Common Implementation Strategy for the Water Framework Directive

Environmental Quality Standards (EQS)

Substance Data Sheet

Priority Substance No. 16

Hexachlorobenzene

CAS-No. 118-74-1

Final version
Brussels, 15 January 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 [18]. 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: 16	Hexachlorobenzene
CAS-Number:	118-74-1
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: 0.013 µg/l Protection against food uptake by man and secondary poisoning (biota): 9.74 µg/kg fishery product (ww)	Protection against direct effects: **0.01 µg/l** Protection of food uptake by man and secondary poisoning (biota): **10 µg/kg fishery product (ww)**	see 8.1, 8.4 & 8.6
MAC-QS (ECO)	0.05 µg/l	**0.05 µg/l**	see section 8.1

2.2 Specific quality standards

Protection Objective #	Quality Standard	Comment:
Pelagic community (freshwater & saltwater)	0.013 µg/l corresponding conc. in SPM: 141 µg/kg dry wt (freshwater) 162 µg/kg dry wt (saltwater)	See section 8.1
Benthic community (sediment)	3.7 µg/kg (wet wt) 16.9 µg/kg (dry wt)	tentative standard based on EP-method see section 8.2
Predators (secondary poisoning)	16.7 µg/kg prey (biota tissue wet wt) corresponding conc. in water: 0.0004 µg/l corresponding conc. in SPM: 4.35 µg/kg dry wt (freshwater) 5 µg/kg dry wt (saltwater)	see section 8.3
Food uptake by man	9.74 µg/kg fishery product (wet wt) corresponding concentration in water: 0.00023 µg/l, corresponding concentration in SPM: 2.5 µg/kg dry wt (freshwater) 2.9 µg/kg dry wt (saltwater)	see section 8.4
Abstraction of water intended for human consumption (AWIHC)	no EU DW abstraction standard set, setting of such a standard is not required	see section 8.5
Water intended for human consumption (WIHC)	no EU standard set	WHO guide value for an additional cancer risk of 10^{-5} is 1.0 µg HCB/L (≈ 0.1 µg/L for additional cancer risk of 10^{-6}); 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
Carc. Cat. 2; R45 - T; R48/25 - N; R50-53	[19]

4 Physical and chemical properties

Property	Value	Reference
Molecular weight	284.8	[7]
Vapour pressure	0.0023 Pa at 25°C 1.1 – 1.45 mPa (20 °C) 2.5 mPa (25 °C)	[7] [5] [5]
Henry's law constant	131 Pa/mol per m^3	[7]
Solubility in water	5 µg/l at 25°C 5 – 6 µg/L (20 – 25°C)	[7] [5]

5 Environmental fate and partitioning

Property	Value	Ref.	Comments
Hydrolysis Photolysis			
Biodegradation			
Partition coefficients			
log Kow	5.5 (5-6.92) 5.31 5.73 3.93 – 6.53	[7] [6] [1] [5]	
Koc	36,308 (3,000-180,000) log Koc 5.11 10,800 – 1,200,000	[7] [6] [5]	 Sediment
Bioaccumulation			
BCF:			
Fish	18,000 (maximum 22,000)	[1]	Geometric mean of whole body BCF of freshwater and marine fish
Fish	8,000 – 230,000	[5]	"average" BCF ≈50,000
Fish	2,040 – 45,000	[7]	(2,040) proposed for risk assessment
Fish	38,795	[15]	90-percentile of 22 individual BCF_{fish}
Fish	78,700	[15]	90-percentile of BCFof cyprinid fish
Bivalves	7,000 4,000 – 10,000	[1] [5]	Calculated BCF
BAF fish (field):	≈42,000		See annex 1

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								
Daphnia magna	Crustacea	21 d	Reproduction	NOEC	0.13	[5]	Scheubel 1984	Test result is valid – quality checked by the German Federal Environmental Agency *
Gammarus lacustris	Crustacea	28 d	Survival	NOEC	1.8	[7], [5]	Nebeker *et al.*, 1989	[7]: RI 2
Micropterus salmoides	Pisces	28 d		EC0	2	[5]	Laseter et al. 1976	
Gammarus lacustris	Crustacea	28 d	Mortality	LC0	2.5	[5]	Alberti 1983	
Oncorhynchus mykiss	Pisces	90 d	Growth, survival	NOEC	3.7	[7]	US EPA (1987) Spehar (2000)	RI 2; NOEC = maximum concn. Tested.
Pimephales promelas	Pisces	28 d	Survival	NOEC	≥ 3.8	[5]	Nebeker et al. 1989	
Lumbriculus variegatus	Annelida	49 d	Survival, growth, asexual reproduction	NOEC	4.7	[7]	Nebeker *et al.*, 1989	RI 2; Worms held in quartz sand
Pimephales promelas	Pisces	32 d	Hatch, survival, growth	NOEC	4.8	[7]	Carlson and Kosian, 1987; Ahmad *et al.*, 1984	RI 1; NOEC = maximum concn. Tested
Daphnia magna	Crustacea	7 d	Mortality	NOEC	5	[7]	Nebeker *et al.*, 1989	RI 2
Selenastrum capricornutum	Algae	96 h	Growth	NOEC	14	[5]	Calamari et al. 1983	
Daphnia magna	Crustacea	21 d	Reproduction	NOEC	17	[7]	Caspers *et al.*, 1993	RI 1
Selenastrum capricornutum	Algae	3 h	Photosynthesis	NOEC	18	[7]	Calamari *et al.*, 1983	RI 2
Daphnia magna	Crustacea	48 h	Mortality	LC50	4.73	[5]	Abernethy et al. 1986	
Daphnia magna	Crustacea	48 h	Immobility	LC50	>5	[7]	Nebeker *et al.*, 1989	RI 1; Solubility limit. Also no mortality after 7 days.
Tanytarsus dissimilis	Insecta	48 h	Mortality	LC50	>5.8	[7]	Call *et al.*, 1983	RI 1
Leuciscus idus	Pisces	48 h	Mortality	LC50	7	[7]	Knie *et al.*, 1983	RI 3
Daphnia magna	Crustacea	24 h	Immobility	EC50	7.5	[6]	Umweltbundesamt (1976), cité dans Rhin-Meuse (1991)	
Scenedesmus abundans	Algae	96 h	Growth	EC50	10	[5]	Geyer et al. 1985	
Procambarus clarki	Crustacea	96 h	Mortality	LC50	>27	[7]	Laska *et al.*, 1978	RI 1; 10d LC50 also >0.027 mg/l. No significant mortality at 0.027 mg/l.
Brachydanio rerio	Pisces	48 h	Mortality	LC50	>30	[7]	Calamari *et al.*, 1983	RI 1No mortality
Selenastrum capricornutum	Algae	96 h	Growth	EC50	<30	[6], [5]	Calamari *et al* (1983	

Species	Taxonomic Group	Duration	Effect	Endpoint	Value µg/l	Master reference	Reference in master reference	Comments on data reliability in master reference [#]
Selenastrum capricornutum	Algae	96 h	Growth	EC50	>30	[7]	Calamari *et al.*, 1983	RI 1; 12% inhibition at this concn.
Selenastrum capricornutum	Algae	3 h	Photosynthesis	EC50	30	[7]	Calamari *et al.*, 1983	RI 2; . Approx. value based on 2 concentrations.
Lepomis macrochirus	Pisces	96 h	Mortality	LC50	>78	[7]	Call *et al.*, 1983	RI 1; No mortality
Oncorhynchus mykiss	Pisces	96 h	Mortality	LC50	>81	[7]	Call *et al.*, 1983; Ahmad *et al.*, 1984	RI 1; No mortality or other symptoms
Bufo bufo japonicus	Amphibia	24 h	Mortality	LC50	4200	[5]	Niimi et al. 1980	
Saltwater								
Thalassiosira pseudonana and Dunaliella tertiolecta (mixed)	Algae	72 h	Growth, cell size	NOEC	>100	[7]	Biggs *et al.,* 1979	RI 3 ; Maximum concn. tested.
Artemia salina	Crustacea	24 h	Mortality	LC50	4.73	[5]	Abernethy et al. 1986	
Crangon septemspinosa	Crustacea	96 h	Mortality	LC50	>7.2	[7]	McLeese and Metcalfe., 1980	RI 1 ; No mortalities. Renewal after 48h.
Lagodon rhomboides	Pisces	96 h	Mortality	LC50	>8.4	[7]	Parrish *et al.*, 1975	RI 1; No mortalities
Cyprinodon variegatus	Pisces	96 h	Mortality	LC50	13	[5]	Mayer 1987	
Cyprinodon variegates	Pisces	96 h	Mortality	LC50	>13.3	[7]	Parrish *et al.*, 1975	RI 1; No mortalities
Palaemonetes pugio	Crustacea	96 h	Mortality	LC50	>17	[7]	Parrish *et al.*, 1975	RI 1
Penaeus duorarum	Crustacea	96 h	Mortality	LC50	>25	[7]	Parrish *et al.*, 1975	RI 1 ; 33% mortality at this concn.
Lagodon rhomboides	Pisces	96 h	Mortality	LC50	100	[5]	Mayer 1987	
Solea solea	Pisces	96 h	Mortality	LC50	142	[5]	Furay et al. 1995	
Platichthys flesus	Pisces	96 h	Mortality	LC50	199	[5]	Furay et al. 1995	
Ophryotrocha diadema	Annelida	48 h	Mortality	LC50	>10000	[7]	Parker, 1984	RI 3; Greatly above solubility.
Crassostrea virginia	Mollusca	48 h	Embryo larval development	EC50	>1000	[7]	US EPA, 1987	RI 3; Embryo-larval development
Crassostrea virginia	Mollusca	48 h	Morphology	EC50	1000	[5]	Zaroogian 1981	

[#] 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)

* The test was conducted according to EU test guideline 79/831 Rev 1. A clear dose-response relationship was observed. Test concentrations were: control, 0.13, 0.25, 0.5, 1.0 and 1.67 µg/l. The respective numbers of offspring produced per adult animal were: 62, 57, 45, 30, 24, 15. Controls met the quality criteria set in the guideline [10]. The report can be borrowed from the Library of the Federal Environmental Agency.

Table 6.2: Toxicity Data of HCB in Sediment Dwelling Organisms

Species	**Treatment**	**Validity** [#]	**Reference in** [7]
Crangon septemspinosa	No evidence of mortality in *Crangon septemspinosa* treated for 96 hours at a concentration of 2.1 mg/kg (normalized to 2% OC).	2	McLeese & Metcalfe, (1980)
Chironomus tentans	No significant mortality or reduction in growth following a 14-day exposure to sediments spiked at a measured concentration of 84 mg/kg (2% OC).	1	Barber *et al* (1997)
Hyella azteca	No significant mortality or reduction in growth following a 14-day exposure to sediments spiked at a measured concentration of 84 mg/kg (2% OC).	1	Barber *et al* (1997)
Leptocheirus plumulosus	No significant mortality or reduction in growth following a 10-day exposure to sediments spiked at a concentration of 120 mg/kg (2% OC).	1	Fuchsman *et al* (1998)
Hyella azteca	No significant mortality or reduction in growth following a 10-day exposure to sediments spiked at a concentration of 120 mg/kg (2% OC) in freshwater and at a salinity of 10‰ .	1	Fuchsman *et al* (1998)
Chironomus tentans)	No significant mortality or reduction in growth following a 10-day exposure to sediments spiked at a concentration of 120 mg/kg (2% OC).	1	Fuchsman *et al* (1998)

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

Species		**Duration**	**Effect**	**NOEC mg/kg food**	**Reference in** [8]
Mustela vision	Mink	1 generation	Mortality, reproduction	0.5	RIVM Rep. No. 679101012
Mustela putorius	European ferret	1 generation	Mortality, reproduction	0.5	
Coturnix c. japonica	Quail	90 d	Reproduction	5	
Rattus norvegicus	Rat	2 and 4 generations	Reproduction	18	
Canis domesticus	Dog	1 y	Mortality, Growth	52	
Felix domesticus	Cat	1 generation	Reproduction	88	

Table 6.4: Summary on Endocrine Disrupting (ED) potential of Hexachlorobenzene

Hexachlorobenzene is a substance with evidence of ED or evidence of potential ED, already regulated or being addressed under existing legislation	[2]
No hints on endocrine disrupting properties of the substance have been found in the information provided by Member States or NGOs	

7 Effect data (human health)

For non-neoplastic effects, based on the lowest reported NOEL (0.05 mg/kg bw/day), for primarily hepatic effects observed at higher doses in studies on pigs and rats exposed by the oral route, and incorporating an uncertainty factor of 300 (10 for interspecies variation, 10 for intraspecies variation, and 3 for severity of effect), a TDI of 0.17 µg/kg bw/ day has been derived (WHO-EHC [16]). The U.S.-EPA has calculated an oral reference dose (RfD) for non-carcinogenic effects of 0.8

µg/kg bw/ day. This RfD is based on a NOAEL for liver effects of 0.08 mg/kg/day in a rat chronic feeding study (LOAEL 0.29 mg/kg/day) and an uncertainty factor of 100 [17].

In the WHO-EHC [16], a health-based guidance value for neoplastic effects of 0.16 µg/kg bw/ day is suggested as well. The approach is based on the tumorigenic dose TD_5, i.e. the intake associated with a 5% excess incidence of tumours in experimental studies in animals. This TD_5 value is 0.81 mg/kg bw/ day for neoplastic nodules of the liver in female rats. Based on consideration of the insufficient mechanistic data, an uncertainty factor of 5000 was used to develop the guidance value.

8 Calculation of quality standards

8.1 Quality standards for water

Freshwater

Long-term toxicity data as well as short-term acute data are available across the 3 trophic levels for the "standard" representatives fish, crustaceans and algae. In addition, tests with insects, amphibia mollusca and annelida have been provided (see table 6.1 of this data sheet).

Based on the available information *Daphnia magna* is the most sensitive species (NOEC 0.13 µg/l). The appropriate assessment factor according to the TGD [3] is 10 (long-term toxicity data across at least 3 trophic levels for 3 different taxonomic groups and the lowest acute toxicity datum is obtained with a representative of these groups):

$QS_{freshwater}$ = 0.13 µg/l / AF (10) = 0.013 µg Hexachlorobenzene /l

HCB is relatively insoluble in water and partitions strongly towards sediment [7]. Koc values between approximately 10,000 and 1,200,000 have been estimated (see section 5 of this data sheet). Hence, the log Kp_{susp}[1] is between 3 and 5.08 and the trigger criterion to calculate the corresponding concentration to the $QS_{freshwater}$ in SPM is met (see section 4.2 & table 1a of the Manual [4]). It is proposed to use a Kp_{susp} of 13,000[2] for the calculation. The $QS_{SPM.freshwat}$ is derived as follows:

$$\mathbf{QS_{SPM.freshwater}} = \frac{QS_{freshwater}\ [0.013\ \mu g/l]}{C_{SPM}\ [15\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(13{,}000\ l/kg)^{-1}]} = \mathbf{141\ \mu g/kg\ SPM\ (dry\ wt)}$$

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).

The detection limit of HCB in water[3] may be higher than the calculated water quality[1] standard. Hence, compliance monitoring in water samples may not be possible.

[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]).

[2] For the calculation of the Kp_{susp} it is suggested to use a Koc of 130,000. This value is reported in the French data sheet and is approximately the geometric mean of the reported Koc range.

[3] Detection limit according to [5] is 0.025 µg/l.

Transitional, coastal and territorial waters

There are mainly short-term acute toxicity tests with saltwater species representing 5 different taxonomic groups available (fish, crustaceans, algae, molluscs and annelida). No obvious differences in the sensitivity of freshwater and saltwater species of the same taxonomic groups are apparent. It is therefore suggested, in line with the conclusions drawn in the TGD, to calculate the $QS_{saltwater}$ from the pooled data set as used for the derivation of the $QS_{freshwater}$.

In addition to the data on marine and freshwater fish, crustaceans and algae there are data for a marine annelid and mollusc species available showing that these groups are apparently not more sensitive to HCB than the before mentioned groups. Further it should be considered that the mode of toxic action of HCB is narcosis [1] [4]. Hence, the resulting saltwater quality standard is equal to the freshwater standard.

$QS_{saltwater}$ = $QS_{freshwater}$ = 0.013 µg Hexachlorobenzene /l

As 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), the quality standard is additionally calculated for a SPM concentration of 3 mg/l:

$$QS_{SPM.saltwat} = \frac{QS_{freshwater}\ [0.013\ \mu g/l]}{C_{SPM}\ [3\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(13000\ l/kg)^{-1}]} = \mathbf{162\ \mu g/kg\ SPM\ (dry\ wt)}$$

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

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. An EC50 and a LC50 of 4.73 µg/l have been obtained for the crustacean species *Daphnia magna* and *Artemia salina* (both results reported from same original reference, see table 6.1).

Based on the guidance given in the TGD on the effects assessment for intermittent releases (see section 4.3.6 of the Manual [4]) it is suggested to apply an assessment factor of 100 in order to derive the MAC-QS.

MAC-QS = 4.73 µg/l / AF (100) = 0.05 µg Hexachlorobenzene /l

8.2 Quality standard for sediment

HCB partitions strongly towards sediment [7]. The log Kp_{susp} is estimated to be 3 – 5. It is therefore required to derive a $QS_{sediment}$ (see table 1a in [4]).

According to the TGD the $PNEC_{sediment}$ ($\approx QS_{sediment}$) may be calculated using the equilibrium partitioning method (see sections 4.3.2.3 & 4.3.2.4 of the Manual [4]).

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

[4] Eurochlor challenges the claim raised in [1] that HCB acts by non-polar narcosis.

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. For compounds with a log Kow greater than 5 the equilibrium method is used in a modified way. It is recommended in the TGD to increase the $PEC_{sed}/PNEC_{sed}$ ratio by a factor of 10 for the risk assessment. However division of the $PNEC_{water}$ by a factor of 10 will result in the same ratio. Thus, it can be inferred that division of the QS_{water} by a factor of 10 will result in a tentative $QS_{sediment}$ that accounts for possible uptake via the mentioned additional routes of exposure.

As the log Kow of hexachlorobenzene is >5 (see section 5 of this data sheet) exposure routes other than direct uptake via the water phase should be considered and the $QS_{sediment}$ is calculated as follows:

$$QS_{sed.wet\_weight}\ [mg.kg^{-1}] = \frac{Kp_{SPM\text{-}water}\ [3{,}250\ m^3/m^3]}{bulk\ density_{SPM.wet}\ [1{,}150\ kg/m^3]} * 1{,}000 * QS_{water}\ [mg/l] * 10^{-1}$$

with:

$K_{SPM\text{-}water}$ = f_{solid} (0.1) * Kp_{susp} (13,000 l/kg) / 1,000 * RHO_{solid} (2,500 kg/m^3) = 3,250 m^3/m^3 (sect 2.3.5 of [3])

$bulk\ density_{SPM.wet}$ = 1,150 kg/m^3

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

10^{-1} = factor to account for possible additional uptake routes for substances with log Kow >5

QS_{water} = 0.000013 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):

$QS_{sediment}$	3.7 µg/kg (wet wt)	16.9 µg/kg (dry wt)

There are some toxicity tests with sediment dwelling organisms available (see table 6.2). Toxic effects have not been found for various invertebrates after 10-14 days exposure to 84 - 120 mg/kg HCB (normalized to 2% OC). A quality standard cannot be derived on the basis of these tests as all results are unbounded NOECs and the exposure time is to short for real long term tests. However, the results give an indication that the quality standard derived for the pelagic community might also be protective for the benthic community ($QS_{sediment}$ calculated with equilibrium partitioning method =169 µg/kg, margin of safety (MOS, corresponding to assessment factor) between minimum "NOEC" of 84 mg/kg and 169 µg/kg =497, the $QS_{sediment}$ derived with the EP-method is calculated for 10% organic carbon in sediment, the minimum "NOEC" normalized to 2% OC ⇒ total MOS approx. 2500).

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 (bounded[5]) NOECs as endpoints are required. For the time being no reliable effects based $QS_{sediment}$ can be derived.

[5] I.e. a significant effect was observed at a higher concentration level (≈ the NOEC was not the highest concentration tested)

8.3 Secondary poisoning of top predators

Hexachlorobenzene has reported bioaccumulation factors (BAF) in fish of ≈ 12,600 – 52,500 (see Annex 1). 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 HCB long-term toxicity studies with birds and mammals are available (see table 6.3). The lowest $NOEC_{food}$ is 0.5 mg/ kg food for effects on survival and reproduction of mink and ferret. This NOEC is used for the calculation of the $QS_{secpois}$.

According to the TGD [3] an assessment factor of 30 is appropriate to derive a $PNEC_{food}$ from a chronic $NOEC_{food}$. The $PNEC_{food}$ is equivalent to the "safe" concentration in the prey of predators and, hence, is the quality standard for biota ($QS_{secpois.biota}$).

Mink, chronic NOEC: 0.5 mg/kg food / AF (30) = 0.0167 mg/kg food

$QS_{secpois.biota}$ = 16.7 µg Hexachlorobenzene / kg biota tissue (wet wt)

Following the invitation of the Expert Group during the Workshop of 12-16 May in Brussels, the German Federal Environmental Agency calculated bioaccumulation factors (BAF) based on field data from the river Elbe (see annex 1) for Bream (*Abramis brama*, mean BAF 12,644) and Eel (*Anguilla anguilla*, mean BAF 41,953). A similar BAF of 52,500 was reported for the Three-Spined Stickleback (*Gasterosteus aculeatus*) in a laboratory two-step aquatic food chain study. Bioaccumulation data reported for molluscs are much lower than for fish. It is therefore suggested to calculate the $QSs_{secpois.water}$ using the higher of the BAF-means calculated on the basis of the eel field data (≈42,000). As most fish species contain less fat in muscle tissue than eel, this BAF value is deemed to be sufficiently high to cover whole body bioaccumulation in most fish species (there may be organs/tissues in fish that accumulate HCB to a higher extent than muscle tissue).

$QS_{secpois.water}$ = $QS_{secpois.biota}$ (16.7 [µg HCB /kg prey]) / BAF (42,000) = 0.000398 µg HCB/l

Hence, it is evident that protection from secondary poisoning requires a considerably lower concentration of HCB in water than calculated for the protection of the freshwater and saltwater pelagic communities.

The corresponding $QS_{SPM.freshwater}$ is derived as follows:

$$QS_{SPM.freshwater} = \frac{QS_{freshwater}\ [0.0004\ \mu g/l]}{C_{SPM}\ [15\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(13{,}000\ l/kg)^{-1}]} = \mathbf{4.35\ \mu g/kg\ SPM\ (dry\ wt)}$$

As 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), the quality standard is additionally calculated for a SPM concentration of 3 mg/l:

$$QS_{SPM.saltwater} = \frac{QS_{freshwater}\ [0.0004\ \mu g/l]}{C_{SPM}\ [3\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(13{,}000\ l/kg)^{-1}]} = \mathbf{5\ \mu g/kg\ SPM\ (dry\ wt)}$$

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}. Therefore, if it is intended to base the compliance monitoring on SPM analysis, special care must be taken to choose a partition coefficient that is representative for the water body examined.

8.4 Quality standard referring to food uptake by humans

Hexachlorobenzene is classified as category 2 R45 (may cause cancer) and R48/25 (danger of serious damage to health by prolonged exposure if swallowed). 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 in [4]).

It is suggested to use the guidance value for neoplastic effects of 0.16 µg/kg bw/ day suggested in the WHO-EHC [16] as starting point for the derivation of the standard.

In the final report [4] it is suggested that the relevant threshold level 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 1.12 µg hexachlorobenzene per day.

The average fish 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 1.12 µg HCB.

$$\mathbf{QS_{hh.food}} = \frac{1.12\ \mu g\ HCB}{115 g\ seafood\ consumption} * 1000\ g = \mathbf{9.74\ \mu g\ HCB\ /\ kg\ seafood}$$

Following the invitation of the Expert Group during the Workshop of 12-16 May in Brussels, the German Federal Environmental Agency calculated bioaccumulation factors (BAF) based on field data from the river Elbe (see annex 1) for Bream (*Abramis brama*, mean BAF 12644) and Eel (*Anguilla anguilla*, mean BAF 41953). It is therefore suggested to calculate the $QSs_{secpois.water}$ using the higher of the BAF-means calculated on the basis of the eel field data (≈42000). This can be considered as a worst case situation since most fish species have a lower fat content in muscle tissue than eel.

$$\mathbf{QS_{hh.food.water} = QS_{hh\text{-}food}\ (9.74\ [\mu g\ HCB\ /kg\ prey])\ /\ BAF\ (42000) = 0.00023\ \mu g\ HCB/l}$$

The corresponding $QS_{SPM.freshwater}$ is derived as follows:

$$\mathbf{QS_{SPM.freshwater}} = \frac{QS_{freshwater}\ [0.00023\ \mu g/l]}{C_{SPM}\ [15\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(13000\ l/kg)^{-1}]} = \mathbf{2.5\ \mu g/kg\ SPM\ (dry\ wt)}$$

As 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), the quality standard is additionally calculated for a SPM concentration of 3 mg/l:

$$\mathbf{QS_{SPM.saltwater}} = \frac{QS_{freshwater}\ [0.00023\ \mu g/l]}{C_{SPM}\ [3\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(13000\ l/kg)^{-1}]} = \mathbf{2.9\ \mu g/kg\ SPM\ (dry\ wt)}$$

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}. Therefore, if it is intended to base the compliance monitoring on SPM analysis, special care must be taken to choose a partition coefficient that is representative for the water body examined.

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 HCB in drinking water applies according to Council Directive 98/83/EC.

Therefore, according to the strategy described in section 4.3.3 of the Manual [4] regarding the derivation of the QS for drinking water abstraction, a provisional drinking water quality standard is calculated based on the recommendations given in the TGD.

The guidance value for neoplastic effects of 0.16 µg/ kg bw/ day [16] is suggested as starting point for the calculation. The provisional quality standard for drinking water is calculated with the provision that uptake by drinking water should in any case not exceed 10% of the threshold level for human health [3].

$$QS_{DW.provisional} \text{ (non cancer effects only)} = \frac{0.1 * TL_{HH} * BW}{Uptake_{DW}} = 0.56 \text{ µg Hexachlorobenzene /l}$$

with:

$QS_{DW.provisional}$	provisional quality standard for drinking water (mg/l)
TL_{HH}	threshold level for human health (0.16 µg HCB /kg bw per day)
BW	body weight (70 kg)
$Uptake_{DW}$	uptake drinking water (2 l per day)

The provisional drinking water quality standard is by far higher than any standard calculated for the other objectives of protection. With regard to the non-cancerogenic and non-mutagenic effects of HCB it is therefore not necessary to set a quality standard referring to drinking water abstraction.

The guide value[6] proposed by WHO for drinking water is 1 µg HCB/l for an additional cancer risk of 10^{-5} (≈ 0.1 µg/L for additional cancer risk of 10^{-6}). This proposal is based on a multiple stage extrapolation of a 2 years study on rats. [9]

8.6 Overall quality standard

As hexachlorobenzene is a carcinogen, the decisive issue for quality standard setting may be human health. The proposed AA-QS of 9.74 µg/kg fishery product (corresponding to a concentration in water of 0.23 ng/l) does cover the tolerable intake limits calculated by experts of the WHO for protection against neoplastic effects due to oral uptake of hexachlorobenzene as well as the WHO drinking water guideline value (see sections 8.4 and 8.5). In view of the carcinogenic properties of HCB and its ecological hazard potential emissions and losses of the substance should be minimised as far and as soon as possible. At the same time, there is a significant variation in the conversion factors when calculating an overall EQS for water only. It may therefore by suitable to set one EQS for water on the basis of the direct effects to the pelagic communities and one EQS for biota accounting for the indirect effects. The proposed AA-EQS for the pelagic communities derived in section 8.1 is slightly more stringent than the current EQS of 0.1 µg/l set by Council Directive 86/280/EEC.

[6] For carcinogenic substances the "guide" value is calculated as the concentration in drinking water corresponding to an additional risk of cancer over the whole life of 10^{-5} (one additional cancer in 100 000 persons drinking during 70 years the water containing the substance at a concentration equal to the guide value). To decrease the risk by a factor of 10 the guide value should be divided by 10. [9]

9 References

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ANNEX 1

Evaluation of the Bioaccumulation Potential of HCB in Fish

by Dieter Schudoma, Federal Environmental Agency, Berlin (June 2003)

Data base

Data on residual levels of HCB in bream (*Abramis brama*) and eel (*Anguial anguila*) are available from investigations carried out for the Environmental Specimen Bank [1], the Joint Working Group Elbe (ARGE Elbe) [2] and the International Commission for the Protection of the Rhine [3]. Using these data and the data generated at the measuring stations of the Joint Water Commission of the Federal States (LAWA) on total HCB concentrations in the water phase [4], a bioconcentration factor (field) or, better still, a bioaccumulation factor (BAF) can be determined for muscle tissue of bream and eel.

At many measuring stations, it has proved to be impossible to determine a BAF value since the HCB concentration in the water phase was below the detection limit. For this reason, BAF values could only be calculated for the Elbe. As HCB accumulates in suspended particulate matter (SPM) and SPM-bearing sediments, HCB concentrations in German inland surface waters are usually above the detection limit. Therefore, a Biota-SPM accumulation Factor (BSAF) can be calculated for most sampling sites for which data on residual levels in fish and in SPM or SPM-bearing sediments are available.

Definitions

Bioaccumulation means the concentration increase (accumulation) of a test substance in an organism (C_{org}) relative to its concentration in the surrounding medium (C_{medium}). Bioaccumulation comprises accumulation via all possible routes of uptake (water, sediment, food).

Bioconcentration means the concentration increase (accumulation) of a test substance in an organism, relative to its concentration in the surrounding medium, that results exclusively from the uptake of the substance via the body surface.

Biota-SPM accumulation factor (BSAF) is the quotient of the concentration of a test substance in an organism, normalised to lipid content (C_{fish} in mg/kg lipid content), and the concentration of the test substance in suspended particulate matter, normalised to organic carbon content (C_{sed} in mg/kg organic carbon).

Bioaccumulation factor for HCB in fish from the Elbe

To calculate the BAF, the HCB content in fish muscle tissue (bream, pooled sample from the Environmental Specimen Bank) was divided by the annual average at the corresponding measuring station. For the Elbe, a BAF referring to muscle tissue wet weight was calculated for 26 value pairs for bream and for 14 value pairs for eel. The data used to calculate the values are contained in the attachment.

Bioaccumulation factor for HCB in bream from the Elbe

(values refer to muscle tissue wet weight)

	BAF (l/kg)
Mean value	12644
Min	2169
Max	39447

Bioaccumulation factor for HCB in eels from the Elbe

(values refer to muscle tissue wet weight)

	BAF (l/kg)
Mean value	41953
Min	8524
Max	146317

Similar BAF values were determined for the three-spined stickleback (*Gasterosteus aculeatus*) in a laboratory two-step aquatic food chain [5]. In this study, artificial sediment was used as the main exposure source. Different routes of uptake were studied by exposing the fish to spiked water, spiked artificial sediment, pre-contaminated prey organisms (freshwater oligochaete *Tubifex tubifex* or the marine polychaete *Capitella capitata*), or combinations of these exposure routes. In the limnic test system (water-sediment-biota), a BAF of 52,500 l/kg, i.e. similar to the one calculated from field data, was determined.

Biota-SPM accumulation factor (BSAF)

The $QS_{secpois.biota}$ (16.7 [µg HCB/kg prey]) can also be transposed into a corresponding concentration in SPM by using a biota-SPM accumulation factor (BSAF) determined for fish using field data.

The average BSAF for bream from the Rhine is about 1.1 [kg (OC) / kg (lipid)]. The data used to calculate the value is contained in the attachment.

Calculation of a Quality standard for SPM corresponding to a QS Secondary Poising

$QS_{secpois.biota}$ = 16.7 [µg HCB /kg prey f.w.]

Assumptions:
Average lipid content in prey organisms (f_lipid) = 0.1 kg/kg
Average TOC content (Rhine data) in SPM (f_oc) = 5% = 0.05 kg/kg

$QS_{secpois.SPM}$	=	$QS_{secpois.biota}$ (16.7 [µg HCB / kg prey f.w.]) * foc / f_lipid*BSAF)
$QS_{secpois.SPM}$	=	$QS_{secpois.biota}$ (16.7 [µg HCB / kg prey f.w.] * 0,05) / (0.1 * 1.1)
	=	7.6 [µg HCB / kg d.w.]

References

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