpois}$	0.00082	0.003

[a] MPC = Maximum Permissible Concentration. The subscript ‘eco’ refers to direct ecotoxicity; the subscript ‘secpois’ refers to secondary poisoning, the subscript ‘hh’ refers to consumption of fish and shellfish by humans.

[b] Dissolved concentrations

[c] Total concentrations

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Appendix A. Bioconcentration data for HCB and HCBD

Table A1 Bioconcentration data for HCB

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Crustacea																
Gammarus lacustris	adults; 5.3% lipids	GC-ECD	F		nw	7	25-35	20	28	3.3	no	24000	SS Cb/Cw	3	1,2,3	Nebeker et al., 1989
Gammarus lacustris	adults; 5.3% lipids	GC-ECD	F		nw	7	25-35	20	28	1.8	no	29400	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Gammarus lacustris	adults; 5.3% lipids	GC-ECD	F		nw	7	25-35	20	28	1	no	33000	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Gammarus lacustris	adults; 5.3% lipids	GC-ECD	F		nw	7	25-35	20	28	0.8	no	18800	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Gammarus lacustris	adults; 5.3% lipids	GC-ECD	F		nw	7	25-35	20	28	0.4	no	20000	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Gammarus lacustris		GC-ECD	R		nw	7.1-8.9	200	20	30	4.5	15	41200	Cb/Cw	2	4	Schuytema et al., 1989
Hyalella azteca	randomly selected adults; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	4.5	no	38200	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	randomly selected adults; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	3.3	no	22100	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	randomly selected adults; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	0.8	no	75000	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	randomly selected adults; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	0.7	no	40000	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	randomly selected adults; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	0.4	no	35000	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	young mated pairs; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	3.8	no	26600	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	young mated pairs; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	2	no	24500	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	young mated pairs; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	0.7	no	38600	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	young mated pairs; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	0.5	no	28000	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	young mated pairs; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	30	0.3	no	28300	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	mixed population of adults and juveniles; 2.3 % lipids	GC-ECD	F		nw	7	25-35	20	49	4.7	17	13200	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca	mixed population of adults and juveniles; 2.3% lipids	GC-ECD	F		nw	7	25-35	20	49	3.2	17	14400	SS Cb/Cw	2	1,2	Nebeker et al., 1989
Hyalella azteca		GC-ECD	R		nw	7.1-8.9	200	20	28	5.7	no	20700	Cb/Cw	2		Schuytema et al., 1989
Portunus pelagicus												590000		4	5	Mortimer and Connell, 1993, in Mortimer and Connell, 1995.

Species	Properties	Analysis	Test type	Purity [%]	Test water	pH	Hardness [mg/L]	Temp [°C]	Exp. Time [d]	Exp. Conc. [µg/L]	Dep. Time [d]	BCF [L/kg]	BCF type	Ri	Notes	Reference
Insecta																
Chironomus riparius	4th instar; about 5 mg ww	GC	S	98	tw	7.6	125	24	13	0.83		29170	k1/k2	2	6	Leslie et al., 2002
Mollusca																
Mytilus edulis	4 cm shell length; field collected	TLC / GC	R		nw		30	10	103 h	0.5	no	>1000	SS Cb/Cw	4	7,8	Bauer et al., 1989
Mytilus edulis			R						96 h	0.5	no	2300	Cf/Cw	4	9	Ernst, 1986
Mytilus edulis												2000		4		Pearson and McConnell 1975 in Taylor et al., 2003
Oligochaeta																
Lumbriculus variegatus	mixed ages; 1.8% lipids	GC-ECD	F		nw	7	25-35	20	28	1.4	no	17100	SS Cb/Cw	3	10,11	Nebeker et al., 1989
Lumbriculus variegatus	mixed ages; 1.8% lipids	GC-ECD	F		nw	7	25-35	20	28	1.1	no	21800	SS Cb/Cw	3	10,12	Nebeker et al., 1989
Lumbriculus variegatus	mature worms; 1.8% lipids	GC-ECD	F		nw	7	25-35	20	49	4.7	17	47500	SS Cb/Cw	2	13	Nebeker et al., 1989
Lumbriculus variegatus	mature worms; 1.8% lipids	GC-ECD	F		nw	7	25-35	20	49	1.9	17	106800	SS Cb/Cw	2	13	Nebeker et al., 1989
Lumbriculus variegatus	mature worms; 1.8% lipids	GC-ECD	F		nw	7	25-35	20	49	1	17	50000	SS Cb/Cw	2	13	Nebeker et al., 1989
Lumbriculus variegatus	mixed ages; 1.8% lipids	GC-ECD	F		nw	7	25-35	20	28	0.8	no	5000	SS Cb/Cw	3	10,14	Nebeker et al., 1989
Lumbriculus variegatus		GC-ECD	F		nw	7.1-8.9	200	20	28	5.8	19	25100	Cb/Cw	2	4	Schuytema et al., 1989
Pisces																
Cyprinus carpio	8 cm		F			6.0-8.5		25	56	0.0005		11000-27000	SS Cb/Cw	4	15	NITE database, accessed august 21, 2009
Cyprinus carpio	8 cm		F			6.0-8.5		25	56	0.00005		6000-30000	SS Cb/Cw	4	15	NITE database, accessed august 21, 2009
Fundulus similis	field-collected	GC-ECD	F	Pest. Grade	rw (salt)				11	0.04-0.45	7	375	fitted curve; model	4	16	Giam et al., 1990
Fundulus similis	field-collected	GC-ECD	F	Pest. grade	rw (salt)				11	0.04-0.45	7	420	fitted curve; model	4	16	Giam et al., 1990
Gambusia affinis	0.19 g; 2.75 cm; adult	GC-ECD	R	>97	dtw	7.6		23.1	4	0.0012; 0.0021; 0.0037	4	3730	k1/k2	2	17,18	Chaiksuksant et al 1997
Gambusia affinis	0.19 g; 2.75 cm; adult	GC-ECD	R	>97	dtw	7.6		23.1	4	0.0012; 0.0021; 0.0037	4	3776	k1/k2	2	17,19	Chaiksuksant et al 1997
Gasterosteus aculeatus	3-8 mo; 300-500 mg ww	LSC	R	>97	rw			18	28	1.8	no	22100	Cf/Cw	2	2,20	Egeler et al., 2001

Species	Properties	Analysis	Test type	Purity [%]	Test water	pH	Hardness [mg/L]	Temp [°C]	Exp. Time [d]	Exp. Conc. [µg/L]	Dep. Time [d]	BCF [L/kg]	BCF type	Ri	Notes	Reference
Ictalurus punctatus	4 g; 6-7 cm	LSC	F	98.9	ftw			22	28	diet	14	11026	k1/k2	2	21,22	Woodburn et al., 2008
Lepomis macrochirus	juveniles	GC-ECD	F		nw	7.5	45.5	15	32			21900	Cf/Cw	2		Veith et al., 1979
Oncorhynchus mykiss	9.4 cm; 8.8 g; 10% lipid	GC-ECD	F	>99				20	20	1.07	no	6500	Cf/Cw	4	17,23	Lu and Wang, 2003
Oncorhynchus mykiss	9.4 cm; 8.8 g; 10% lipid	GC-ECD	F	>99				20	20	1.07	no	12126	Cf/Cw	2	17,24	Lu and Wang, 2002
Oncorhynchus mykiss	4-5 inches; 8-10 g			>99	dnw nw	8		12				7762	k1/k2	4	25	Neely et al., 1974
Oncorhynchus mykiss	250 g; hatchery-reared	GC-ECD	F		(filt.) nw			15	119	0.00032	no	12000	Cf/Cw	3	17,26	Oliver and Niimi, 1983
Oncorhynchus mykiss	250 g; hatchery-reared	GC-ECD	F		(filt.)			15	119	0.008	no	20000	SS Cb/Cw	3	17,27	Oliver and Niimi, 1983
Oncorhynchus mykiss	0.99 g; 2.8% lipids							14	10	diet	14	16708	k1/k2	2	21,28	Exxon Mobil database v.1.0
Oncorhynchus mykiss	2.3 g; 4.8% lipids							15.5	13	diet	21	15804	k1/k2	2	21,28	Exxon Mobil database v.1.0
Oncorhynchus mykiss	0.88 g; 2.4% lipids							13.2 14.7333	10	diet	10	10785	k1/k2	2	21,28	Exxon Mobil database v.1.0
Oncorhynchus mykiss	1.2 g; 3.2% lipids							3	13	diet	21	10120	k1/k2	2	21,28	Exxon Mobil database v.1.0
Oncorhynchus mykiss	1.4 g; 3.5% lipids							16.2	13	diet	21	22162	k1/k2	2	21,28	Exxon Mobil database v.1.0
Oncorhynchus mykiss	1.9 g; 5.6% lipids							14	11	diet	21	15028	k1/k2	2	21,28	Exxon Mobil database v.1.0
Oncorhynchus mykiss	fingerlings	GC-ECD	F		nw	7.5	45.5	15	32	low diet		5500	Cf/Cw	2		Veith et al., 1979
Oncorhynchus mykiss	juveniles; 2-4 g	GC-ECD	F		tw			10	30	conc high diet	160	20262	k1/k2	3	21,30,31	Fisk et al., 1998
Oncorhynchus mykiss	juveniles; 2-4 g	GC-ECD	F		tw nw			10	30	conc	160	19477	k1/k2	2	21,30	Fisk et al., 1998
Pimephales promelas	4-12 hr old	GC	F	97	(filt.) Nw	7.3-7.6	44-46	25	32-33	0.3		26700	SS Cb/Cw	2	32,33	Carlson and Kosian, 1987
Pimephales promelas	4-12 hr old	GC	F	97	(filt.) nw	7.3-7.6	44-46	25	32-33	0.7		21400	SS Cb/Cw	2	32,33	Carlson and Kosian, 1987
Pimephales promelas	4-12 hr old	GC	F	97	(filt.) nw	7.3-7.6	44-46	25	32-33	1.2		22500	SS Cb/Cw	2	32,33	Carlson and Kosian, 1987
Pimephales promelas	4-12 hr old	GC	F	97	(filt.) nw	7.3-7.6	44-46	25	32-33	2.6		17700	SS Cb/Cw	2	32,33	Carlson and Kosian, 1987
Pimephales promelas	4-12 hr old	GC	F	97	(filt.)	7.3-7.6	44-46	25	32-33	4.8		20200	SS Cb/Cw	2	32,33	Carlson and Kosian, 1987
Pimephales promelas	6 months old	GC-ECD	F		Nw	7.5	45.5	25	32-120	5		16600	Cf/Cw	2		Veith et al., 1979
Pimephales promelas	30 d old	GC-ECD	F		Nw	7.5	45.5	25	32-120	5		18200	Cf/Cw	2		Veith et al., 1979
Pimephales promelas	90 d old	GC-ECD	F		Nw	7.5	45.5	25	32-120	5		17800	Cf/Cw	2		Veith et al., 1979
Pimephales promelas	fry	GC-ECD	F		Nw	7.5	45.5	25	32-120	5		45700	Cf/Cw	2		Veith et al., 1979
Pimephales promelas	6 months old	GC-ECD	F		Nw	7.5	45.5	15	32			16200	Cf/Cw	2		Veith et al., 1979
Pimephales promelas	6 months old	GC-ECD	F		Nw	7.5	45.5	25	32	2.6		18500	Cf/Cw	2	34	Veith et al., 1979
Pimephales promelas	20-50 d old; 10-35 mm; 6.9% lipids	GC-ECD	F		Nw	7	25-35	20	28	3.8	no	12200	SS Cb/Cw	2	2,33,35	Nebeker et al., 1989
Pimephales promelas	20-50 d old; 10-35 mm;	GC-ECD	F		nw	7	25-35	20	28	2	no	15300	SS Cb/Cw	2	2,33,35	Nebeker et al., 1989

Species	Properties	Analysis	Test type	Purity [%]	Test water	pH	Hardness [mg/L]	Temp [°C]	Exp. Time [d]	Exp. Conc. [µg/L]	Dep. Time [d]	BCF [L/kg]	BCF type	Ri	Notes	Reference
	6.9% lipids															
	20-50 d old; 10-35 mm;															
Pimephales promelas	6.9% lipids	GC-ECD	F		nw	7	25-35	20	28	0.7	no	21100	SS Cb/Cw	2	2,33,35	Nebeker et al., 1989
	20-50 d old; 10-35 mm;															
Pimephales promelas	6.9% lipids	GC-ECD	F		nw	7	25-35	20	28	0.5	no	12600	SS Cb/Cw	2	2,33,35	Nebeker et al., 1989
	20-50 d old; 10-35 mm;															
Pimephales promelas	6.9% lipids	GC-ECD	F		nw	7	25-35	20	28	0.3	no	13300	SS Cb/Cw	2	2,33,35	Nebeker et al., 1989
	20-50 d old; 10-35 mm;															
Pimephales promelas	6.9% lipids	GC-ECD	F		nw	7	25-35	20	48	3.8	18	11500	SS Cb/Cw	2	2,33,35	Nebeker et al., 1989
	20-50 d old; 10-35 mm;															
Pimephales promelas	6.9% lipids	GC-ECD	F		nw	7	25-35	20	48	3.8	18	20700	SS Cb/Cw	2	2,33,35	Nebeker et al., 1989
Pimephales promelas												23400		4		Ahmad et al., 1979, in Nebeker et al., 1989
Pimephales promelas												48000-52000		4		Kosian et al., 1980 in Nebeker et al., 1989
Pimephales promelas		GC-ECD	R		nw	7.1-8.9	200	20	28	3.5	28	95400	Cb/Cw	3	36,37	Schuytema et al., 1989
Pimephales promelas		GC-ECD	R		nw	7.1-8.9	200	20	28	5	22	93800	Cb/Cw	2	36	Schuytema et al., 1989
	female, 0.62g; 5.4% lipid															
Poecilia reticulata	weight	GC	F		tw		89	21	7	0.3	60	15660	SS Cb/Cw	2	17,38	Konemann & van Leeuwen, 1980
					2/3 tw;											
Poecilia reticulata	150 mg; 18 mm; 5% lipids		S	>95	1/3 dw				290 h	1.5	no	27000	k1/k2	3	17,39	Schrap and Opperhuizen, 1990
	2y old; 15-20 mm; 206-															Opperhuizen et al., 1988
Poecilia reticulata	283 mg; 5% lipids	GC-ECD	S	>97	tw/dw			13	48h		no	18600	SS Cb/Cw	3	17,40	
	2y old; 15-20 mm; 206-															
Poecilia reticulata	283 mg; 5% lipids	GC-ECD	S	>97	tw/dw			19	48h		no	20800	SS Cb/Cw	3	17,40	Opperhuizen et al., 1988
	2y old; 15-20 mm; 206-															
Poecilia reticulata	283 mg; 5% lipids	GC-ECD	S	>97	tw/dw			28	48h		no	22900	SS Cb/Cw	3	17,40	Opperhuizen et al., 1988
	2y old; 15-20 mm; 206-															
Poecilia reticulata	283 mg; 5% lipids	GC-ECD	S	>97	tw/dw			33	48h		no	28800	SS Cb/Cw	3	17,40	Opperhuizen et al., 1988
Poecilia reticulata	0.15 g; 4% lipids	GC-ECD	S		ftw				230	diet	40	7664	k1/k2	2	21,41	Clark and Mackay, 1991
	6.24 g; 8.41 cm; 2.31%															
Salmo salar	lipids	GC/MS	S		dtw		14		96 h	see note	no	690	Cf/Cw	3	17,42	Zitko and Hutzinger, 1976
												K_{SPME} or K_{SPMD}				
Artifical																
SPME fibers	2 cm long 15µm	GC	S	98	tw	7.6	125	24	13	0.83		68320	k1/k2	2	6	Leslie et al., 2002
SPME fibers	1 cm polyacrylate fiber	GC-MS	S	'high'					2.5 h	0.21		66000	k1/k2	2	1744	Verbruggen et al., 2000
SPMD	triolein-SPMDs	GC-ECD	F	>99				20	20	1.07		18000	Cf/Cw	3	17,43	Lu and Wang, 2003

Notes:

1	Animals were fed twice per week
2	Steady state was reached
3	Significant mortality occurred
4	Steady state was approached, not reached
5	lipid-based
6	Midges exposed without substrate
7	unclear if BCF is based on ww, lw or dw
8	No steady state
9	Value in table is 2300; value in text is 1300
10	system contained sediment
11	sediment exposed to water HCB concentration of 1.4 µg/L for 1 month prior to test start
12	sediment exposed to water HCB concentration of 1.1 µg/L for 2 months prior to test start
13	system contained quartz sand
14	sediment was not pre-exposed to HCB
15	Data may be for hexachlorobiphenyl; report of data requested by NITE but not available.
16	Amount of fish per litre not reported; unclear if BCF is based on wet weight or dry weight; fish were fed
17	Exposure in a mixture
18	Lipid = 3.1%; Value according to author; exposure time relatively short to determine k_1 but k_1-value reported agrees with k_1 value calculated by weight
19	Lipid = 3.1%; Average of 3 steady state kinetic values at 3 different exposure concentrations; value calculated by dividing reported values for k_1 by k_2; exposure time relatively short to determine k1 but k1-value reported agrees with k1 value calculated by weight
20	Lipid = 2.7%; Cfish/Cw = 23100 L/kg.
21	Dietary study
22	Fish fed 2% of their weight; food 14.5% lipid
23	BCF estimated from figure; steady state may not have been reached yet. BCFs from figure 1 do not agree with figure 2.
24	BCF from text and figure 3. Steady state may not have been reached yet.
25	Based on muscle concentrations; method described by Branson et al., 1974
26	Equilibrium does not seem to be reached; 8.2% lipids at end of experiment; Fish loading too high (18g/L); exposure concentration too low for valid aqueous measurements
27	8.7% lipids at end of experiment; Fish loading too high (18 g/L); exposure concentration too low for valid aqueous measurements

28 BCF calculated using weights (k1) and reported half-lives (k2); fish fed diet at 0.03 g food/ww/day; mean lipid content of diet is 15.6%
29 Food spiked with a mixture of 16 PCBs, HCB and Mirex; fish fed 1.5% of their weight; Food lipid = 14%; value may be incorrect due to contaminated food at depuration fase
30 Food spiked with a mixture of 16 PCBs, HCB and Mirex; fish fed 1.5% of their weight; Food lipid = 14%;
31 Value may be incorrect due to contaminated food at depuration fase
32 Exposure from embryos to juveniles
33 No toxicity observed
34 Value selected by author
35 Fish were fed daily
36 BCFs are relatively high, but based on wet weight.
37 Steady state does not seem to be reached
38 Total exposure was 19 d, but BCF was calculated after 7d of exposure. No elimination constant could be determined. Original value (290000) was based on lipid content and recalculated.
39 Total concentration showed toxicity by lower activity of fish and mortality at day 4.
40 Equilibrium was reached in a preliminary study at 48h but this does not seem to be reliable; original BCF in ref reported based on lipid contents, recalculated using 5% lipids
41 BCF calculated using weights (k_1) and reported half-live (k_2); fish fed diet at 4% of ww per day, mean lipid content of diet is 6.7%
42 >6g Fish/L; water concentrations decreased from 6.6 µg/L (initially) to 0.22 µg/L after 96 hours
43 BCF estimated from figure; BCFs from figure 1 do not agree with figure 2.
44 Exposure concentration based on measured concentrations, which were 50% of nominal.

Table A2. Bioconcentration data for hexachlorobutadiene

Species	Species properties	Analysis	Test type	Purity [%]	Test water	pH	Temp. [°C]	Exposure time [d]	Exposure concentration [µg/L]	BCF [L/kg ww]	BCF type	Ri	Notes	Reference
Cyprinus carpio	6.2 % lipids (4.9-7.5) in the beginning; 5.1% lipids in the end (range 3.8-8.5%; n = 3); 8 +/- 4 cm; 5 grams	Y; GC/MS	F	96	carbon-filtered tapwater	6.0-8.5	24	60	0.831	6608	Cfish/Cwater	2	1	NITE database; accessed august 21, 2009
Cyprinus carpio	6.2 % lipids (4.9-7.5) in the beginning; 5.1% lipids in the end (range 3.8-8.5%; n = 3); 8 +/- 4 cm; 5 grams	Y; GC/MS	F	96	carbon-filtered tapwater	6.0-8.5	24	60	0.087	7555	Cfish/Cwater	2	1	NITE database; accessed august 21, 2009
Oncorhynchus mykiss	250 g; hatchery-reared	GC-ECD	F		nw (filtered)		15	119	0.0001	5800	steady state Cf/Cw	3	2	Oliver and Niimi, 1983
Oncorhynchus mykiss	250 g; hatchery-reared	GC-ECD	F		nw (filtered)		15	119	0.00034	17000	steady state Cf/Cw	3	2	Oliver and Niimi, 1983

Notes:

1 Solvent = HCO-40 0.02 mg/L; 2 weeks elimination time; 60 fish in 50 litres; test equipment 'improved for a volatile substance'; BCF calculated using data provided by author

2 Exposure together with other chlorobenzenes; 8.7% lipids at end of experiment; Fish loading too high (18 g/L); exposure concentration too low for valid measurements

Appendix B. Biomagnification data for HCB

Biomagnification factors (BMFs)

Field studies

Borgå et al. (2001) measured biomagnification of organochlorines along a Barents Sea food chain, from invertebrates (copepods, euphasiids, amphipods) and codfish to seabirds. All organisms except the two Guillemot birds were collected in the Barents Sea near Bjørnøya from May to June 1995. Guillemots were collected during the same period in the marginal ice zone further north in the Barents Sea. Biomagnification factors ($ng.g_{predator}^{-1}$/ $ng.g_{prey}^{-1}$) were based on lipid weights. In the lower end of the foodchain (excluding seabirds), the cod (predator)/polar cod (prey) BMF was 1.7; the average cod/invertebrate BMF was 4.0 and the average polar cod/invertebrate BMF was 2.4. Regarding the four species of birds, the bird/cod BMF was 63, 13, 5.2, and 8.9 for Glaucous gull, Kittiwake, Black guillemot and Brunnich's guillemot, respectively. (Ri = 2)

Hop et al. (2002) reported biomagnification factors for fish (cod), birds and seals from the Barents Sea. Samples from 7 locations were taken in June 1995. BMFs were calculated according to $(C_{predator,\ lipid}/C_{prey,lipid})/(TL_{predator}-TL_{prey})$. Because the trophic levels of predators in most cases were not a full trophic level above the prey based on $\delta^{15}N$ values, BMFs was corrected to unity for trophic level increase ($TL_{predator}-TL_{prey}$). BMFs for fish were 3.4 or 2.6, depending on the prey composition in the calculations. BMFs for harp seal and ringed seals were 7.3 and 0.5 respectively (with different prey compositions for each seal species). For birds, the BMFs were determined to range from 9.3 to 36.6. However, when these data are recalculated the values of Hop et al (2002) do not correspond to their measured values, except for the values for fish. If recalculated using data in the article, the BMF for harp seal adjusted to trophic level is 13.2 and not adjusted to trophic level the BMF is 5.7. (Ri = 4; results do not correspond to data and cannot be reproduced).

Hoekstra et al (2003). determined trophic transfer within an Arctic marine food web from the southern Beaufort-Chukchi Seas. The foodweb contained zooplankton, fish species and mammals such als ringed seals, bearded seals, bowhead whales and beluga whales. Samples were collected form 1999 to 2000 at two locations; results were not further specified per location. Trophic levels of each organism were determined using $\delta^{15}N$. BMFs were calculated according to $(C_{predator,\ lipid}/C_{prey,lipid})/(TL_{predator}/TL_{prey})$ and adjusted for trophic level based on $\delta^{15}N$. BMFs measured in this study were 8.7, 2.6, 0.3, 0.2 and 5.5 for bowhead whale, cod, ringed seal, bearded seals and beluga whales, respectively. However, the calculation of the BMFs is not correct and should be adjusted for $TL_{predator} - TL_{prey}$ instead of $TL_{predator}/TL_{prey}$. (Ri = 3 due to wrong TL-correction).

Fraser et al. (2002). used data from Wolkers et al (2000) to model biomagnification of HCB in harp seals of the Barents Sea, with crustaceans and polar cods as food. BMFs were calculated using two methods: (1) based on concentrations in wet weights of the organisms (not lipid-normalised) and (2) based on lipid-normalised fugacities. The BMFs were 14.44 and 3.58, respectively. The ratio of lipid contents between seal and prey was reported to be about 4.0. (Ri = 4; data from Wolkers unknown).

Fisk et al. (2001) measured biomagnification factors for individual species in a foodweb in the Baffin Bay in the Canadian Arctic, according to $(C_{predator,\ lipid}/C_{prey,lipid})/(TL_{predator}-TL_{prey})$, with lipid-corrected concentrations. Samples were collected during the April-July 1998 voyage of a research vessel through the Northwater Polynya strait. Trophic levels of each organism were

determined using $\delta^{15}N$. BMFs for amphipods and fish were 3.8 and 6.1, respectively. For ringed seals, the BMF was 0.2. For seabirds, the BMF ranges from 5.0 to 21.6. Please note that in the text Fisk et al. give a wrong equation where $TL_{predator}$ is divided by TL_{prey}, but in the table TL_{prey} is correctly abstracted from $TL_{predator}$. (Ri = 2)

Goerke et al. (2004) measured biomagnification in the antarctic food web (krill, cephalopod, fish, penguin, seal) of the area around Elephant Island and from the Weddell Sea. Samples were taken between 1986 and 2000. Lipid normalised concentrations of the species (not specified whether geographic locations were taken into account) were compared to determine biomagnification factors. For the krill-feeding mackerel icefish *Champsocephalus gunnari*, the BMF was determined to be 3. For three other fish species, the BMF was 1.6, 2.2 and 2.0; for squid the BMF was 1.1. For the adelie penguin the BMF was 8.1, but this species does not directly feed on krill. For the top predators (Weddell seal and southern elephant seal) the BMF compared to krill was 1, which means that the BMF compared to their food sources (fish, penguins) was much lower than 1, pointing to metabolic transformation of HCB in these seals. (Ri = 3, samples not taken in the same year).

Morrissey et al. (2005) measured biomagnification factors in eggs from the American dipper (a bird; *Cinclus mexicanus*) from the Chilliwack River watershed in British Columbia, Canada, collected in 1999, 2000, and 2001. Prey was sampled in April 2002 at 15 different locations. Diet was supposed to consist of 67% invertebrates and 33% salmon fry. BMFs were based on lipid-normalised concentrations. For HCB, the BMF was 4.7. (Ri = 3, samples not taken in the same year).

Strandberg et al. (1998a) reported data from four specimens of harbour porpoise (*Phocoena phocoena*) found dead in fishing nets during 1991-1993 and three herring (*Clupea harengus*), caught close to the porpoise catch in 1992. The age of the porpoises was 2-4 years. The average BMF (based on lipid normalised concentrations) was 4.9. (Ri = 3, samples not taken at the same time and the same location).

Strandberg et al. (1998b) collected zooplankton, *Mysis* sp.and herring (*Clupea harengus*) at two different stations in the northern part of the Baltic Sea. Only a few samples/specimens (2-4) of each trophic level were analyzed. The BMF can be calculated from reported lipid-normalised concentrations and is 1.3 and 0.7 for zooplankton to mysis, 2.2 and 8.6 for zooplankton to herring, and 1.7 and 12.8 for mysis to herring for the two respective locations. However, these calculated BMF values do not agree with BMFs reported in a figure in the article. (Ri = 4, figures and tables do not match).

Ruus et al. (1999) determined biomagnification factors in a marine food chain including the lesser sandeel, cod, harbour seal and grey seal, from the Jarfjord in Norway. Animals were caught in 1989 and 1990 and blubber of seals, liver of cod and homogenised individuals of sandeels were sampled. Lipid-normalised BMFs were only calculated where there were significant differences in HCB concentrations between the trophic levels (Kruskal-Wallis multiple comparisons, $p<0.05$), which was not the case for harbour seal to sandeel and grey seal to cod. For Cod/Sandeel the BMF was 2.1; for Grey seal/Sandeel the BMF was 2.7; and for Harbour seal/Cod the BMF was 0.3. (Ri = 2)

Catalan et al. (2004) reported the distribution of organochlorine compounds in a food web in a high mountain lake in the Pyrenees in Spain. Dates of sampling were not specified. The food web comprised chironomids, terrestrial isnects, cladocerans, molluscs, cyanobacteria and brown trout. Water concentrations were also measured. Brown trout diet was estimated by analysis of fish stomach contents and $\delta^{15}N$-analysis. Using average diet proportions and the concentrations in diet, the lipid-normalised BMF is 6.8. (Ri = 2)

Russel et al. (1995) determined biomagnification of organochlorines in Lake Erie White Bass caught in 1990 by analysing muscle and intestinal contents of the bass and pooled whole body samples of their prey (emerald shiner). The lipid-normalised biomagnification factor for HCB was 0.79. (Ri = 2)

Ramu et al. (2006) analysed organohalogen compounds in the blubber of male finless porpoises (*Neophocaena phocaenoides*) collected in 1990 (7 animals) and 2000/2001 (5 animals) in the South China Sea. Stomach contents in semi-digested form in two finless porpoises were also analysed. The average lipid-normalised BMF for porpoise/stomach content was 0.84. (Ri = 3; stomach content concentrations may have changed, BMF only based on two stomach samples).

Jarman et al. (1996) measured trophic positions and HCB concentrations in a food web of the Gulf of the Farallones (USA). Two species of krill were sampled in February 1994 with a research vessel; two fish species were sampled in July 1993 at the Farallon Islands; eggs from four bird species were collected in the summer of 1993 at the Farallon Islands. $\delta^{15}N$ Concentrations were determined, as well as concentrtions of organochlorines. From the data provided in the article, not only a TMF can be calculated, but also lipid-normalised BMF values can be derived using $(C_{predator,\ lipid}/C_{prey,lipid})/(TL_{predator}-TL_{prey})$. BMF values for fish/krill were 2.1 and 1.2; BMF values for birds/average fish were 2.5, 5.2, 11.2, and 14.8. (Ri = 3; samples not taken at the same time and the same location).

Laboratory studies

Clark and Mackay (1991) determined biomagnification of HCB by guppy (Poecilia reticulata) from contaminated food. Food was spiked commercial fish food. HCB contents in the guppy achieved steady state after approximately 30 days. When the guppies were fed clean food, HCB was rapidly eliminated, suggesting that this chemical may be metabolized. They state that significant biomagnification is unlikely for this fish species. A BMF of 0.1 (based on lipid normalised concentrations) and a BCF of 7700 L/kg can be calculated using data provided in the article, although it is not clear if k_1 and k_2 were taken from the same experiment. (Ri = 2).

Woodburn et al. (2008) determined the dietary absorption efficiency of haxachlorobenzene with the channel catfish (*Ictalurus punctatus*). Catfish were exposed to 340 ng ^{14}C-radiolabeled HCB /g food (14.5% lipids) over a 28-day exposure period followed by a 14-day clearance period. The fish were maintained in a flow-through system to minimize uptake through the gills, with Lake Huron water which was filtered, pH-adjusted and UV-irradiated. The BMF was calculated using a two-box kinetic model as k1/k2 and determined to be 0.59. This BMF was not lipid-normalised. Using concentrations and lipid contents reported in the article, a lipid-normalised BMF of 0.35 can be calculated. Using data provided in the article, a BCF of 11000 L/kg can be calculated. (Ri = 2)

Fisk et al. (1998) measured biomagnification factors in the laboratory using juvenile rainbow trout (*Oncorhynchus mykiss*) and spiked fish food. Rainbow trout were exposed for 30 days in a flow-through system with carbon dechlorinated tap water at 10 ºC. Fish food was spiked at two concentrations (13.7 ng/g ww and 103 ng/g ww). After 30 days, steady state was not reached. BMFs were calculated using feeding rates and assimilation efficiencies and were lipid-corrected. Because the control food also contained some HCB, the BMF from the lower food concentration (2.3) was suggested to be less reliable. The BMF from the higher food concentration was 1.4. BCFs can also be calculated using the data provided in the article, and are 20300 and 19500 for the low and high food concentration, respectively. (Ri = 2)

Trophic magnification factors (TMFs)

Trophic magnification factors are calculated using measured $\delta^{15}N$ and HCB concentrations in the animals. Trophic levels of the organisms are determined using $\delta^{15}N$ concentrations, and then TMFs or FWMFs (Food Web Magnification Factors) are usually calculated from the slope of the relationship of $\log_{10}$- or ln- transformed, lipid normalised HCB concentrations versus trophic levels for all species.

Muir et al. (2003) measured food web magnification factors (FWMFs; comparable to TMFs) in the White Sea pelagic food web, including harp seals, ringed seals, bearded seals as well as fish and invertebrates. Marine mammals were collected in 1998 and 2001, while prey speceis were collected in 1999 and 2000. Samples were all taken in the White Sea, but not at the same locations. The resulting FWMF (or TMF) was 2.3. (Ri = 3, species not collected at the same time and the same location).

Houde et al. (2008) determined trophic magnification factors in 17 Canadian lakes differing in trophic status and food web characteristics. Samples were taken between 1998 and 2001, but samples within each lake were taken at the same time. Sampling locations in each lake were not specified. Trophic levels of each organism were determined using $\delta^{15}N$. TMFs were calculated based on the antilog value of the regresion slope between log HCB concentrations based on lipid weights versus trophic levels for all species. All food webs contained at least two fish species and two invertebrate groups. The resulting TMF values ranged from -0.9 to 6.9 with an average value of 2.9. Per geographic area the TMFs were 4.2, 2.1, and 2.1 for the Northern, Northwest Ontario, and Southern lakes, respectively. (Ri = 2)

Hop et al. (2002) reported food web magnification factors (FWMFs; comparable to TMFs) for the Barents Sea food web, which included invertebrates, fish, birds and seals. Samples from 7 locations were taken in June 1995. FWMFs were reported for both poikilotherms and homeotherms (cold- and warm-blooded animals) for the whole lake (without reference to the sampling locations). FWMFs were calculated using a linear regression model with HCB concentrations based on lipid weights versus trophic levels (determined using $\delta^{15}N$) for all species. For both poikilotherms and homeotherms the FWMF (TMF) was determined to be 4.7. (Ri = 2)

Wan et al. (2005) reported TMFs for a number compounds in the marine food web of Bohay Bay in North China, consisting of primary producers, invertebrates, fish and one seabird species. Aquatic samples were taken during the summer of 2002; while birds were sampled in November 2002. HCB was used as a benchmark for trophic transfer. Trophic levels of each organism were determined using $\delta^{15}N$. TMFs were calculated from the slope of the relationship of HCB concentrations based on lipid weights versus trophic levels for all species. The resulting TMF for HCB was 2.96. (Ri = 2)

Hoekstra et al. (2003) determined trophic transfer within an Arctic marine food web from the southern Beaufort-Chukchi Seas. Samples were collected form 1999 to 2000 at two locations; results were not further specified per location. The foodweb contained zooplankton, fish species and mammals such as ringed seals, bearded seals, bowhead whales and beluga whales. Trophic levels of each organism were determined using $\delta^{15}N$. FWMFs were calculated from the slope of the relationship of $\log_{10}$-transformed, lipid normalised HCB concentrations versus trophic levels for all species. The FWMF measured in this study was 1.36. Hoekstra et al. further recalculated FWMFs from other studies to exclude avian data and benthic oriented species. This results in a FWMF for North Baffin Bay of 1.75 (data from Fisk et al., 2001) and a FWMF for Barents Sea of 1.55 (data from Borgå et al., 2001; Hop et al., 2002). (Ri = 2)

Fisk et al. (2001) measured food web magnification factors (FMWFs) for a foodweb in the Baffin Bay in the Canadian Arctic. Samples were collected during the April-July 1998 voyage of a research vessel through the Northwater Polynya strait. HCB was measured in zooplankton, an invertebrate, cod, 6 species of seabirds, and ringed seal. Trophic levels of each organism were determined using $\delta^{15}N$. The FWMF were calculated from the slope of the relationship of ln-transformed, lipid normalised HCB concentrations versus trophic levels for all species and was reported to be 4.1. (Ri = 2)

Jarman et al. (1996) measured trophic positions and HCB concentrations in a food web of the Gulf of the Farallones (USA). Two species of krill were sampled in February 1994 with a research vessel; two fish species were sampled in July 1993 at the Farallon Islands; eggs from four bird species were collected in the summer of 1993 at the Farallon Islands. $\delta^{15}N$ Concentrations were determined, as well as concentrtions of organochlorines. From the data provided in the article, a TMF can be calculated from the slope of the relationship of log-transformed, lipid normalised HCB concentrations versus trophic levels for all species. This TMF is 3.5. (Ri = 3, species not collected at the same time and the same location)

Furthermore, a number of studies have not been able to show any food web accumulation. Ruus et al. (2002) determined food web accumulation for a marine food web from southeastern Norway from April 1998 to November 1999, consisting of polychaetes, fish, harbor seal and gull. No significant regression was found between the concentration of HCB and trophic level. They suggest that this is caused by the lower concentration of HCB in harbor seal than in fish and herring gull, which, according to the authors, may be attributed to higher metabolic capacity in this species (Ri = 2). Ikemoto et al. (2008) were also not able to show food web accumulation for a tropical aquatic food web in the Mekong Delta in Vietnam. No significant increase in HCB concentrations relative to $\delta^{15}N$ contents were detected (Ri = 4).

Appendix C. Bioaccumulation data for HCB

Bioaccumulation factors (BAFs) are the ratio of a compound in the organism over the concentration in water. This is similar to a BCF, but the BAF also includes exposure through food while the BCF only includes exposure through the water. BAFs are often determined in the field, while BCFs are mostly determined in the laboratory. For HCB, only studies with water concentrations measured as dissolved concentrations are valid.

Kucklick et al. (1996) measured BAFs for hexachlorobenzene in the pelagic food web of Lake Baikal. Zooplankton, amphipods, and fish were collected in August and September 1993. Fish were sampled at one location, while water samples were taken at seven different locations throughout the lake. Water samples were filtrated before analysis, so BAFs are based on dissolved concentrations. Since HCB concentrations in the zooplankton and the amphipods were below detection limits, no TMF or BMF could be calculated. Water and biota samples (composite year classes) were analysed using GC-ECD and GC-NIMS. For the pelagic sculpin *Comephorus dybowskii* the average BAF over all year classes (4-8 years) was 7,440,500 L/kg lipid. For *Comephorus baikalensis* the BAF increased with nearly an order of magnitude with age. The BAF for the white fish *Coregonus atumnalis migratorious* was relatively constant over the year classes from 3 – 13 years and was on average 1,805,384 L/kg lipid. (Ri = 2)

Besides a BMF, a BAF can also be calculated using the data provided by Catalan et al. (2004; see above). Using dissolved concentrations of HCB in lake water, the BAF for muscle of the brown trout (*Salmo trutta*) is 2.4 x 10^5 L/kg based on dry weight and 8.7 x 10^6 based on lipid weight. (Ri = 2)

Burkhard et al. (1997) reported BAF values for four different species of fish from Bayou d'Inde in Louisana, USA. They were caught in october 1990, while water samples were taken in september/october 1990 at the same locations. Water samples were not filtered, but TOC and DOC concentrations were measured and dissolved water concentrations were calculated using a partitioning model. This model uses a K_{OC} value for sorption to TOC that is equal to K_{OW}, which in our view is not correct. Moreover, there are serious doubts on the measured TOC (too low?) and DOC (too high?) concentrations. BAF values based on freely dissolved and lipid-based concentrations were 1.1 × 10^6, 6.3 × 10^5, 4.8 × 10^6, and 2.0 × 10^6 L/kg lipid for the fish *Fundulus heteroclitus*, *Callinectes sapidus*, *Brevoortia patronus*, and *Micropoganias undulatus,* respectively. Lipid contents of the fish were not reported. (Ri = 3 because data are based on total water concentrations and because there are serious doubts on the method to recalculate these data to dissolved water concentrations).

Pereria et al. (1998) measured BAFs based on total water concentrations for four species: the atlantic croaker *Micropogonias undulatus*, the blue crab *Callinectes sapidus*, the spotted sea trout *Cynoscion nebulosis* and the blue catfish *Ictalurus furcatus* in the Calcasieu River estuary in Louisiana, USA. Except for the blue catfish all these species are migratory. Water (not filtered) and suspended sediments were also sampled, probably on the same date (Burkhard et al., 1997). Lipid based BAFs based on total water concentrations were 2.6 × 10^6, 5.1 × 10^6, 9.1 × 10^5, and 9.6 × 10^5 L/kg lipid for *Micropoganias undulatus*, *Callinectes sapidus*, *Cynoscion nebulosis* and *Ictalurus furcatus*, respectively. Burkhard et al. (1997) reported corrected BAF values from this study. Where Pereria et al. (1988) measured BAFs based on total water concentrations, Burkhard corrected these to BAFs based on dissolved water concentrations (see above) using a partitioning model with DOC and POC values reported by the United states Geological Survey. For HCB, lipid-based BAFs based on dissolved water concentrations using the data from Pereria et al. were 4.7 × 10^6, 9.1 × 10^6, 1.6 × 10^6, and 1.7 × 10^6 L/kg lipid for

Micropoganias undulatus, *Callinectes sapidus*, *Cynoscion nebulosis* and *Ictalurus furcatus*, respectively. These fish were caught in the same river ecosystem but at a different location than the fish used by Burkhard et al. (1997). (Ri = 3 for non-corrected data because these are based on total water concentrations because there are serious doubts on the method to recalculate these data to dissolved water concentrations).

Oliver and Niimi (1988) reported HCBD concentrations in a number of species sampled at different locations in Lake Ontario in 1981 and 1982. Water samples (centrifuged to remove particulates) were collected at various locations in 1984. No significant concentration trends were apparent in sediment trap materials collected from 6-month deployments of the traps in the three lake basins over the same 5-year period. Lipid-normalised BAFs can be calculated using the data reported in the paper. For mysids (*Mysis relicta*; composite of 2 samples taken 3 years apart), the BAF was 8.9×10^5 L/kg lipid. For amphipods (*Pontoporeia affinis*) the BAF was 4.0×10^6; for sculpin (*Cottus cognatus*) 3.2×10^6; for alewife (*Alosa pseudoharengus*) 1.9×10^6; for smelt (*Osmerus mordax*) 1.3×10^6 and 2.3×10^6 L/kg lipid for smaller and larger species, respectively. For a composite sample of a number of salmonids (*Oncorhynchus kisutch*, *Oncorhynchus mykiss*, *Salvelinus namaycush* and *Salmo trutta*) the BAF was 2.3×10^6. Burkhard et al. (1997) recalculated the BAFs (see above) for fish from this study for non-DOC containing water, using a partitioning model with an assumed DOC concentration of 2 mg/L. The resulting lipid-based BAFs were 3.4×10^6, 2.0×10^6, 1.4×10^6, and 2.5×10^6 L/kg lipid for *Cottus cognatus*, *Alosa pseudoharengus* and *Osmerus mordax* (small and large), respectively. However, the data recalculated by Burkhard are deemed to be not valid because of limitations of the calculation method. (Ri = 2 for the original data)

Egeler et al. (2001) exposed three-spined stickleback (*Gasterosteus aculeatus*) to HCB in a laboratory setting. Juvenile sticklebacks (3-8 months old; 300-500 mg ww) were exposed at 18 ºC in glass aquaria with reconstiuted freshwater with 1% reconstituted seawater, which was renewed once per week. Uptake from water only (bioconcentration) was studied for 28 days (for results see bioaccumulation table); uptake in systems with sediment or sediment and worms was studied for 63 days. Steady state was reached after 30 days. All samples (water samples were not filtered) were measured by LSC. From the data provided in the article, a wet-weight based BAF of 51800 can be calculated, which corresponds to a lipid-based BAF of 7.8×10^5 L/kg lipid. The BMF for fish to worm was 0.54 in systems without sediment, and 1.3 in systems with sediment. (Ri = 3 for BAF; water samples were not filtered).

Appendix D. Bioaccumulation data for HCBD

Burkhard et al. (1997) determined BAF values for four different species of fish from Bayou d'Inde in Louisana, USA. Fish were caught in October 1990, water samples were taken in September/October 1990 at the same locations. Water samples were not filtered, but TOC and DOC concentrations were measured and dissolved water concentrations were calculated using a partitioning model. This model uses a K_{OC} value for sorption to TOC that is equal to K_{OW}, which in our view is not correct. Moreover, there are serious doubts on the measured TOC (too low?) and DOC (too high?) concentrations. Lipid-based BAF-values based on freely dissolved concentrations were 575000, 339000, and 282000 L/kg lipid for the fish *Fundulus heteroclitus* (mummichog), *Brevoortia patronus* (Gulf menhaden) and *Micropoganias undulatus (*Atlantic croaker) respectively. The BAF for the blue crab *Callinectes sapidus* was 6760 L/kg lipid. Lipid contents of the animals were not reported. (Ri = 3 because data are based on total water concentrations and because there are serious doubts on the method to recalculate these data to dissolved water concentrations)

Pereria et al. (1998) also measured BAFs for the atlantic croaker *M. undulatus* and the blue crab *C. sapidus*, and additionally for the spotted sea trout *Cynoscion nebulosis* and the blue catfish *Ictalurus furcatus*. Animals were caught in the Calcasieu River estuary in Louisiana, USA. This belongs to the same river basin as used by Burkhard et al. (1997), but refers to a different location. Except for the blue catfish all these species are migratory. Water (not filtered) and suspended sediments were also sampled, probably on the same date (Burkhard et al., 1997). Lipid based BAFs based on total water concentrations were 31600, 9200, 11600, and 35400 L/kg lipid for *M. undulatus*, *C. sapidus*, *C. nebulosis* and *I. furcatus*, respectively. However, reported total water concentrations for HCBD were much higher than what would be expected on basis of the suspended sediment concentrations and the concentrations of other compounds. This could have caused an underestimation of the BAFs.
Next to their own experimental data, Burkhard et al. (1997) also reported corrected BAF values from this study. Where Pereria et al. (1988) measured BAFs based on total water concentrations, Burkhard et al. (1997) corrected these to BAFs (see above) based on dissolved water concentrations using a partitioning model with DOC and POC values reported by the United states Geological Survey. Resulting estimated lipid-based BAFs based on dissolved water concentrations were 36300, 10700, 13200, and 40700 L/kg lipid for *M. undulatus*, *C. sapidus*, *C. nebulosis* and *I. furcatus*, respectively. These values are about an order of magnitude lower than the BAF determined earlier by Burkhard et al. (1997) themselves. This is most likely caused by erroneous total water concentrations for HCBD in the Pereria paper. (Ri = 3 because of possible erroneous water concentrations).

Oliver and Niimi (1988) reported HCBD concentrations in a number of species sampled at different locations in Lake Ontario in 1981 and 1982. Water samples (centrifuged to remove particulates) were collected at various locations in 1984. No significant concentration trends were apparent in sediment trap materials collected from 6-month deployments of the traps in the three lake basins over the same 5-year period. Lipid-based BAFs can be calculated using the data reported in the paper. For mysids (*Mysis relicta*; composite of 2 samples taken 3 years apart), the BAF was 185200 L/kg lipid. For amphipods (*Pontoporeia affinis*) and sculpin (*Cottus cognatus*) the BAFs were 5000000 and 347200 L/kg lipid, respectively. Burkhard et al. (1997) recalculated the BAF (see above) for sculpin from this study for non-DOC containing water, using a partitioning model with an assumed DOC concentration of 2 mg/L. The resulting lipid-based BAF based on dissolved concentrations was 355000 L/kg lipid for *Cottus cognatus*. However, the data recalculated by Burkhard are deemed to be not valid because of limitations of the calculation method. (Ri = 2 for the original data)

Published by:

National Institute for Public Health and the Environment
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