Common Implementation Strategy for the Water Framework Directive

Environmental Quality Standards (EQS)

Substance Data Sheet

Priority Substance No. 27

Pentachlorophenol

CAS-No. 87-86-5

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 [19]. 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: 27	Pentachlorophenol
CAS-Number:	87-86-5
Classification WFD Priority List *:	PSR

* 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 types of waters bodies addressed by the WFD	0.35 µg/l	0.4 µg/l	see 8.1.2 & 8.6
MAC-QS (ECO)	1 µg/l	1 µg/l	see section 8.1.1

2.2 Specific quality standards

Protection Objective #	Quality Standard	Comment
Pelagic community (freshwater & saltwater)	0.35 µg/l	see section 8.1.2
Benthic community (freshwater & marine sediment)	25.9 µg/kg wet wt (119 µg/kg dry wt)	tentative standard (EP method); see section 8.2
Predators (secondary poisoning)	1.83 mg/kg prey (biota tissue wet wt) corresponding concentration in water: 2.4 µg/l	see section 8.3
Food uptake by man	18.3 mg/kg fishery product (wet wt) corresponding concentration in water: 23.7 µg/l	oral toxicity data with relevance to human health not available; see section 8.4
Abstraction of water intended for human consumption (AWIHC)	< 1 µg/l	A1-value for Σpesticides in CD 75/440/EEC; see section 8.5
Water intended for human consumption (WIHC)	0.1 µg/l	Drinking water standard set in CD 98/83/EC

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. 3; R40 - T+; R26 - T; R24/25 - Xi; R36/37/38 - N; R50-53	[20]

4 Physical and chemical properties

Property	Value	Reference
Vapour pressure	0.00415 Pa (20° C) 0.0051 Pa (20 °C)	[10] [5]
Henry's law constant		
Solubility in water	14 mg/l (20° C) 330 g/l Na-salt	[10]
Dissociation constant	4.92 pK_a = 4.28 - 5.77	[10] [5]

5 Environmental fate and partitioning

Property	Value	Ref.
Hydrolytic stability (DT_{50})	no hydrolisation	[10]
Photostability (DT_{50}) (aqueous, sunlight, state pH)	reported half lifes in water range from 1h to 4.6 d	[10]
Readily biodegradable (yes/no)		
Degradation in Water/sediment -DT_{50} water - DT_{50} whole system	aerobic aquatic incl. sediment DT50 4.9 d; anaerobic aquatic incl sediment Dt50 33.8 d	[10]
Mineralization		
Bound residue		
Distribution in water / sediment systems (active substance)		
Residues relevant to the aquatic environment		
Partition co-efficient (log P_{OW})	3.32 - 5.08 (depending on pH) 5.12 3.32 at pH 7; 4.5 at pH 4; 1.3 at pH 10 4.74 5 at pH 2; 3 at pH 7; 3.32 at pH 7.7	[9] [1] [10] [7] [5]
Koc	log Koc 3.97 (≈9330) 706 –3420 (4 soil types) 700 – 4580 (soils) 33000 – 53000 (sediment)	[1] [10] [5] [5]
BCF <u>Fish</u> *Jordanella floridae* Fathead Minnow Bluegill Rainbow Trout Killifish (saltwater) Fish (experimental freshwater & marine) (whole body) Fish (various species) <u>Bivalves</u> Marine Bivalves (experimental) Mytilus edulis (Blue mussel, marine) *Anodonta anatina* (Duck mussel, freshw.) Oyster Blue Mussel <u>Other</u> *Lanice conchilega* (marine polychaete) Neanthes virens *Daphnia magna* (pelagic crustacean)	 216 (whole fish) 174-770 (whole body) 490 (whole body) 91 – 771 (whole body) 64 (whole body) average: 140 (maximum 770) 100 – 1000 (most values <500) 88 (maximum 130) 390 305 34-82 300 -390 3820 280 100 - 400	 [9; 14] [10] [10] [10] [10] [7] [5] [7] [9] [9] [5] [5] [9, 16] [15] [5]

6 Effect data (aquatic environment)

Table 6.1: Overview on pentachlorobenzene aquatic toxicity data for most sensitive species from different sources (master reference). The data highlighted in bold are used for the SSD based derivation of the QS, see section 8.1.

Species	Taxon. Grp.	Duration	Effect	Endpoint	Value	Unit	Master Ref.	Reference in master ref.
Freshwater								
Micropterus salmoides	Pisces	52 d	Growth	NOEC	**1**	µg/l	[1]	Johansen et al (1985)
Daphnia magna	Crustacea	21 d	Reproduction	NOEC	**1.8**	µg/l	[5]	Korte et al. 1984
Salmo gairdneri	Pisces	≥4 w	Survival, growth	NOEC	**11**	µg/l	[6]	risk limits PIII, geometric mean (n=3)
Lymnea stagnalis	Mollusca	40 d	Hatching	NOEC	**3.2**	µg/l	[9], [6]	Slooff and Canton (1983)
Pimephales promelas	Pisces	90 d	Survival / Growth	NOEC	8	µg/l	[9]	Hamilton et al (1986)
Pimephales promelas	Pisces	90 d	Growth	NOEC	28.3	µg/l	[6]	risk limits PIII
Pimephales promelas	Pisces	90 d	Growth	NOEC	**15**	µg/l		geometric mean
Gammarus fasciatus	Crustacea	42 d	Survival	NOEC	**23**	µg/l	[6]	risk limits PIII
Xenophus laevis	Amphibia	100 d	Survival	NOEC	**32**	µg/l	[6]	Slooff et al. 1983; risk limits PIII
Hydra oligactis	Coelenterata	21 d	Growth	NOEC	**32**	µg/l	[6]	risk limits PIII
Oryzias latipes	Pisces	42 d	Survival, hatching, growth	NOEC	**32**	µg/l	[6]	risk limits PIII
Physa gyrina	Mollusca	36 d	Growth	NOEC	**55**	µg/l	[1]	Brown and Pascoe (1989)
Scenedesmus pannonicus	Algae	4d	Growth	NOEC	**100**	µg/l	[6]	risk limits PIII
Lemna minor	Macrophyta	7 d	Growth	NOEC	**1000**	µg/l	[6]	risk limits PIII
Culex pipiens	Insecta	25 d	Development, survival	NOEC	**3200**	µg/l	[6]	risk limits PIII
Cyprinus carpio	Pisces	96 h	Mortality	LC50	10	µg/l	[9]	Verma et al (1981a)
Salmo clarki	Pisces	96 h	Mortality	LC50	10 - 100	µg/l	[9]	Meyer and Ellersieck (1986)
Oncorhynchus mykiss	Pisces	96 h	Mortality	LC50	18	µg/l	[5]	Van Leeuwen 1985
Carassius auratus	Pisces	96 h	Mortality	LC50	23	µg/l	[5]	Inglis et al. 1972
Ictalurus punctatus	Pisces	96 h	Mortality	LC50	54	µg/l	[1]	Phipps and Holcombe (1985)
Scenedesmus quadricauda	Algae	96 h	Life Cycle	EC50	80	µg/l	[9]	Adema and Vink (1981)
Scenedesmus costatum	Algae	96 h	Growth	EC50	80	µg/l	[1]	Crossland and Wolff (1985)
Daphnia magna	Crustacea	48 h	Mortality	LC50	82	µg/l	[9]	Stephenson et al (1991a)
Bufo bufo japonicus	Amphibia	96 h	Mortality	LC50	100	µg/l	[5]	Nishiuchi 1976
Chironomus thummi	Insecta	48 h	Mortality	LC50	110	µg/l	[5]	Slooff 1983
Dreissena polymorpha	Mollusca	96 h	Mortality	LC50	110	µg/l	[5]	Adema et al. 1981
Gammarus pseudolimnaeus	Crustacea	96 h	Mortality	LC50	121	µg/l	[1]	Spehar et al (1985)

Species	Taxon. Grp.	Duration	Effect	Endpoint	Value	Unit	Master Ref.	Reference in master ref.
Saltwater								
Ophryotrocha diadema	Annelida	30 d	Reproduction	NOEC	**10**	µg/l	[10], [6]	Adema & Vink 1981; risk limits PIII
Pleuronectes platessa	Pisces	56 d	Egg & larvae mortality, growth, development	NOEC	**10**	µg/l	[10], [6]	Adema & Vink 1981; risk limits PIII
Skeletonema costatum	Algae	5 d	Growth	NOEC	**11**	µg/l	[10]	Hoberg 1993e
Meiobenthic Nematode	Nematoda	91 d	Biomass & density	NOEC	**16**	µg/l	[10]	Cantelmo & Rao 1978
Cyprinodon variegatus	Pisces	Life Cycle	Survival and growth	NOEC	**47**	µg/l	[10], [6]	Parrish et al 1978; risk limits PIII
Marinogammarus marinus	Crustacea	56 d	Growth	NOEC	**100**	µg/l	[6]	risk limits PIII
Crassostrea virginica	Mollusca	96 h	Embryo development (Na-salt of PCP)	EC50	40	µg/l	[9]; [6]	Borthwick and Schimmel (1978); risk limits PIII
Lagodon rhomboides	Pisces	96 h	Growth, mortality	L(E)C50	44.9	µg/l	[6]	risk limits PIII
Lagodon rhomboides	Pisces	96 h	Mortality (Na-salt of PCP)	LC50	53	µg/l	[9]	Schimmel et al (1978)
Crassostrea virginica	Mollusca	14 d	Survival	EC50	70	µg/l	[9]	Davis and Hidu (1969)
Monochrysis Sp.	Algae	96 h	Growth	EC50	200	µg/l	[9]	Adema and Vink (1981)
Cyprinodon variegatus	Pisces	96 h	mortality	LC50	442	µg/l	[6]	risk limits PIII
Palaemonetes pugio	Crustacea	96 h	mortality	LC50	531.9	µg/l	[6]	risk limits PIII
Brachionus plicatilis	Rotatoria	24 h	mortality	LC50	1360	µg/l	[6]	risk limits PIII

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) [6]

Species		**Duration**	**Effect**	**Endpoint**	**mg/kg food**	**Reference in [6]:**
Rattus norvegicus	Rat	5 m	Reproduction	NOEC	55	679101012
Mus musculus	Mouse	2 y	Growth	NOEC	200	679101012
Gallus domesticus	Hen	8 w	Reproduction	NOEC	245	679101012
Colinus virginianus	Quail	5 d	Mortality	LC50	3400	601640001
Phasianus colchicus	Phesant	5 d	Mortality	LC50	4331	601640001
Anas platyrhynchos	Mallard Duck	5 d	Mortality	LC50	4500	601640001
Coturnix c. japonica	Quail	5 d	Mortality	LC50	5204	601640001

Table 6.3: Summary on Endocrine Disrupting Potential

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

7 Effect data (human health)

The U.S.-EPA has developed an oral Reference Dose (**RfD) of 0.03 mg/ kg bw/ day** for pentachlorophenol [18], based on a NOEC of 3 mg/kg/day for liver and kidney pathology (LOEC 10 mg/kg/day) obtained in a chronic oral rat study [17] and an associated uncertainty factor of 100. The 100-fold factor accounts for the expected intra- and inter- species variability to the toxicity of this chemical in lieu of specific data.

The RfD is an estimate (with uncertainty spanning perhaps an 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.

A number of studies that have investigated the teratogenicity of orally administered pentachlorophenol in rodents are as well available in the literature [18]. Although these studies did not reveal teratogenic effects, feto- maternal toxicity was seen at 30 mg/kg/day. Since pentachlorophenol apparently does not cross the placental barrier, the observed fetotoxicity may be a reflection of maternal toxicity. The NOAEL in these studies was concluded to be 3.0 mg/kg/day (U.S. EPA, 1984), which is the same as for the chronic study reported earlier.

8 Calculation of quality standards

8.1 Quality standards for water

Aquatic toxicity data collated from different sources are summarized in table 6.1. There are many long-term no effect and short-term acute toxicity data for a broad range of species from different taxonomic groups available. Apparently, the sensitivity of marine species is in general comparable with the sensitivity of freshwater species of the same taxonomic group although the most sensitive species are freshwater organisms.

The TGD [3] offers the option to support the effects assessment performed with the assessment factor method by a statistical extrapolation method if the database is sufficient for its application. The TGD requires reliable NOECs from chronic/long-term studies for a minimum of 15 different species from at least 8 taxonomic groups. In the PCP database long-term/chronic NOECs are available for 10 different taxonomic groups (freshwater & saltwater together). The minimum species requirements as mentioned in section 3.3.1.2 of the TGD are fulfilled and there are more than a minimum of 15 NOEC data available that could serve as input data for statistical extrapolation. Therefore the method of Aldenberg & Jaworska [11] has been applied in order to explore to which extent the result of this method differs from the outcome of the standard TGD assessment factor method. Details of application and the result of the SSD method are described in section 8.1.2.

8.1.1 Calculation of quality standards for water using the assessment factor method

Freshwater

The differences in sensitivity to pentachlorophenol are apparently not significant for the most susceptible fish, crustacean, mollusc and algae species. The lowest chronic endpoint is the 52 d NOEC of 1 µg/l for the Largemouth Bass *(Micropterus salmonides)*. 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. Hence, the appropriate assessment factor according to the TGD [3] is 10.

$QS_{freshwater}$ = 1 µg/l / AF (10) = 0.1 µg Pentachlorophenol /l

Koc values between 700 and 53000 have been reported for pentachlorophenol (see section 5 of this data sheet). Hence, the log Kp_{susp}[1] is 1.85 – 3.72 and the trigger criterion to calculate the corresponding concentration to the $QS_{freshwater}$ in SPM is normally met (see section 4.2 of the Manual [4]). As pentachlorophenol is partially dissociated under environmental conditions (pKa ≈5) the sorption to organic matter is pH-dependent (i.e. the Koc value increases when the pH decreases). Therefore, analysis of pentachlorophenol in SPM is not considered a good alternative to water samples, given that the detection limit of pentachlorophenol in water is 1 ng/l [5]. Hence, it should be no problem to conduct compliance monitoring for the derived water quality standard of 100 ng/l in water samples.

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]).

Transitional, coastal and territorial waters

Toxicity tests with species of marine fish, crustacea, algae, molluscs, annelida, nematoda and rotatoria are available beside the freshwater data, which also cover a broad range of taxonomic groups (see table 6.1). Apparently, the sensitivity of marine species is in general comparable with the sensitivity of freshwater species of the same taxonomic group although the most sensitive species are freshwater organisms. A reason for this observation may be that due to the prevailing pH in marine waters a higher percentage of pentachlorophenol is dissociated than in less alkaline freshwaters. Ionized pentachlorophenol is believed to be less toxic than the undissociated form [10]. However, given the relatively small differences in the NOECs of the most sensitive freshwater and saltwater organisms and taking into account the limited availability of data these differences are not considered significant. 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 draft revised TGD [3], it appears appropriate to use 10 as assessment factor for the derivation of the saltwater QS (there are toxicity tests with marine species other than fish, crustaceans and algae available showing that the representatives of the additional groups are apparently not more sensitive to pentachlorophenol).

$QS_{saltwater}$ = 1 µg/l / AF (10) = 0.1 µg Pentachlorophenol /l

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

Acute toxicity data are available for a broad range of taxonomic groups (see table 6.1). The lowest acute toxicity values available are two LC50 values for fish (*Cyprinus carpio*, *Salmo clarki*) of 10 µg/l each.

It is suggested to derive the MAC-QS on the basis of this LC50 and the guidance given in the TGD on the effects assessment for intermittent releases (Manual, section 4.3.6[4]).

As information is available for a broad range of taxonomic groups it is suggested to use a reduced assessment factor of 10 to derive the quality standard for transient concentration peaks.

MAC-QS = 10 µg/l / AF (10) = 1 µg Pentachlorophenol /l

8.1.2 Calculation of the quality standard for water using statistical extrapolation

The 5th-percentile cut-off value was calculated with the method of Aldenberg & Jaworska [11] (for details see section 4.3.4 of the Manual [4]). The program ETX-2000 [12] was used for the calculation and for assessing the fit of the input data to the supposed log-normal distribution.

The toxicity tests highlighted in bold in table 6.1 were used as input-data. The selected data fit very well to the expected distribution curve (see figure 8.1). The Kolomogorov-Smirnov and Anderson-Darling tests for goodness of fit are passed on the highest level of significance.

The calculated 5th-percentile cut off-value is 1.05 µg/l (see table 8.1).

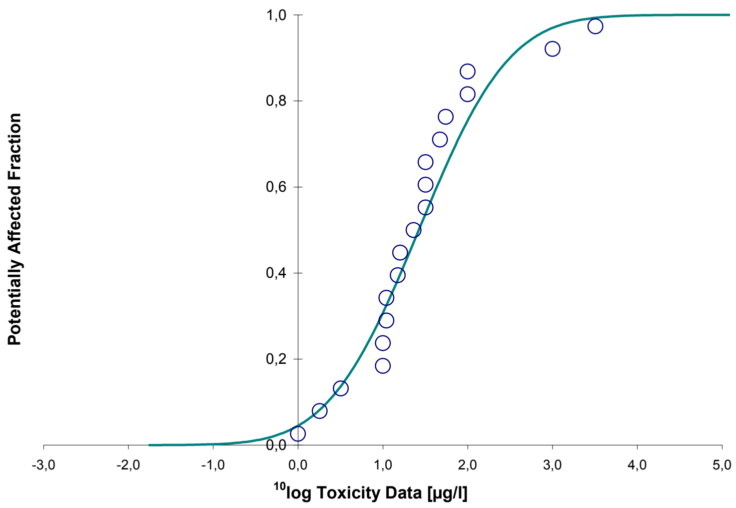

Figure 8.1: Cumulative frequency distribution of the combined freshwater and saltwater data set used for the derivation of the 5th-percentile cut-off value by the method of Aldenberg and Jaworska [11]

Table 8.1: Results of the SSD calculation (NOEC data; n=19)

		90 % Confidence Interval	
Data set	**5-Percentile Cut-Off Value (50% confidence)**	**5P-COV (95% conf.)**	**5P-COV (5% conf.)**
NOECs highlighted bold in table 6.1	1.05 µg/l	0.25 µg/l	2.79 µg/l

In order to derive the PNEC (≈ Quality Standard) it is suggested in the TGD to divide the 5-percentile cut off value by an appropriate assessment factor between 1 and 5, reflecting further uncertainties identified.

The exact value of the AF must depend on an evaluation of the uncertainties around the derivation of the 5th percentile. As a minimum, the following points have to be considered when determining the size of the assessment factor:

- The overall quality of the database and the endpoints covered, e.g., if all the data are generated from "true" chronic studies (e.g., covering all sensitive life stages).

  Many of the studies included in the SSD are no "true" chronic studies covering all sensitive life stages of the species examined. Exceptions are the algae studies, the life cycle test of *Cyprinodon variegatus* and the study with the meiobentic nematode species.

- The diversity and representativity of the taxonomic groups covered by the database, and the extent to which differences in the life forms, feeding strategies and trophic levels of the organisms are represented.

  The database is rather comprehensive. Although some important (marine) taxonomic groups are not covered, the species requirements of the TGD are fulfilled. A broad spectrum of life forms and feeding strategies is covered. Trophic levels from primary producers to secondary consumers are included.

- Knowledge on presumed mode of action of the chemical (covering also long-term exposure).

  It is widely believed that pentachlorophenol affects by uncoupling mitochondrial oxidative phosphorylation, thereby causing accelerated aerobic metabolism and increasing heat production. It causes loss of membrane electrical resistance. [13] This mode of action explains why pronounced differences in the susceptibility of sensitive representatives of different taxonomic groups do apparently not occur.

- Statistical uncertainties around the 5th percentile estimate, e.g., reflected in the goodness of fit or the size of confidence interval around the 5th percentile, and consideration of different levels of confidence (e.g. by a comparison between the 5% of the SSD (50%) with the 5% of the SSD (95%)).

  The fit of the log-transformed data to the assumed normal distribution is very good. The spread of the 5th-percentile estimate between the 5% and the 95% confidence level is ≈11 (i.e. the figure of the 5th-percentile 95% confidence level is eleven times lower than the figure of the respective 5% confidence level).

- Comparisons between field and mesocosm studies, where available, and the 5th percentile and mesocosm/field studies to evaluate the laboratory to field extrapolation.

  Field or meso/microcosm data are not available.

On the one hand, the database used for the calculation of the 5-percentile cut-off value does not comprise very many "true" chronic studies covering all sensitive life stages of the species examined. Further, the spread between the 5% and 95% confidence levels of the 5th-percentile is larger than one order of magnitude (≈11) and therefore considered quite high. On the other hand the mode of action of the chemical suggests that pronounced differences in the susceptibility of sensitive representatives of different taxonomic groups need not to be anticipated (see table 6.1, with the exception of *Lemna* and *Culex* the NOECs of the most sensitive representatives of the different taxonomic groups differ not more than approximately one order of magnitude).

Based on the above considerations an assessment factor of 3 is suggested for the derivation of the water quality standard.

$QS_{water.SSD}$ = 5th-percentile cut-off (1.05 µg/l) / AF (3) = 0.35 µg Pentachlorophenol /l

It is suggested to use the value derived by statistical extrapolation according to the method of Aldenberg & Jaworska as water quality standard as this value is based on a rather broad range of NOEC data covering 10 different taxonomic groups.

8.2 Quality standard for sediment

The log Kp_{susp} of pentachlorophenol is 1.85 – 3.72 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 $PNEC_{sediment}$ (≈ $QS_{sediment}$) 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. As the log Kow of pentachlorphenol is < 5 at pH values occurring in the environment (see section 5 of this data sheet) exposure routes other than direct uptake via the water phase need not to be considered.

Depending on the prevailing pH, a certain percentage of pentachlorophenol is dissociated under environmental conditions (pKa ≈5). Hence, the sorption to organic matter in sediment is also pH dependent (i.e. the Koc value increases when the pH decreases). It is therefore suggested to use a Koc from the lower end of the reported range for the calculation of the partition coefficients required for the derivation of the sediment quality standard (i.e. Kp_{susp} and $K_{SPM\text{-}water}$). This is considered a worst case approach since with rising Koc the amount of pentachlorophenol partitioned to sediment in a sediment – water system gets higher at equilibrium. A Koc of 3400 l/kg is suggested for the calculation resulting in a Kp_{susp} of 340 l/kg (see footnote 1).

The $QS_{sediment}$ is calculated as follows:

$$QS_{sed.wet\_weight}\ [mg.kg^{-1}] = \frac{K_{SPM\text{-}water}\ [85\ m^3/m^3]}{bulk\ density_{SPM.wet}\ [1150\ kg/m^3]} * 1000 * QS_{water}\ [mg/l]$$

with:
$K_{SPM\text{-}water}$ = f_{solid} (0.1) * Kp_{susp} (340 l/kg) / 1000 * RHO_{solid} (2500 kg/m^3) = 85 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} = 0.00035 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):

$QS_{sediment}$	25.9 µg/kg (wet wt)	119 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

Pentachlorophenol is subject to bioaccumulation with reported BCF values (fish) up to 1000 (see section 5 of this data sheet). Therefore, the trigger criterion to derive a quality standard referring to the protection of top predators from secondary poisoning is met (see table 8.1 of the final report [4]).

The NOEC of 55 mg/kg food for oral toxicity in rat (see table 6.2) is the lowest value available.. From this $NOEC_{food}$ a $PNEC_{oral}$ is calculated according to the procedure described in section 5.1.4.2 of the final report [4] (based on section 3.8.3.5 of the TGD [3]). The $PNEC_{oral}$ is equivalent to the $QS_{secpois.biota}$.

$PNEC_{oral}$ = $NOEC_{oral}$ (55 (mg/ kg food) / AF (30) = 1.83 mg/kg food

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

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

$QS_{secpois.biota}$ = 1.83 mg Pentachlorophenol / kg food (fish; wet weight)

Pentachlorophenol has been shown to bioaccumulate. Reported BCF_{fish} range up to 1000 although most values are <500. The BCFs reported for invertebrates are in general somewhat lower (up to 400) but for the marine polychaete species *Lanice conchilega* a BCF of 3820 was found whereas for a second polychaete species, *Neanthes virens*, a BCF of only 280 has been observed [15, 16]. The huge difference in bioconcentratation between these two species cannot be explained on the basis of the information provided in the references.

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. However, according to the Dutch "Criteria Document Chlorphenols" (RIVM 1991 [8], cited in [10]) biomagnification does not play a significant role in the aquatic environment.

The water concentration that corresponds to the $QS_{secpois.biota}$ is therefore calculated as follows:

$QS_{secpois.water}$ = $QS_{secpois.biota}$ (1.83 [mg Pentachlorophenol /kg prey]) / BCF

It is suggested to use a BCF_{fish} of 770 for the calculation (considered as kind of "realistic worst case", see section 5). This results in:

$QS_{secpois.water}$ = 2.4 µg Pentachlorophenol / l

Thus, the protection of the pelagic community does require a lower quality standard than the protection of top predators from secondary poisoning (i.e. top predators are protected by the QS for freshwater or saltwater).

8.4 Quality standard referring to food uptake by humans

Pentachlorophenol is classified as a category 3 carcinogen and as toxic if swallowed. It further has a BCF > 100. Thus the trigger criteria to derive a quality standard referring to the protection of humans from adverse effects on health due to the ingestion of food from aquatic environments are met (see table 1a of the Manual [4]).

The oral reference dose of **0.03 mg/ kg bw/ day** derived by the U.S.-EPA can be used as a starting point for the assessment since its concept is similar to that of a TDI or ADI (see section 7).

In the Manual (section 4.3.2.6) [4] it is suggested that an ADI/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 2.1 mg pentachlorophenol 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 2.1 mg pentachlorophenol.

$$QS_{hh.food} = \frac{2.1 \text{ mg Endosulfan}}{115\text{g fishery product consumption}} * 1000 \text{ g} = \mathbf{18.26 \text{ mg PCP / kg fishery products}}$$

In the TGD approach for the assessment of secondary poisoning (see sections 4.3.2.5 & 4.3.2.6 of the Manual [4]) it is foreseen to consider bioconcentration and biomagnification as relevant factors affecting body burdens and the PEC, respectively. If no information on BMF values is available, it is proposed in the TGD to use default BMFs for substances with a BCF_{fish} >2000. However, the

BCF of pentachlorophenol remains usually well below this trigger value and further, according to the Dutch "Criteria Document Chlorphenols" (RIVM 1991 [8], cited in [10]) biomagnification does not play a significant role in the aquatic environment.

It is suggested to use a BCF_{fish} of 770 for the calculation (considered as kind of "realistic worst case", see section 5). The water concentration that corresponds to the $QS_{hh.food}$ is therefore calculated as follows:

$$\mathbf{QS_{hh.food.water}} = \frac{QS_{hh.food}\ (18.26\ mg/kg)}{BCF\ (770) * BMF\ (1)} = \mathbf{23.7\ \mu g\ PCP/l}$$

Thus, the protection of the pelagic community does require a by far lower quality standard than the protection of human health against adverse effects due to the ingestion of fishery products.

8.5 Quality standard for drinking water abstraction

Pentachlorophenol is used as a biocide in some Member States while its use is prohibited in others. Hence, the limits set for pesticides in Council Directives 75/440/EEC and 98/83/EC may apply. The imperative A1 value referring to drinking water abstraction by simple treatment is 1 µg/l for the total amount of pesticides (Council Directive 75/440/EEC). The drinking water standard set in CD 98/83/EC is 0.1 µg/l for individual pesticides.

The DWS is a limit value never to be exceeded at the tap. The MAC-QS (ECO) derived for the protection of the freshwater community (1 µg/l) may therefore not suffice to allow for compliance with the DWS if only simple purification techniques (category A1 of CD 75/440/EEC, i.e. filtration and disinfection) are used for the abstraction of drinking water from surface water bodies according to Art. 7 of the WFD.

An assessment by experts in drinking water technology with regard to the question which fraction of the amount of pentachlorophenol present in raw water can be removed by usual simple treatment procedures might be helpful. If the respective fraction were known, this figure could be used together with the drinking water standard to set the maximum acceptable concentration in surface water bodies designated for the **a**bstraction of **w**ater **i**ntended for **h**uman **c**onsumption (AWIHC).

MAC-QS (AWIHC) = DWS (0.1 µg/l) / fraction not removable by simple treatment

8.6 Overall quality standard

It is suggested to adopt the quality standard of 0.35 µg PCP/l derived for the protection of the pelagic communities in inland waters as well as transitional, coastal and territorial waters as overall annual average quality standard. It covers the protection of human health against adverse effects due to the ingestion of fishery products and the protection of predators against secondary poisoning as well.

In areas designated for the abstraction of water intended for human consumption in accordance with Art. 7 of the WFD a specific MAC-QS (AWIHC) should apply. This standard may be derived as proposed in section 8.5.

9 References

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