Common Implementation Strategy for the Water Framework Directive

Environmental Quality Standards (EQS)

Substance Data Sheet

Priority Substance No. 17

Hexachlorobutadiene

CAS-No. 87-68-3

Final version
Brussels, 31 July 2005

Disclaimer

This data sheet provides background information on the setting of the Environmental Quality Standard in accordance with Article 16 of the Water Framework Directive (2000/60/EC). The information was compiled, evaluated and used as outlined in the Manual [4] and has been discussed in a consultative process with the Expert Advisory Forum on Priority Substances and the Expert Group on Quality Standards. Furthermore, it has been peer-reviewed by the SCTEE[9]. The substance data sheet may, however, not necessarily represent the views of the European Commission.

New upcoming information was considered and included up to the date of finalisation of this data sheet. Information becoming available after finalisation of this document will be evaluated in the review process of priority substances according to Art. 16(4) of the Water Framework Directive. If necessary, the Environmental Quality Standard substance data sheets will then be revised in the light of technical and scientific progress.

1 Identity of substance

Priority Substance No: 17	Hexachlorobutadiene
CAS-Number:	87-68-3
Classification WFD Priority List*:	PHS

* PS: priority substance; PHS: priority hazardous substance; PSR: priority substance under review according to Decision 2455/2001.

2 Proposed quality standards

2.1 Overall quality standards

Ecosystem	**Quality Standard**	**Quality Standard "rounded values"**	**Comment:**
AA-QS all surface waters covered by the WFD	Protection against direct effects: 0.44 µg/l Protection against secondary poisoning: 55.3 µg/kg prey (biota tissue wet wt)	Protection against direct effects: **0.1 µg/l** Protection against secondary poisoning: **55 µg/kg prey (biota tissue wet wt)**	The proposed rounded EQS is not based on the derivation in section 8.1 but consistent with the existing EQS in Council Directive 86/280/EEC. Secondary poisoning and human health are the most critical protection objectives; see sections 8.3, 8.4 & 8.6
MAC-QS (ECO)	0.59 µg/l	**0.6 µg/l**	see section 8.1

2.2 Specific quality standards

Protection Objective#	**Quality Standard**	**Comment:**
Pelagic community (freshwater)	0.44 µg/l corresponding conc. in SPM: 485 µg/kg dry wt	see section 8.1
Pelagic community (saltwater)	0.44 µg/l corresponding conc. in SPM: 491 µg/kg dry wt	see section 8.1
Benthic community (freshwater & saltwater sediment)	107 µg/kg (wet wt) 493 µg/kg (dry wt)	tentative standard based on EP-method see section 8.2
Predators (secondary poisoning)	55.3 µg/kg prey (biota tissue wet wt) corresponding conc. in water: 0.003 µg/l corresponding conc. In SPM 3.3 µg/kg dry wt	see section 8.3
Food uptake by man	12.2 µg/kg seafood (wet wt) corresponding conc. in water: (0.0007 - 0.0174 µg/l)	based on WHO TDI see section 8.4
Abstraction of water intended for human consumption (AWIHC)	no EU DW abstraction standard set; derivation of such a QS is not required	see section 8.5
Water intended for human consumption (WIHC)	no EU DW standard set	WHO guide value is 0.6 µg/l; see section 8.5

If justified by substance properties or data available, QS for the different protection objectives are given independently for freshwater environments, transitional waters or coastal and territorial waters

3 Classification

R-Phrases and Labelling	Reference:
This chemical substance is not classified in the Annex I of Directive 67/548/EEC.	[11]
According to Annex 1 of Directive 93/72/EEC hexachlorobutadiene should be classified as: Harmful in contact with skin or if swallowed (R21/22), irritating to eyes and respiratory system (R36/37), possible risk of irreversible effects (R40), may cause sensitisation by skin contact (R43), very toxic to aquatic organisms. May cause long-term adverse effects in the aquatic environment (R 50/53).	[1]

4 Physical and chemical properties

Property	Value:	Ref.
Molecular weight	260.8 (g/mol)	[1]
Vapour pressure	20 Pa at 20°C 36 Pa (20 °C)	[1] [5]
Henry's law constant	1630 Pa.m^3/mol at 25°C	[1]
Solubility in water	3.2 mg/l at 20°C 4 mg/L (20 °C) 3 mg/L 2 mg/L 3.23 (25 °C)	[1] [5] [5] [5] [5]

5 Environmental fate and partitioning

Property	Value:	Ref:	Comments:
Hydrolysis	not relevant under enviromental conditions	[5]	
Biodegradation	half life in natural water 4-52 weeks	[1]	
Partition coefficients			
log Kow	4.78 to 4.9 4.9	[1], [5] [6]	
Koc	log Koc 3.95-4.05 log Koc 4.51 1260000 l/kg (sediment) 25100 L/kg (sediment) 2400 L/kg (soil, calculated)	[1] [6] [5] [5] [5]	
Bioconcentration			
BCF fish:			
Salmo gairdneri	5800 - 17000	[1]	17,000 used for risk assessment in [1]
Poecilia latipinna & *Micropterus salmonides*	although variable normally below 50	[1]	
Pleuronectes patessa & *Limanda limanda*	500 – 700 (flesh) 7000 – 10000 (liver)	[1]	
Oncorhynchus mykiss	2000 - 19000	[5]	
Micropterus salmonides	1.4 – 112.9	[5]	
Poecilia latipinna	1.7 – 196	[5]	
Cynoscion nebulosis	264	[5]	
Micropogonias undulatus	696	[5]	
Ictalurus furcatus	1171	[5]	
BCF bivalves:			
Mytilus edulis	900 – 2000	[5]	
BCF oligochaete worms:	29000 (based on dry wt)	[1]	

Property	Value:	Ref:	Comments:
Biomagnification:	[1]: 2 publications: fish were fed with food contaminated with HCBD. In one study no clear evidence on bioconcentration but results variable and inconclusive. In other study no evidence of bioaccumulation was seen. [1]: A number of authors have examined data to determine if HCBD might biomagnify through the food chain. For example Goldbach *et al.* (1976) examined levels of HCBD in fish of prey and found that concentrations in fish such as pike and perch were in fact lower than in the prey fish. No correlation between age and HCBD residues was found. Based on these findings the authors concluded there is no significant biomagnification to higher trophic levels. This conclusion is supported by Pearson and McConnell (1975) who concluded that there was little evidence for biomagnification of HCBD up the food chain. Similarly Laseter *et al.* (1976) concluded that HCBD was not concentrated to a great extent and accumulated irregularly. [1]: Studies in mammalian species have shown that when rats received oral doses of HCBD as part of a mixture of seven different chlorinated hydrocarbons, there was no evidence of accumulation in the selected organs examined (Jacobs *et al.*, 1974). No other data have been found concerning the accumulation of HCBD in mammalian tissues.		

6 Effect data (aquatic environment)

Table 6.1: Overview on toxicity data of most sensitive species from different sources (master reference).

Species	Taxonomic Group	Duration	Effect	Endpoint	Value µg/l	Master reference	Reference in master reference	Comments on data reliability in master reference [#]
Freshwater								
Brachydanio rerio	Pisces	14 d	feeding behaviour and position	NOEC	5	[5], [1]	Röderer 1990	The study was evaluated by DE-EPA and is considered valid [1]: RI 4
Carassius auratus	Pisces	67 d	growth	NOEC	9.6	[1]	Leeuwangh et al. (1975)	RI 2;
Pimephales promelas	Pisces	32 d	larval survival	NOEC LOEC	6.5 13	[1], [5]	Benoit et al. 1982), Walbridge et al. (1983)	[1]: RI 1
Daphnia magna	Crustacea	21 d	reproduction	NOEC LOEC EC10 EC50	4.4 9.1 14 30	[10]		RI 1
Haematococcus pluralis	Algae	4 h	growth	EC10	>2000	[1]	Knie et al. (1983)	RI 3
Scenedesmus quadricauda	Algae	8 d	growth	toxicity threshold (NOEC)	>25000	[1], [5]	Bringmann & Kuehn (1977)	[1]: RI 3
Scenedesmus subspicatus	Algae	7 d	growth	EC3	>25000	[5]	Niemitz et al. 1979	
Carassius auratus	Pisces	96 h	mortality	LC50	90	[1]	Leeuwangh et al. (1975), EPA (1980)	RI 2
Oncorhynchus mykiss	Pisces	96 h	mortality	LC50	320	[1]	Call et al. (1983), EPA (1980)	RI 2; also 192h LC50 of 0.121 mg/l
Oncorhynchus mykiss	Pisces	192 h (8d)	mortality	LC50	121	[6]	Call et al (1983)	
Pimephales promelas	Pisces	96 h	larval survival and weight	LC50	90	[1], [5]	Geiger et al. (1985)	[1]: RI 1
Asellus aquaticus	Crustacea	96 h	mortality	LC50	130	[1], [6], [5]	Leeuwangh et al. (1975)	[1]: RI 2
Daphnia magna	Crustacea	24 h	mortality	LC50	500	[1], [7]	Knie et al. 1983	[1]: RI 3
Lymnaea stagnalis	Mollusca	96 h	mortality	LC50	210	[1], [5]	Leeuwangh et al. (1975)	[1]: RI 2

[#] RI = reliability index (by Euro Chlor, based on IUCLID system): 1 (valid without restriction); 2 (valid with restrictions, to be considered with care); 3 (invalid); 4 (not assignable)

Table 6.1: (continued) Overview on toxicity data of most sensitive species from different sources (master reference).

Saltwater								
Eliminius modestus (nauplii)	Crustacea	48 h	mortality	LC50	870	[1]	Pearson & McConnell (1975)	RI 2
Mysidopsis bahia	Crustacea	96 h	mortality	LC50	59	[5], [1]	EPA 1980	[1]: RI 4
Cyprinodon variegatus	Pisces	96 h	mortality	LC50	3600	[1]	Dow Chemical Company (1978)	RI 2; Limited method information
Limanda limanda	Pisces	96 h	mortality	LC50	450	[1]	Pearson & McConnell (1975)	RI 1; Method designed for compounds with high volatility
Crassostrea gigas	Mollusca	48 h	larval development	EC50 EC10 NOEC	≥ 21 ≥ 21 ≥ 21	[10]		RI 1
Psammechinus miliaris	Echinoder-mata	48 h	larval development	EC50 EC10 NOEC	≥ 21 ≥ 21 ≥ 21	[10]		RI 1

[#] RI = reliability index (by Euro Chlor, based on IUCLID system): 1 (valid without restriction); 2 (valid with restrictions, to be considered with care); 3 (invalid); 4 (not assignable)

Table 6.2: Mammal and bird oral toxicity data relevant for the assessment of non compartment specific effects relevant for the food chain (secondary poisoning) [1]

Species	Type of study	NOAEL	Reference in [1]
Rat, Mouse	chronic toxicity	0.2 mg/kg bw/d	WHO-IPCS 1994
Rat	reproductive toxicity	20 mg/kg bw/d	WHO-IPCS 1994
Japanese Quail	sub-chronic toxicity	3 mg/kg bw/d	

Summary on endocrine disrupting potential

Hexachlorobutadiene is not mentioned in [2]. No hints on endocrine disrupting properties of the substance have been found in the information provided to the consultant by Member States or other experts.

7 Effect data (human health)

No experimental data with relevance to human health have been provided. The WHO drinking water limit for HCBD is 0.6 µg/l based on a TDI of 0.2 µg/kg bw/d [8].

8 Calculation of quality standards

8.1 Quality standards for water

Freshwater

Long-term toxicity data are available for fish, daphnia and algae, short-term acute data for fish, crustaceans and one mollusc species (see table 6.1 of this data sheet).

Based on the available information the crustacean species *Daphnia magna* appears to be the most sensitive species in long-term tests (NOEC 4.4 µg/l). The appropriate assessment factor according to the TGD [3] is 10 as long-term toxicity data across the 3 trophic levels algae, daphnia and fish are available:

$QS_{freshwater}$ = 4.4 µg/l / AF (10) = 0.44 µg Hexachlorobutadiene /l

Koc values between approximately 10,000 and 1,260,000 have been estimated for hexachlorobutadiene (HCBD) (see section 5 of this data sheet). Hence, the log Kp_{susp}[1] ranges between 3 and 5.1 and the trigger criterion to calculate the corresponding concentration to the $QS_{freshwater}$ in SPM is met (see section 4.3.1 of the Manual [4]).

[1] Kp_{susp} is the partition coefficient solid-water in suspended matter = Koc * foc (with foc 0.1; see TGD section 2.3.5.3 [3]).

It is proposed to use a Kp_{susp} of 1120[2] for the calculation. The $QS_{SPM.freshwat}$ is derived as follows:

$$\mathbf{QS_{SPM.freshwat}} = \frac{QS_{freshwater}\ [0.44\ \mu g/l]}{C_{SPM}\ [15\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(1120\ l/kg)^{-1}]} = \mathbf{484.7\ \mu g/kg\ SPM\ (dry\ wt)}$$

It should be kept in mind that because of the large reported Koc range there is considerable uncertainty associated with the calculation of a reliable $QS_{SPM.freshwater}$. Therefore, if it is intended to base the compliance monitoring on monitoring of SPM, special care must be taken to choose a partition coefficient that is representative for the river(basin).

Transitional, coastal and territorial waters

There are short-term toxicity tests with saltwater species representing 4 different taxonomic groups available (fish, crustacea, mollusca, echinodermata). It is not possible to judge on the basis of the available data whether saltwater and freshwater species of the same taxonomic groups are equally sensitive to HCBD. However, in the EURO CHLOR risk assessment for HCBD it is stated that *"from an evaluation of the available toxicity data for other chlorinated aliphatic compounds (e.g. Calow, 1998f), it is reasonable to conclude that the sensitivity of marine and freshwater organisms is quite similar"*. It is therefore suggested to calculate the $QS_{saltwater}$ from the same data set as used for the derivation of the $QS_{freshwater}$. To this end, the TGD assessment factor method as proposed for the marine effects assessment is used (section 4.3.2.2 of the Manual [4]).

Additional data on 2 marine taxa beside fish, crustaceans and algae are available (molluscs, echionodermata) and these additional taxa do not appear to represent the most sensitive species. Therefore, the appropriate assessment factor for the derivation of the $QS_{saltwater}$ is 10. The lowest NOEC is 4.4 µg/l for the crustacean species *Daphnia magna*.

$QS_{saltwater}$ 4.4 µg/l / AF (10) = 0.44 µg Hexachlorobutadiene /l

The SPM concentration in marine waters is significantly lower than in freshwater (discussed in the context of the marine risk assessment: approx. 3 mg/l as standard concentration). Therefore the quality standard for SPM corresponding to the concentration in the "total" water sample is calculated for a SPM concentration of 3 mg/l:

$$\mathbf{QS_{SPM.saltwat}} = \frac{QS_{saltwater}\ [0.44\ \mu g/l]}{C_{SPM}\ [3\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(13000\ l/kg)^{-1}]} = \mathbf{491.1\ \mu g/kg\ SPM\ (dry\ wt)}$$

With regard to the uncertainties associated with the $QS_{SPM.saltwater}$ see the section on $QS_{SPM.freshwater}$ above.

[2] For the calculation of the Kp_{susp} it is suggested to use a Koc of 11,200. This value is the upper level reported in the EURO CHLOR risk assessment (log Koc 4.05). The selection of a Koc from the lower end of the reported range (see section 5) can be considered as a realistic worst case approach for the calculation of the concentration in SPM corresponding to the concentration in the "total" water sample.

Quality standard accounting for transient concentration peaks (MAC-QS)

It is suggested to derive the MAC-QS on the basis of the lowest acute toxicity test available in the combined freshwater and saltwater database (table 6.1). This is the LC50 of 59 µg/l obtained for the crustacean species *Mysidopsis bahia*.

Based on the guidance given in the TGD on the effects assessment for intermittent releases (section 3.3.2 of part II of [3]) it is suggested to apply an assessment factor of 100 in order to derive the MAC-QS.

MAC-QS = 59 µg/l / AF (100) = 0.59 µg Hexachlorobutadiene /l

8.2 Quality standard for sediment

The log Kp_{susp} of HCBD is estimated to be 3 – 5.1. It is therefore required to derive a $QS_{sediment}$ (see table 1a of the Manual [4]).

No toxicity data for sediment dwelling organisms have been provided by the stakeholders. According to the TGD [3], the $PNEC_{sediment}$ ($\approx QS_{sediment}$) may be calculated by the equilibrium partitioning method in the absence of ecotoxicological data of sediment-dwelling organisms.

The equilibrium partitioning approach only considers uptake via the water phase. However, uptake may also occur via other exposure pathways like ingestion of sediment and direct contact with sediment. There is evidence from studies in soil that the proportion of the total dose remains low for chemicals with a log Kow up to 5. As the log Kow of HCBD is < 5 (see section 5 of this data sheet) exposure routes other than direct uptake via the water phase need not to be considered and the $QS_{sediment}$ is calculated as follows:

$$QS_{sed.wet\_weight}\ [mg.kg^{-1}] = \frac{K_{SPM\text{-}water}\ [280\ m^3/m^3]}{bulk\ density_{SPM.wet}\ [1150\ kg/m^3]} * 1000 * QS_{water}\ [mg/l]$$

with:

$K_{SPM\text{-}water}$ = f_{solid} (0.1) * Kp_{susp} (1120 l/kg) / 1000 * RHO_{solid} (2500 kg/m^3) = 280 m^3/m^3 (sect 2.3.5 of [3])

bulk $density_{SPM.wet}$ = 1150 kg/m^3

1000 = conversion factor m^3/kg to l/kg

QS_{water} (freshwater & saltwater) = 0.00044 mg/l

The TGD defines wet SPM as 90% vol/vol water (density 1 kg/l) and 10% vol/vol solids (density 2.5 kg/l), thus giving a wet density of (0.9 × 1) + (0.1 × 2.5) = 1.15 kg/l. The dry weight of solids is therefore 0.25 kg (per litre wet SPM) and thus the wet:dry ratio is 1.15/0.25 = 4.6.

This results in the following quality standards for sediment (wet and dry weight):

$QS_{sediment}$ (freshwater & saltwater)	107 µg/kg (wet wt)	493 µg/kg (dry wt)

The values derived by the EP-method should only be considered as tentative standards. In order to refine the quality standards for the sediment compartment long term tests conducted with benthic organisms and NOECs as effect levels are required. For the time being no reliable $QS_{sediment}$ can be derived.

8.3 Secondary poisoning of top predators

Hexachlorobutadiene has a BCF > 100. Thus the trigger criterion to derive a quality standard referring to the protection of top predators from secondary poisoning is met (see table 1a of the Manual [4]).

For HCBD long-term toxicity studies with birds and mammals are available (see table 6.2). The lowest $NOAEL_{oral}$ is 0.2 mg/kg bw/d for chronic effects in rats and mice. This NOAEL is used for the calculation of the $QS_{secpois}$.

According to section 4.3.2.5 of the Manual [4] a $NOAEL_{oral}$ may be converted to a $NOEC_{food}$ by multiplication with a conversion factor (CONV) accounting for the ratio between body weight and food uptake. For rats >6 weeks a CONV of 20 is recommended, the respective factor for mice is 8.3.

$NOEC_{food.rat}$ = $NOAEL_{rat}$ (0.2 mg/kg bw.d) * CONV 20 (kg bw/ kg food.d) = 4 mg HCBD / kg food
$NOEC_{food.mouse}$ = $NOAEL_{mouse}$ (0.2 mg/kg bw.d) * CONV 8.3 (kg bw/ kg food.d) = 1.66 mg HCBD / kg food

As the $NOEC_{food}$ calculated for rats is higher than the respective NOEC for mice the NOEC of the mice is used to derive the quality standard.

An assessment factor of 30 is appropriate to derive a $PNEC_{food}$ from a chronic $NOEC_{food}$. The $PNEC_{food}$ is equivalent to the "save" concentration in the prey of predators and thus is the quality standard for biota ($QS_{secpois.biota}$).

Mouse, chronic NOEC: 1.66 mg/kg food / AF (30) = 0.0553 mg/kg food

$QS_{secpois.biota}$ = 55.3 µg HCBD / kg biota tissue (wet wt)

Reported BCF values for fish range up to 19,000. It therefore appears reasonable to use the same BCF of 17,000 that was used in the EURO CHLOR risk assessment [1] as a realistic worst case for the calculation of the concentration in water that corresponds to the $QS_{secpois.biota}$.

There is no "hard" information on biomagnification (i.e. BMF figures) available. However, the issue is addressed in the EURO CHLOR risk assessment [1]. From the information given there it can be assumed that HCDB does not biomagnify up through the food chain (see section 5 of this data sheet).

According to the provisions given in the TGD [3] with regard to the assessment of secondary poisoning of top predators, biomagnification factors (BMF) should be taken into account for the calculation of the PEC_{oral} of top predators. Ideally the BMF should be based on measured data but if such data is not available the use of default values is recommended. These default values are defined in the TGD based on the Kow or the BCF of the substance (see section 4.3.2.5 of the Manual for details). For a BCF >5000 the use of a default BMF of 10 is suggested for freshwater environments and for marine environments a BMF of 100 (10*10) in order to take account of the more complex and longer trophic pathways in marine ecosystems.

Because there are no "hard facts" regarding biomagnification available some scenario calculations may highlight the potential of HCBD for secondary poisoning (table 8.1).

The $QS_{secpois.water}$ is calculated as follows:

$QS_{secpois.water}$ = $QS_{secpois.biota}$ (55.3 [µg/kg prey]) / BCF * BMF

Table 8.1: Scenario calculations for "safe" water concentrations with respect to secondary poisoning

Scenario	**BCF**	**$BMF_{freshwater}$**	**BMF_{marine}**	**$QS_{secpois.freshw}$**	**$QS_{secpois.saltw}$**
worst case	17,000	10 (TGD default)	100 (TGD default)	0.00033 µg/l	0.000033 µg/l
best case (no biomagnifcation)	17,000	1	1	0.0033 µg/l	0.0033 µg/l

From the figures calculated in table 8.1 it is evident that any scenario requires a lower $QS_{secpois.water}$ than the quality standards calculated for the protection of the freshwater and saltwater pelagic communities. Hence, an in depth assessment of the bioaccumulation potential of HCB is required in order to derive a reliable quality standard for the protection of predators from secondary poisoning.

For the time being, it is suggested to adopt 0.003 µg/l as standard for protection from secondary poisoning as, based on the information available, there is no evidence for biomagnification of HCBD.

$QS_{secpois.water}$ = 0.003 µg Hexachlorobutadiene / l

The $QS_{SPM.water}$ corresponding to the above $QS_{secpois.water}$ is derived as described in section 8.1 of this data sheet. It should be kept in mind that because of the uncertainty associated with the estimation of an appropriate partition coefficient the calculation of the $QS_{SPM.water}$. is a crucial step. Therefore, if it is intended to base the compliance monitoring on monitoring of SPM, special care must be taken to choose a partition coefficient that is representative for the river(basin).

$QS_{SPM.water}$ (freshwater & saltwater) = 3.3 µg/kg SPM (dry wt)

8.4 Quality standard referring to food uptake by humans

According to the information provided in the EURO CHLOR risk assessment [1] hexachlorobutadiene is classified as "harmful in contact with skin or if swallowed" (R21/22) and with "possible risk of irreversible effects" (R40). In addition, the substance is subject to bioaccumulation. Therefore the derivation of a quality standard addressing the protection of human health from adverse effects due to the uptake of food originating from aquatic environments is required (trigger criteria met, see table 1b of the Manual [4]).

Mammalian oral toxicity NOAELs with relevance to human health are not available to the consultant. However, the WHO has established a drinking water standard that is based on a tolerable daily intake (TDI) of 0.2 µg/kg bw [8]. This TDI is used for the calculation.

In the Manual (section 4.3.2.6) [4] it is suggested that the relevant threshold level (i.e. the TDI) may not be exhausted for more than 10% by consumption of food originating from aquatic sources. For a person weighing 70 kg this results in an acceptable daily intake of 1.4 µg HCBD per day.

The average fishery product consumption of an EU citizen is 115 g d-1 (TGD [3]). Thus, 115 g edible fish tissue (or seafood) must not contain more than 1.4 µg HCBD.

$$QS_{hh.food} = \frac{1.4 \text{ µg HCBD}}{115\text{g fishery product consumption}} * 1000 \text{ g} = \textbf{12.2 µg HCBD / kg food}$$

Hence, the $QS_{hh.food}$ is 4.5 times lower than the $QS_{secpois.biota}$.

HCBD has been shown to bioconcentrate. The whole body BCF_{fish} of 17,000 which was used in the assessment for secondary poisoning (section 8.3) might be considered to high for the calculation of the water concentration corresponding to the $QS_{hh.food}$ because humans usually do not eat whole fish but only the fillets. The fillet BCF appears to be lower than the whole body BCF or the BCF in the liver (see section 5). Therefore, it is proposed to use 3 different BCFs for scenario calculations: 17,000 (whole body); 2,000 (BCF reported for blue mussel, most reported values for fish species other than Rainbow trout are below this level); 700 (BCF reported for fillet of Plaice).

According to the guidance given in the TGD [3] regarding the assessment of secondary poisoning of top predators, biomagnification factors (BMF) should be taken into account for the calculation of the PEC_{oral}. The use of default BMFs as proposed in the TGD is recommended, if the bioconcentration factor of the substance concerned exceeds a level of 2,000 and measured BMFs are not available (see section 54.3.2.5of the Manual [4] for details).

However, based on the available information (see section 5 of this data sheet) HCBD is apparently not subject to biomagnification in fish. Therefore, it appears not justified to use default BMF values for the calculation of the water concentration corresponding to the $QS_{hh.food}$.

The $QS_{hh.water}$ is therefore calculated as follows:

$QS_{hh.water}$ = $QS_{hh.food}$ (12.2 [µg/kg]) / BCF

See table 8.2 for results.

Table 8.2: Scenario calculations for "safe" water concentrations with respect to protection of human health from adverse effects due to seafood ingestion

Scenario	**BCF**	**$QS_{secpois.water}$**
BCF_{fish} (whole body)	17,000	0.0007 µg/l
BCF Blue mussel	2,000	0.0061 µg/l
BCF in Plaice fillet	700	0.0174 µg/l

From the figures calculated in table 8.2 it is concluded that the water quality standard proposed for the protection of predators from secondary poisoning ($QS_{secpois.water}$) can also be considered as low enough to protect humans from adverse effects due to ingestion of food from aquatic environments.

However, an in depth assessment of the bioaccumulation potential of HCBD should be conducted in order to enable the calculation of a standard associated with less uncertainties.

8.5 Quality standard for drinking water abstraction

No "A1-value" has been set for drinking water abstraction in Council Directive 75/440/EEC and also no limit value for HCBD in drinking water applies according to Council Directive 98/83/EC.

However, the World Health Organization (WHO) has proposed a guide value of 0.6 µg/l for drinking water [8]. This value is higher than all the other quality standards derived for the other objectives of protection, including the MAC-QS addressing the protection of the pelagic community from adverse effects exerted by transient concentration peaks. Hence, the calculation of a specific QS referring

to the abstraction of water intended for human consumption in areas designated in accordance with Art. 7 of the WFD is not necessary.

8.6 Overall quality standard

Protection of predators from secondary poisoning and of humans from adverse effects due to seafood ingestion are the most critical objectives that require water concentrations of at most 0.003 µg/l.[3]

It may be considered to monitor the overall quality standard as concentration in biota instead as corresponding concentration in water. This would avoid uncertainties associated with the choice of an appropriate bioaccumulation factor. Quality standard proposals referring to biota tissue concentrations have been calculated in section 8.3. If the approach is chosen where a separate biota-EQS is established, the water-EQS for protection against direct effects on the pelagic communities should be at least as stringent as the water quality objective of 0.1 µg/l set in Council Directive 86/280/EEC.

[3] In its opinion of 28 May 2004 on the proposed QS for this substance [9] the CSTEE stated that it does not support the (formerly) proposed QS because for the most sensitive group of organisms (crustaceans) only acute toxicity data were available.

In an attempt to find long-term toxicity data for crustaceans / aquatic invertebrates, representatives of the Member States and industry branch organisations were asked to provide such data at the 7th Expert Advisory Forum (15-16 June 2004), further a data search was conducted by the Fraunhofer Institute (US-EPA ECOTOX database and STN International, a portal to search most relevant databases in one go). The data search by FHI was unsuccessful. However, the Netherlands provided newly generated long-term toxicity data for daphnia and short-term data for 2 marine species belonging to the groups of molluscs and echinoderms [10]. Due to the availability of the new data it was possible to reduce the assessment factors from 100 to 10 with regard to the protection of the freshwater pelagic community and from 1000 to 10 with regard to the saltwater pelagic community. However, the availability of new data has no influence on the overall QS because this value refers to the protection from secondary poisoning.

9 References

[1] Euro Chlor Risk Assessment for the Marine Environment. OSPARCOM Region: North Sea – Hexachlorobutadiene. Draft - Status January 2002

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