Common Implementation Strategy for the Water Framework Directive

Environmental Quality Standards (EQS)

Substance Data Sheet

Priority Substance No. 26

Pentachlorobenzene

CAS-No. 608-93-5

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 [13]. 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: 26	Pentachlorobenzene
CAS-Number:	608-93-5
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	Comment
AA-QS inland waters	$QS_{overall\cdot freshwater}$ = 0.007 µg/l corresponding conc. in SPM: 12 µg/kg dry wt	Secondary poisoning is the protection objective that requires the lowest concentration in aquatic ecosystems; see sections 8.3 & 8.6
AA-QS transitional, coastal and territorial waters	$QS_{overall\cdot saltwater}$ = 0.0007 µg/l corresponding conc. in SPM: 1.3 µg/kg dry wt	Secondary poisoning is the protection objective that requires the lowest concentration in aquatic ecosystems; see sections 8.3 & 8.6
MAC-QS (ECO) *	1 µg/l	see section 8.1

* The proposal by the Commission may include a MAC-QS value which is based on the calculation of 12 * AA-EQS. This derivation is based on the minimum annual frequency of monitoring of priority substances in accordance with the Water Framework Directive. The derivation of such a MAC-QS is based on monitoring, compliance and reporting considerations rather than derived from effect data as presented in this EQS datasheet.

2.2 Specific Quality Standards

Protection Objective#	Quality Standard	Comment
Pelagic community (freshwater & saltwater)	1 µg/l corresponding conc. in SPM: 3.77 mg/kg dry wt	see section 8.1
Benthic community (freshwater & saltwater sediment)	87 µg/kg wet wt (400 µg/kg dry wt)	tentative standard (EP method); see section 8.2
Predators - secondary poisoning (freshwater)	$QS_{secpois.biota}$ = 367 µg/kg prey (biota tissue wet wt) corresponding $QS_{secpois.freshwater}$ = 0.007 µg/l corresponding conc. in SPM: 26 µg/kg dry wt	see section 8.3
Predators - secondary poisoning (saltwater)	$QS_{secpois.biota}$ = 367 µg/kg prey (biota tissue wet wt) corresponding $QS_{secpois.saltwater}$ = 0.0007 µg/l corresponding conc. in SPM: 2.6 µg/kg dry wt	see section 8.3; the difference in the corresponding concentrations of freshwater and saltwater are due to the different foodchain scenarios used for assessment of secondary poisoning in freshwater and marine environments
Food uptake by man	30 - 49 µg/ kg food (fishery products	Indicative value, not suitable as quality standard; see section 8.4
Abstraction of water intended for human consumption (AWIHC)	no EU DW abstraction standard set and the derivation of a specific QS addressing DW abstraction is not required	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
F; R11 - Xn; R22 - N; R50-53	[14]

4 Physical and chemical properties

Property	Value	Ref.
Vapour pressure	4.84 Pa 20°C 0.86 Pa 25°C 2.2 Pa	[1] [1] [5]; [7]
Henry's law constant		
Solubility in water	0.83 mg/L (25 °C) 0.24 mg/L (22°C) 1.33 mg/L (25 °C)	[1], [5]
Dissociation constant		

5 Environmental fate and partitioning

Property	Value:	Ref.
Hydrolytic stability (DT_{50})	Presumably no significant removal process	[5]
Photostability (DT_{50}) (aqueous, sunlight, state pH)		
Readily biodegradable (yes/no)	Chlorobenzenes are stable under aerobic and anaerobic conditions	[1]
Degradation in Water/sediment -DT_{50} water - DT_{50} whole system	Aerobic biodegradation presumably no significant removal process	[5]
Mineralization		
Bound residue		
Distribution in water / sediment systems (active substance)	Pentachlorobenzene adsorbs on suspended particles and sediment	[1]
Residues relevant to the aquatic environment	<u>anaerobic:</u> DT_{50} (adapted sediment) 17 d metabolites: 1,2,3,4-tetrachlorobenzene, 1,3,5-trichlorobenzene, 1,2,4-trichlorobenzene, 1,2,3-trichlorobenzene, 1,3-dichlorobenzene, 1,2-dichlorobenzene, monochlorobenzene	[5], [1]
Partition co-efficient (log P_{OW}) Koc	5.2 5.03 – 5.18 5.18 log Koc 3.5-5.1 58700 l/kg 40000 (suspended sediment of river water) 25120 – 125900 (sediment)	[1] [5] [7] [1] [5] [5] [5]
BCF Fish *Poecilia reticulata* (Guppy) Golden Orfe Sunfish Trout Carp Freshwater fish (whole body) Fish Bivalves	 1100 – 6800 (general range , HSDB) 260000 3000 3400 13000 – 20000 1100 – 6800 5300 (geometric mean exp. data, maximum 8100) 7300 (calculated) 2000 (calculated)	 [1] [1] [5] [5], [11] [5] [5] [7] [7] [7]

6 Effect data (aquatic environment)

Table 6.1: Overview on Pentachlorobenzene aquatic toxicity data for most sensitive species from different sources (master reference)

Species	Taxon. Grp.	Duration	Effect	Endpoint	Value	Unit	Master Ref.	Reference in master ref.
Freshwater								
Daphnia magna	Crustacea	16 d	Reproduction	NOEC	10	µg/l	[5]	Hermens et al. 1984
Daphnia magna	Crustacea	16 d	Reproduction	NOEC	16	µg/l	[1]	Hesse et al 1991
Daphnia magna	Crustacea	21 d	Reproduction / Mortality	NOEC	21	µg/l	[1]	Hesse et al. 1991
Danio rerio	Pisces	28 d	Reproduction	NOEC	34	µg/l	[1]	Van Leeuwen et al. 1990
Selenastrum capricornutum	Algae	96 h	Growth	NOEC	100	µg/l	[1]	EPA, 1978
Oncorhynchus mykiss	Pisces	6 d	Behaviour	EC50	100	µg/l	[5]	Ahamd et al. 1984
Poecilia reticulata	Pisces	8 d	Mortality	LC50	100	µg/l	[1]	Van Hoogen & Opperhuizen 1988
Chironomus thummi	Insecta	48 h	Mortality	LC50	230	µg/l	[5]	Roghair et al. 1994
Daphnia magna	Crustacea	48 h	Mortality	LC50	300	µg/l	[1]	Abernethy et al. 1986
Ceriodaphnia dubia	Crustacea	7 d	Reproduction	IC50	520	µg/l	[5]	Oris et al. 1991
Selenastrum capricornutum	Algae	96 h	Growth	EC50	6630	µg/l	[1]	EPA, 1978
Saltwater								
Cyprinodon variegatus	Pisces	28 d	Growth	NOEC	18	µg/l	[5]	Hansen et al. 1991
Mysidopsis bahia	Crustacea	96 h	Mortality	LC50	160	µg/l	[5]	US-EPA 1978
Skeletonema costatum	Algae	96 h	Physiology	EC50	2230	µg/l	[5]	US-EPA 1978
Crassostrea gigas	Mollusca	48 h	Larval development	EC50 EC10 NOEC	>49 >49 >49	µg/l	[8]	
Psammechinus miliaris	Echinodermata	48 h	Larval development	EC50 EC10 NOEC	>19 >19 >19	µg/l	[8]	

Table 6.2: Mammal oral toxicity data relevant for the assessment of non compartment specific effects relevant for the food chain (secondary poisoning). Data collated from Health Canada [11] and EPA-IRIS [9] documents

Species	Duration	Dosage	Endpoint	Effect observed	Reference:
Mouse *Mus musculus*	90 d	0, 33, 100, 330, 1000 or 2000 ppm	LOEC: 33 mg/kg food ≈ 5.2 mg/kg bw/d	functional effects on the tyroid	NTP 1991
Rat *Rattus norvegicus*	90 d	0, 33, 100, 330, 1000 or 2000 ppm	NOEC: 33 mg/kg food ≈ 5.2 mg/kg bw/d	increased liver and kidney weights, hepatocellular hypertrophy, renal histopatological defects	NTP 1991
Rat *Rattus norvegicus*	180 d	male rats 0, 125 or 1000 ppm; female rats 0, 125, 250, 500 or 1000 ppm	NOEC: 125 mg/kg food ≈ 8.3 mg/kg bw/d (LOAEC: 250 mg/kg food)	increased liver to body weight ratios in dams and pups; tremors in succling pups of dams fed with the substance	Linder 1980
Rat *Rattus norvegicus*	180 d	male rats 0, 125 or 1000 ppm; female rats 0, 125, 250, 500 or 1000 ppm	LOAEC: 125 mg/kg food ≈ 8.3 mg/kg bw/d	significantly increased kidney weight, decrased heart weight and an increase in hyaline droplets in proximal kidney tubules	Linder 1980

Table 6.3: Summary on endocrine disrupting potential

Comment	Reference
There is insufficient data on pentachlorobenzene available (in the BKH-report)	[2]

7 Effect data (human health)

Upon evaluation of the pentachlorobenzene data-sheet, the CSTEE recommended to re-consider the NOEC used and the assessment factor applied in order to derive a human health based QS referring to the ingestion of fishery products. This recommendation was followed and toxicological data better suitable as basis for the derivation of a quality standard were searched for.

- The U.S.-EPA has calculated an Oral Reference Dose (RfD) of 0.8 µg per kg body weight per day for non-cancerogenic effects of pentachlorobenzene [9]. The RfD is an estimate (with uncertainty spanning perhaps one order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime. It hence is comparable with a tolerable daily intake (TDI).

  The RfD of 0.8 µg /kg bw /d is based on a LOAEL of 8.3 mg/kg bw/d obtained in acute and subchronic oral bioassays with rats (including weanlings) [10] and an uncertainty factor of 10,000. A statistically significant increase in kidney weights, a decreased heart weight, and an increase in hyaline droplets in proximal kidney tubules was noted in rats receiving 8.3 mg/kg/day. Female rats receiving the next highest dose, 18 mg/kg/day, and their offspring showed increased liver/body weight ratios. Suckling pups of dams receiving 18 mg/kg/day and higher doses of pentachlorobenzene developed tremors. The composite uncertainty factor of 10000 represents 10 each for the expected interspecies and interhuman variability to the toxicity of this compound in lieu of specific data, 10 to extrapolate a subchronic effect level to its chronic counterpart, and 10 to drop the LOAEL into the expected range of a NOAEL.

Confidence in the RfD can be considered low to medium. The study rates a medium confidence because several effects were monitored, and both adult animals and neonates were tested. The study does not rate higher than medium because a NOAEL was not established and only a moderate number of animals was used. The database rates a low confidence because few data exist to support this analysis.

- Health Canada has derived a TDI for pentachlorobenzene on the basis of sub-chronic investigations, which were the longest-term studies available [11]. Pentachlorobenzene was administered in the diet to rats (Linder *et al.,* 1980 [10]) and to rats and mice (NTP, 1991 [12]), the lowest dietary concentration (and associated dose on a body weight basis) at which compound-related effects were observed was that to which male mice were exposed (33 ppm [mg/kg] in the diet; 5.2 mg/kg bw/day) in the NTP bioassay (NTP, 1991). At this concentration, there was minimal to moderate centrilobular hepatocellular hypertrophy and occasional necrosis of hypertrophied hepatocytes(considered to be secondary to the hypertrophy) [NTP, 1991]. On the basis of this LOEL, a tolerable daily intake of 0.5 µg/kg bw/d is conservatively (owing to the paucity of available data) derived with an uncertainty factor of 10000 (x 10 for intraspecies variation; x 10 for interspecies variation; x 10 for less than chronic study; x 10 for lack of data on carcinogenicity and chronic toxicity; additional factor of 10 for LOEL rather than NOAEL not incorporated since observed effects at the LOEL were minimal).

8 Calculation of quality standards

8.1 Quality standards for water

Freshwater

Aquatic toxicity data collated from different sources are summarized in table 6.1.

Fish and crustaceans appear to be more sensitive to pentachlorobenzene than algae. The lowest chronic endpoint is the 16 d NOEC of 10 µg/l for the freshwater crustacean *Daphnia magna*. As long-term NOEC data across the three trophic levels (fish, daphnia and algae) are available and the species most sensitive in the acute toxicity tests belongs to the mentioned groups the appropriate assessment factor according to the TGD [3] is 10.

$QS_{freshwater}$ = 10 µg/l / AF (10) = 1 µg Pentachlorobenzene /l

Koc values between 3160 -125900 have been reported for pentachlorobenzene (see section 5 of this data sheet). Hence, the log Kp_{susp}[1] is 3.5 – 5.1 and the trigger criterion to calculate the corresponding concentration to the $QS_{freshwater}$ in SPM is met (see section 4.2 of the Manual [4]). It is proposed to use a Kp_{susp} of 4000 l/kg[2] for the calculation, based on a measured Koc of 40000 l/kg in suspended sediment of river water [5]. The $QS_{SPM.freshwat}$ is derived as follows:

$$\mathbf{QS_{SPM.freshwat}} = \frac{QS_{freshwater}\ [1\ \mu g/l]}{C_{SPM}\ [15\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(4000\ l/kg)^{-1}]} = \mathbf{3.77\ mg/kg\ SPM\ (dry\ wt)}$$

[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} (Koc * 0.1) it is suggested to use the Koc for SPM in river water (40000 l/kg) reported in [5].

Transitional, coastal and territorial waters

5 toxicity tests with one species each of marine fish, crustaceans, algae, molluscs and echinoderms are available beside the freshwater data (see table 6.1). Apparently, the sensitivity of marine species is comparable with the sensitivity of freshwater species of the same taxonomic group. Therefore, it is suggested to use the pooled data of freshwater and saltwater organisms for the derivation of the $QS_{saltwater}$. Taking into account the recommendations for marine risk assessment of the TGD [3] it appears appropriate to use 10 as assessment factor for the derivation of the saltwater QS (there are 2 toxicity tests with marine species other than fish, crustaceans and algae available).

$QS_{saltwater}$ = 10 µg/l / AF (10) = 1 µg Pentachlorobenezene /l

As the log Kp_{susp} is >3 (see footnote 2), the QS for water is additionally given as concentration in SPM. For the TGD standard water, the concentration corresponding to the $QS_{saltwater}$ is 1/10 of that calculated for freshwater (0.377 mg/kg SPM dry wt). However, 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 is, as an example, also calculated for a SPM concentration of 3 mg/l:

$$\mathbf{QS_{SPM.saltwat}} = \frac{QS_{freshwater}\ [1\ \mu g/l]}{C_{SPM}\ [3\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(4000\ l/kg)^{-1}]} = \mathbf{3.95\ mg/kg\ SPM\ (dry\ wt)}$$

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

Acute toxicity data are available for fish, crustaceans, algae and insects (see table 6.1). The lowest acute toxicity values available are two LC50 or EC50 values for fish of 100 µg/l each.

It is suggested to derive the MAC-QS on the basis of these values and the guidance given in the TGD on the effects assessment for intermittent releases (section 3.3.2 of part II of [3]).

As information is only available for the 3 trophic levels fish, invertebrates and algae, it is suggested to use 100 as assessment factor to derive the quality standard for transient concentration peaks.

MAC-QS = 100 µg/l / AF (100) = 1 µg Pentachlorobenzene /l

8.2 Quality standard for sediment

The log Kp_{susp} of pentachlorobenzene is >3 (see footnotes 1 & 2) and therefore the trigger criterion to calculate a sediment quality standard is met.

No toxicity data are available for sediment dwelling organisms. According to the TGD [3], the $PNEC_{sediment}$ ($\approx QS_{sediment}$) may be calculated using the equilibrium partitioning method in the absence of ecotoxicological data for 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. 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 pentachlorobenzene is 5.03 – 5.2 (range given in 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:

$$QS_{sed.wet\_weight}\ [mg.kg^{-1}] = \frac{Kp_{SPM\text{-}water}\ [1000\ m^3/m^3]}{bulk\ density_{SPM.wet}\ [1{,}150\ kg/m^3]} * 1{,}000 * QS_{water}\ [mg/l] * 10^{-1}$$

with:
$K_{SPM\text{-}water}$ = f_{solid} (0.1) * Kp_{susp} (4000 l/kg) / 1000 * RHO_{solid} (2500 kg/m^3) = 1000 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
10^{-1} = factor to account for possible additional uptake routes for substances with log Kow >5

$QS_{freshwater}$ & $QS_{saltwater}$ = 0.001 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):

$QS_{sediment}$	87 µg/kg (wet wt)	400 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

Pentachlorobenzene is bioaccumulating (BCF >>100). Therefore, 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]).

The NOEC of 33 mg/kg food for sub-chronic (90d) oral toxicity in rats (see table 6.2) is the lowest value available. It refers to increases in organ weights, liver hypertrophy and renal defects. Especially the latter observations are considered to be of ecological relevance because they could cause early death in long-living top-predators and thus have an impact on reproduction of the population[3]. From this $NOEC_{food}$ a $PNEC_{oral}$ is calculated according to the procedure described in section 4.3.2.5 of the Manual [4] (based on section 3.8.3.5 of the TGD [3]). The $PNEC_{oral}$ is equivalent to the $QS_{biota.secpois}$.

$PNEC_{oral}$ = $NOEC_{oral}$ (33 (mg/ kg food) / AF (90) = 0.367 mg/kg food

AF: assessment factor for the extrapolation to PNEC, depending on duration of test
(90 for a 90 day study with mammals)

[3] Upon evaluation of this data sheet the CSTEE recommended to reconsider the NOEC used as basis for the derivation of a PNEC referring to secondary poisoning because its ecological relevance was unclear. This recommendation has been followed and the formerly used NOAEL was discarded and replaced by the now used value.

Thus, the $QS_{biota.secpois}$ is:

$QS_{biota.secpois}$ = 367 µg Pentachlorobenzene / kg food (fish; wet weight)

Pentachlorobenzene has been shown to be liable to bioconcentration (see section 5 of this data sheet). However, the available BCF data cover a very wide range and, hence, it is difficult to select one figure representing a realistic worst case. Therefore, 3 different BCFs (3000, 5300, 20000) are used in a scenario approach to calculate the concentration in water that corresponds to the $QS_{biota\cdot secpois}$. No information is available on observations regarding biomagnification.

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 [4] or sections 3.8.3 and 4.4.3 of the TGD [3] 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. For substances with a BCF between 2000 and 5000 the respective default BMFs are 2 (freshwater) and 4 (marine, 2*2).

Because of the large BCF range found for pentachlorobenzene and the uncertainty regarding possible biomagnification no firm figure for a "safe" water concentration with regard to protection from secondary poisoning can be calculated. However, some scenario calculations may highlight the potential of pentachlorobenzene for secondary poisoning (table 8.1).

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

$QS_{secpois.water}$ = $QS_{secpois.biota}$ (367 [µg pentachlorobenzene /kg prey]) / BCF * BMF

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

Scenario	**BCF**	**default $BMF_{freshwater}$**	**default BMF_{marine}**	**$QS_{secpois.freshw}$ µg/l**	**$QS_{secpois.saltw}$ µg/l**
worst case	20000	10	100	0.002	0.0002
intermediate	5300	10	100	0.007	0.0007
best case	3000	2	4	0.061	0.031
best case without default BMFs	3000	1 (no biomagnifcation)	1 (no biomagnifcation)	0.12	0.12

From the figures calculated in table 8.1 it is evident that any scenario requires a considerably lower $QS_{secpois.water}$ as the quality standard calculated for the protection of the freshwater and saltwater pelagic communities.

The Expert Group on Quality Standards (Workshop 12-16 May 2003, Brussels) agreed on the use of the "intermediate" scenario in table 8.1 with the geometric mean of experimental data as BCF (=5300) and the default BMF values of 10 and 100 for freshwater and saltwater, respectively. Hence, the respective quality standards are:

$QS_{secpois.freshwater}$ = 0.007 µg Pentachlorobenzene /l

$QS_{secpois.saltwater}$ = 0.0007 µg Pentachlorobenzene /l

As the trigger criteria to calculate the corresponding concentration to the $QS_{secpois.water}$ in SPM are met (see section 8.1) the $QSs_{SPM.water}$ are derived as follows:

$$\mathbf{QS_{secpois.freshw.SPM}} = \frac{QS_{secpois.freshwater}\ [0.007\ \mu g/l]}{C_{SPM}\ [15\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(4000\ l/kg)^{-1}]} = \mathbf{26\ \mu g/kg\ SPM\ (dry\ wt)}$$

$$\mathbf{QS_{secpois.freshw.SPM}} = \frac{QS_{secpois.freshwater}\ [0.0007\ \mu g/l]}{C_{SPM}\ [3\ mg/l] * 10^{-6}\ [kg/mg] + Kp^{-1}\ [(4000\ l/kg)^{-1}]} = \mathbf{2.6\ \mu g/kg\ SPM\ (dry\ wt)}$$

8.4 Quality standard referring to food uptake by humans

Pentachlorobenzene is subject to bioaccumulation and it is classified as harmful if swallowed (R22). Therefore, the trigger criteria to derive a quality standard referring to protection of human health from adverse effects due to the ingestion of food from aquatic environments is met (see table 1b of the Manual [4]).

The TDI of 0.5 µg/kg bw /d and the Oral Reference Dose of 0.8 µg/kg bw /d derived by Health Canada and the U.S.-EPA, respectively, may be used as starting point for the QS derivation. However, both standards are derived on the basis of an extraordinarily high composite uncertainty factor of 10000. Therefore, any quality standard derived on the basis these values should be used with care.

In the Manual [4] (section 4.3.2.6) 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 3.5 - 5.6 µg pentachlorobenzene per day.

The average fish consumption of an EU citizen is 115 g d-1 (TGD [3]). Thus, 115 g edible fishery products must not contain more than 3.5 - 5.6 µg pentachlorobenzene.

$$\mathbf{QS_{hh.food}} = \frac{3.5 - 5.6\ \mu g\ PentaClbenzene}{115g\ fishery\ products} * 1000\ g = \mathbf{30.4 - 48.7\ \mu g\ PentaClbenzene\ /\ kg\ food}$$

Transformation of the derived $QShh.food$ to the corresponding concentration in water, using the approach described for secondary poisoning in section 8.3, would result in a 7-12 times lower QS proposal than derived for the secondary poisoning scenario.

However, as the assessment factors used by US-EPA and Health Canada to derive the oral Reference Dose (RfD) or the Tolerable Daily Intake (TDI) sum already up to a factor of 10,000 [9, 11] it appears not meaningful to transform the concentration in fishery products based $QS_{hh.food}$ already associated with so much uncertainty to a water-based concentration, adding further bioaccumulation related uncertainty to the calculation. Overall, because of the huge uncertainty associated with the calculation, neither the derived $QS_{hh.food}$ nor the corresponding $QS_{hh.water}$ should be imposed as quality standards. They can be considered as indicative values only.

8.5 Quality standard for drinking water abstraction

No "A1 value" for pentachlorobenzene is set in Council Directive 75/440/EEC and also no drinking water limit value has been fixed in Council Directive 98/83/EC. However, Health Canada has derived a TDI of 0.5 µg/kg bw/d and the US-EPA an Oral Reference Dose (RfD) of 0.8 µg/kg bw/d (see section 7). It is suggested to use these values as starting point for the derivation of a tentative QS.

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].

$$QS_{DW.provisional} = \frac{0.1 * TL_{HH} * BW}{Uptake_{DW}} = 1.8 – 2.8 \text{ µg Pentachlorobenzene /l}$$

with:

$QS_{DW.provisional}$	provisional quality standard for drinking water (mg/l)
TL_{HH}	threshold level for human health (TDI or RfD = 0.05 – 0.08 µg/kg bw/d)
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 the standards required to protect the pelagic freshwater community or predators and humans from secondary poisoning. It is therefore not necessary to set a specific quality standard referring to abstraction of water intended for human consumption (AWIHC) as objective of protection.

8.6 Overall quality standard

Protection of predators from secondary poisoning is the objective that requires the lowest quality standard. Hence, the quality standards addressing secondary poisoning of predators derived in section 8.3 are suggested as overall annual average quality standards.

9 References

[1] Les Etudes des Agences de l'Eau Nº 64: Systéme d'Évaluation de la Qualite de l'Eau des Cours d'Eau. SEQ-Eau (version 1) Annexe A – Grilles de seuils par altération avec justifications (Annexe 4: Classes d'Aptitude Pour Divers Micropollutants, Fonction "Potentialites Biologiques de l'Eau", Pentachlorobenzene - Fiche de Donnees). Agences de l'Eau, Janvier 1999. ISSN 1161-0425

[2] COM(2001)262 final: Communication from the Commission to the Council and the European Parliament on the implementation of the Community Strategy for Endocrine Disrupters – a range of substances suspected of interfering with the hormone system of humans and wildlife.

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