Summary report for Formaldehyde

SUMMARY

Substance name	**Formaldehyde**	
CAS-number	**50-00-0**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	0.004 mg/L	0.042 mg/L
SSD	**0.13 mg/L**	**1.3 mg/L**
Sediment	**/**	**/**
Remarks	**SSD method was selected due to the large number of data**	

*** marine and freshwater data**

1. IDENTITY

Substance name	Formaldehyde
CAS-number	50-00-0
Substance group	Organics
Synonyms	/
Molecular formula	CH_2O
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	30.0262	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	5.19E+05	SRC exp.
Water Solubility (mg/L)	400 000	SRC exp.
Log Kow	0.4	SRC exp.
Log Koc	0.0	SRC est.
Log K_{SED}	-1.3	est. from Koc - 5% OC
Henry-coefficient (Pa-m3/mol)	0.034	SRC exp.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	3	SRC est.
(Aerobic bio)degradation	Readily biodegradable	HSDB, SRC

4. ECOTOXICITY

4.1.1 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Chlorococcales (alg)	1d-EC50	6.5			RIVM database	1	F				
Scenedesmus quadricauda (alg)	1d-EC50	14.7			RIVM database	1	F				
Invertebrates											
Artemia sp (cru)	2d-LC50	1072.4			RIVM database	9	M				
Ceriodaphnia dubia (cru)	2d-EC50	13			RIVM database	1	F				
Cypridopsis sp (cru)	4d-EC50	**0.42**			RIVM database	1	F	10*	100	**42**	**4.2**
Crangon crangon (cru)	2d-LC50	574.5			RIVM database	2	M				
Daphnia magna (cru)	1d-EC50	5			RIVM database	7	F				
Daphnia pulex (cru)	2d-EC50	5.8			RIVM database	1	F				
Macrobrachium rosenbergii (cru)	1d-LC50	423			RIVM database	1	M				
Metapenaeus ensis (cru)	1d-LC50	633			RIVM database	1	M				
Palaemonetes kadiakensis (cru)	4d-EC50	186			RIVM database	1	F				
Penaeus duorarum (cru)	4d-LC50	81.6			RIVM database	6	M				
Penaeus japonicus (cru)	1d-LC50	136			RIVM database	1	M				
Penaeus monodon (cru)	1d-LC50	168			RIVM database	1	M				
Penaeus penicillatus (cru)	1d-LC50	275			RIVM database	1	M				
Penaeus semisulcatus (cru)	1d-LC50	184			RIVM database	1	M				
Uca pugilator (cru)	4d-LC50	332			RIVM database	2	M				
Corbicula manilensis (mol)	4d-LC50	109.4			RIVM database	2	F				
Corbicula sp (mol)	4d-EC50	50.4			RIVM database	1	F				
Crassostrea virginica (mol)	2d-EC50	0.93			RIVM database	4	M				
Helisoma sp (mol)	4d-EC50	37.2			RIVM database	1	F				
Notonecta sp (ins)	4d-EC50	334			RIVM database	1	F				
Fish											
Ameiurus melas (pis)	4d-LC50	39.2			RIVM database	2	F				
Anguilla japonica (pis)	2d-LC50	400			RIVM database	1	F				
Anguilla rostrata (pis)	4d-LC50	183.8			RIVM database	3	F				
Carassius auratus (pis)	1d-LC50	35			RIVM database	1	F				
Chanos chanos (pis)	4d-LC50	232			RIVM database	1	M				

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Danio rerio (pis)	4d-LC50	41			RIVM database	1	F				
Gambusia affinis (pis)	4d-LC50	113.4			RIVM database	4	F				
Ictalurus punctatus (pis)	4d-LC50	31.3			RIVM database	18	F				
Lepomis cyanellus (pis)	4d-LC50	109.4			RIVM database	2	F				
Lepomis macrochirus (pis)	4d-LC50	28.1			RIVM database	19	F				
Leuciscus idus melanotus (pis)	4d-LC50	22			RIVM database	3	F				
Menidia menidia (pis)	4d-LC50	69			RIVM database	1	M				
Micropterus dolomieui (pis)	4d-LC50	86.01			RIVM database	2	F				
Micropterus salmoides (pis)	4d-LC50	90.4			RIVM database	2	F				
Morone saxatilis (pis)	3d-LC50	15			RIVM database	22	F				
	4d-LC50	12.4			RIVM database	4	M				
Oncorhynchus mykiss (pis)	4d-LC50	61.4			RIVM database	28	F				
Oryzias latipes (pis)	2d-LC50	55.2			RIVM database	3	F				
Pimephales promelas (pis)	4d-LC50	24.1			RIVM database	1	F				
Platichthys flesus (pis)	2d-LC50	181.7			RIVM database	2	M				
Salmo salar (pis)	4d-LC50	109.4			RIVM database	2	F				
Salmo trutta (pis)	2d-LC50	185			RIVM database	1	F				
Salvelinus fontinalis (pis)	2d-LC50	157			RIVM database	1	F				
Salvelinus namaycush (pis)	4d-LC50	63.2			RIVM database	3	F				
Tanichthys albonubes (pis)	2d-LC50	2.3			RIVM database	4	F				
Tilapia nilotica (pis)	4d-LC50	162.8			RIVM database	2	F				
Trachinotus carolinus (pis)	4d-LC50	71.1			RIVM database	4	M				
Other											
Saprolegnia sp. (fun)			15-60min-LOEC**	300	EPA	1	F				

*** a factor of 10 was thought sufficient due to the large number of data**

**** additional data**

Deriving MAC-QS: 3.96 mg/L (AF=3; 49 species from 5 major taxonomic groups from 3 trophic levels) → 1.3 mg/L
Deriving AA-QS: 1.3/10 = 0.13 mg/L

Input toxicity data

Data no.	Toxicity data	Label
1	6,5	alg-RIVM
2	14,7	alg-RIVM
3	1072,4	cru-RIVM
4	13	cru-RIVM
5	0,42	cru-RIVM
6	574,5	cru-RIVM
7	5	cru-RIVM
8	5,8	cru-RIVM
9	423	cru-RIVM
10	633	cru-RIVM
11	186	cru-RIVM
12	81,6	cru-RIVM
13	136	cru-RIVM
14	168	cru-RIVM
15	275	cru-RIVM
16	184	cru-RIVM
17	332	cru-RIVM
18	109,4	mol-RIVM
19	50,4	mol-RIVM
20	0,93	mol-RIVM
21	37,2	mol-RIVM
22	334	ins-RIVM
23	39,2	pis-RIVM
24	400	pis-RIVM
25	183,8	pis-RIVM
26	35	pis-RIVM

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Input toxicity data

Data no.	Toxicity data	Label
27	232	pis-RIVM
28	41	pis-RIVM
29	113,4	pis-RIVM
30	31,3	pis-RIVM
31	109,4	pis-RIVM
32	28,1	pis-RIVM
33	22	pis-RIVM
34	69	pis-RIVM
35	86,01	pis-RIVM
36	90,4	pis-RIVM
37	15	pis-RIVM
38	12,4	pis-RIVM
39	61,4	pis-RIVM
40	55,2	pis-RIVM
41	24,1	pis-RIVM
42	181,7	pis-RIVM
43	109,4	pis-RIVM
44	185	pis-RIVM
45	157	pis-RIVM
46	63,2	pis-RIVM
47	2,3	pis-RIVM
48	162,8	pis-RIVM
49	71,1	pis-RIVM
50		
51		
52		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	1,78E0	mean of the log toxicity values
s.d.	7,14E-1	sample standard deviation
n	4,90E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	2,001E0	3,012E-1	lower estimate of the HC5
HC5	3,959E0	5,976E-1	median estimate of the HC5
UL HC5	6,798E0	8,324E-1	upper estimate of the HC5
sprHC5	3,398E0	5,312E-1	spread of the HC5 estimate

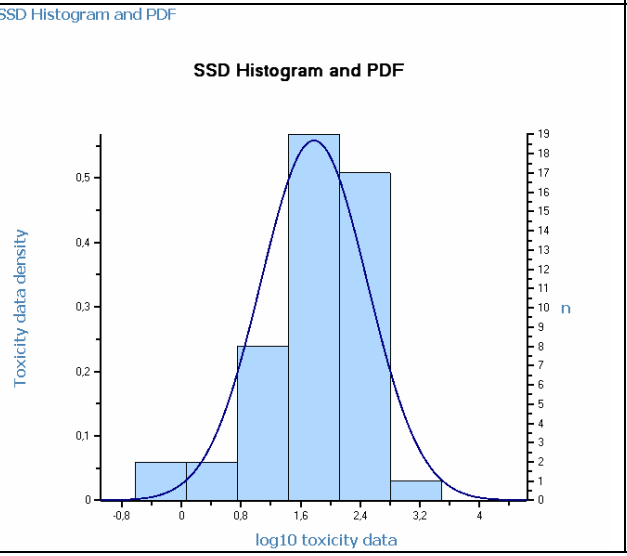
FA At HC5 results

Name	Value	Description
FA lower	2,20	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	8,03	95% confidence limit of the FA at standardised median logHC5

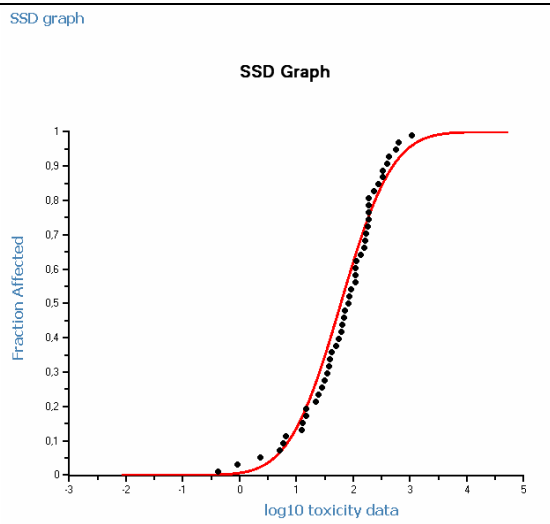
HC50 results

Name	Value	log10(Value)	Description
LL HC50	4,064E1	1,609E0	lower estimate of the HC50
HC50	6,028E1	1,780E0	median estimate of the HC50
UL HC50	8,940E1	1,951E0	upper estimate of the HC50
sprHC50	2,200E0	3,424E-1	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph

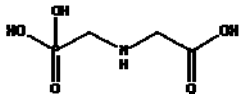


Summary report for Glyphosate

SUMMARY

Substance name	**Glyphosate**	
CAS-number	**1071-83-6**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**20 µg/L**	**200 µg/L**
Sediment	**/**	**/**
Remarks	**data from dossier**	

1. IDENTITY

Substance name	Glyphosate
CAS-number	1071-83-6
Substance group	Herbicide-Phosphonoglycine
Synonyms	/
Molecular formula	$C_3H_8NO_5P$
Structural formula	

Substance name	Aminomethylphosphonic acid*
CAS-number	/
Substance group	Metabolite
Synonyms	AMPA
Molecular formula	/
Structural formula	/

*** Metabolite AMPA is not relevant due to the low toxicity**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**		**ref.**
Substance	Glyphosate	AMPA	
Molecular weight (g/mol)	169	/	dossier
Vapour Pressure (Pa)	1.31E-05	/	dossier
Water Solubility (mg/L)	10500	/	dossier
Log Kow	-3.2	/	dossier
Log Koc	2.9-4.8 → 3.86	3.06-4.39 → 3.73	dossier
Log K_{SED}	1.6-3.5 → 2.56	1.76-3.09 → 2.43	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	2.10E-07	/	dossier
pKa	5.73	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic			**ref.**
Substance	Glyphosate	AMPA	
BCF	Not relevant	/	dossier
(Aerobic bio)degradation	Not biodegradable (degradation in days), hydrolytically stable	/	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity Glyphosate

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Unknown species			(EC50) → extrapolated NOEC=EC50/3	(0.6) → 0.6/3=**0.2**	PPP dossier	MS	F	1	10	**200***	**20**
Daphnids											
Daphnia sp.	EC50	40	NOEC	9.0	PPP dossier	MS	F				
Fish											
Unknown species	EC50	38	NOEC	25.7	PPP dossier	MS	F				
Other											
Lemna sp.			(EC50) → extrapolated NOEC=EC50/3	(25.5) → 25.5/3=8.5	PPP dossier	MS	F				

*** MAC-QS derived from NOEC (AF = 1) is protective for algae, which are the most sensitive species**

4.1.2 Aquatic toxicity AMPA

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Unknown species			(EC50)	(89.9)	PPP dossier	MS	F				
Daphnids											
Daphnia sp.	EC50	>180			PPP dossier	MS	F				
Fish											
Unknown species	EC50	>180			PPP dossier	MS	F				

Aquatic toxicity of the metabolite AMPA is between 10-100 mg/L or >100 mg/L → metabolite is not relevant due to the low toxicity

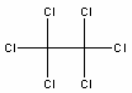
Summary report for Hexachloroethane

SUMMARY

Substance name	**Hexachloroethane**	
CAS-number	**67-72-1**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	7.1 µg/L	71 µg/L
SSD	**24 µg/L**	**240 µg/L**
Sediment	**/**	**/**
Remarks	**MPC= 83 µg/L**	**/**

*** marine and freshwater data**

1. IDENTITY

Substance name	Hexachloroethane
CAS-number	67-72-1
Substance group	Chlorinated alkanes
Synonyms	
Molecular formula	C_2Cl_6
Structural formula	

2. FHYSICO-CHEMICAL CHARACTERISTICS

Property	**values**	**ref.**
Molecular weight (g/mol)	236.74	ChemFinder
Vapour Pressure (Pa)	39.5	SRCexp
Water Solubility (mg/L)	50	SRCexp
Log Kow	4.1	SRCexp
Log Koc	2.35	SRCest
Log K_{SED}	1.05	Est. 0.05% OC
Henry-coefficient (Pa-m3/mol)	394	SRCexp
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	308	SRCest
(Aerobic bio)degradation	recalcitrant	SRCest

4. ECOTOXICITY

4.1 Aquatic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum (alg)	4d-EC50	87			RIVM database	1	F				
			4d-NOEC	<5,6			F				
Skeletonema costatum (alg)	4d-EC50	8.57			RIVM database	1	M				
Invertebrates											
Americamysis bahia (cru)	4d-LC50	0.94			RIVM database	1	M				
Aplexa hypnorum(mol)	4d-LC50	2.1			RIVM database	1	F				
Arbacia punctulata (ech)	2d-EC50	8.9			RIVM database	2	F				
Ceriodaphnia reticulate (cru)	2d-EC50	4.7			RIVM database	2	F				
Ceriodaphnia dubia (cru)	2d-EC50	4.3			RIVM database	1	F				
Daphnia magna (cru)	2d-EC50	2.8			RIVM database	>3	F				
Daphnia pulex (cru)	2d-EC50	11.4			RIVM database	1	F				
Orconectes immunis (cru)	4d-EC50	2.5			RIVM database	3	F				
Simocephalus vetulus (cru)	2d-EC50	5.8			RIVM database	1	F				
Tanytarsus dissimilis (ins)	3d-EC50	1.4			RIVM database	3	F				
Fish					RIVM database						
Carassius auratus (pis)	4d-EC50	1.6			RIVM database	3	F				
Cyprinodon variegates (pis)	4d-LC50	2.4			RIVM database	1	F				
			4d-NOEC	1	RIVM database		F		100		10
Gambusia affinis (pis)	4d-LC50	1.4			RIVM database	1	F				
Ictalurus punctatus (pis)	4d-LC50	1.9			RIVM database	6	F				
Lepomis macrochirus (pis)	4d-LC50	0.93			RIVM database	3	F				
Oncorhynchus mykiss (pis)	8d-LC50	**0.71**			RIVM database	3	F	10*	100	**71**	**7.1**
Pimephales promelas (pis)	4d-LC50	1.3			RIVM database	7	F				
Other											
Rana catesbeiana (amp)	4d-LC50	2.8			RIVM database	3	F				

*** a factor of 10 was thought sufficient due to the large number of data**

Deriving MAQ-QS: 0.47 mg/L (AF=2; 20 species from 7 major taxonomic groups from 3 trophic levels) → 0.24 mg/L
AA-QS: 0.24/10 = 0.024 mg/L

Input toxicity data

Data no.	Toxicity data	Label
1	87	alg-RIVM
2	8,6	alg-RIVM
3	0,94	cru-RIVM
4	2,1	mol-RIVM
5	8,9	ech-RIVM
6	4,7	cru-RIVM
7	4,3	cru-RIVM
8	2,8	cru-RIVM
9	11,4	cru-RIVM
10	2,5	cru-RIVM
11	5,8	cru-RIVM
12	1,4	ins-RIVM
13	1,6	pis-RIVM
14	2,4	pis-RIVM
15	1,4	pis-RIVM
16	1,9	pis-RIVM
17	0,93	pis-RIVM
18	0,71	pis-RIVM
19	1,3	pis-RIVM
20	2,8	amp-RIVM
21		
22		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	4,81E-1	mean of the log toxicity values
s.d.	4,85E-1	sample standard deviation
n	2,00E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	2,090E-1	-6,798E-1	lower estimate of the HC5
HC5	4,693E-1	-3,285E-1	median estimate of the HC5
UL HC5	8,168E-1	-8,790E-2	upper estimate of the HC5
sprHC5	3,907E0	5,919E-1	spread of the HC5 estimate

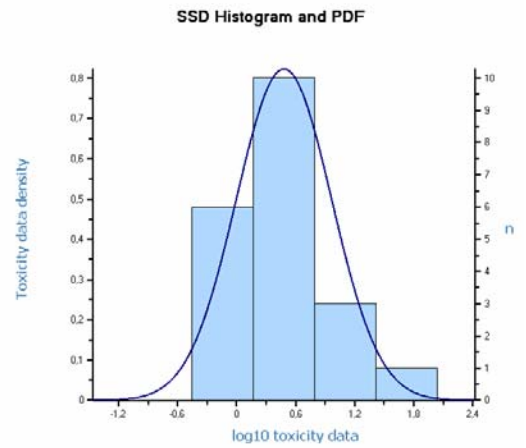
FA At HC5 results

Name	Value	Description
FA lower	1,28	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	13,98	95% confidence limit of the FA at standardised median logHC5

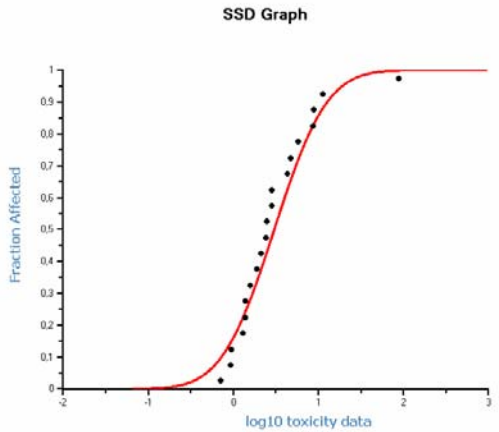
HC50 results

Name	Value	log10(Value)	Description
LL HC50	1,968E0	2,939E-1	lower estimate of the HC50
HC50	3,029E0	4,813E-1	median estimate of the HC50
UL HC50	4,663E0	6,687E-1	upper estimate of the HC50
sprHC50	2,370E0	3,747E-1	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph



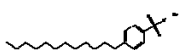
Summary report for LAS

SUMMARY		
Substance name	**LAS**	
CAS-number	**42615-29-2**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**0.25 mg/L $C_{11.6}$****	**2.5 mg/L $C_{11.6}$**
Sediment	**/**	**/**
Remarks	**Data from RIVM Report*** **AA-QS=MPC** **MAC-QS=MPC*10**	

*** Feijtel, T.C.J., Plassche, E.J., Enviromental Risk Characterisation of 4 Major Surfactants Used in the Netherlands, RIVM report 679101 025, 1995**

****800 data. PNEC(SSD) was overrun by results of field studies**

1. IDENTITYž

Substance name	Linear alkyl benzenesulfonate C_{10}-C_{13} (mean $C_{11.6}$) example: Dodecyl benzenesulfonic acid, sodium salt C_{12}
CAS-number	25155-30-0
Substance group	Organics
Synonyms	Surfactant
Molecular formula	$C_{12}H_{25}$-$C_6H_4SO_3$-Na^+ (LAS: $RC_6H_4SO_3$-Na^+)
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	values	ref.
Molecular weight (g/mol)	348.47507	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	3.0E-13	SRC est.
Water Solubility (mg/L)	800	SRC exp.
Log Kow	3.0	SRC est.
Log Koc	4.23	SRC est.
Log K_{SED}	2.92	est. from K_{OC}-5% OC
Henry-coefficient (Pa-m3/mol)	6.1E-12	SRC est.
pKa	/	/

1. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		ref.
BCF	71	SRCest
(Aerobic bio)degradation	Ready biodegradable	HSDB

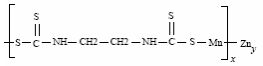
Summary report for Mancozeb

SUMMARY

Substance name	**Mancozeb**		**ETU***	
CAS-number	**8018-01-7**		**/**	
Proposed Quality Standard	**Freshwater**		**Freshwater**	
	AA-QS	**MAC-QS**	**AA-QS**	**MAC-QS**
Water **Sum of ethylene bisdithiocarbamates (metiram and mancozeb)**	**0.07 µg/L**	**0.7 µg/L**	**200 µg/L**	**325 µg/L**
Sediment	**/**	**/**	**/**	**/**
Remarks	**data from dossier; metiram and mancozeb has the same mode of action**			

*** QS for ETU is derived also in Summary report for Metiram**

1. IDENTITY

Substance name	Mancozeb
CAS-number	8018-01-7
Substance group	Fungicide-Dithiocarbamate, Inorganic-Zinc
Synonyms	/
Molecular formula	$(C_4H_6MnN_2S_4)_x(Zn)_y$
Structural formula	 Mancozeb is a polymeric complex of the monomer illustrated which contains 20% manganese and 2.5% zinc

Substance name	Ethylene-thiourea, Ethylene-urea
CAS-number	/
Substance group	Metabolite
Synonyms	ETU
Molecular formula	/
Structural formula	/

Substance name	Ethyleneurea*
CAS-number	/
Substance group	Metabolite
Synonyms	EU
Molecular formula	/
Structural formula	/

***Metabolite is not relevant due to the lack of toxicity data**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**		**ref.**
Substance	Mancozeb	ETU	
Molecular weight (g/mol)	271.3	/	dossier
Vapour Pressure (Pa)	1.33E-05	/	dossier
Water Solubility (mg/L)	2-20	/	dossier
Log Kow	1.80	-0.82	dossier
Log Koc	2.56-3.37 → 3.00	1.53-2.16 → 1.85	dossier
Log K_{SED}	1.26-2.07 → 1.70	0.23-0.86 → 0.55	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	<5.9E-04	/	dossier
pKa	10.3	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic			**ref.**
Substance	Mancozeb	ETU	
BCF	No	/	dossier
(Aerobic bio)degradation	Not readily degradable, rapid hydrolytic degradation (days)	/	dossier

2. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
/											
Daphnids											
Daphnia magna	2d-EC50	**0.073**			PPP dossier	MS	F	100	1000	**0.73**	**0.073**
Fish											
Rainbow trout	4d-LC50	0.074			PPP dossier	MS	F				

4.1.2 Aquatic toxicity metabolite ETU

Species	Endpoint-chronic	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Pseudokirchneriella subcapitata	3d-EC50	93.8	(3d-NOECextrapolated)	(NOEC→ 93.8/3= 31.3)	PPP dossier						
Pseudokirchneriella subcapitata	4d-EC50	>119	4d-NOEC	119	PPP dossier						
Daphnids											
Daphnia magna	2d-EC50	**32.5**	21d-NOEC	**2.0**	PPP dossier			100	10	**325**	**200**
Fish											
Rainbow trout	4d-LC50 4d-NOEC	>122 122			PPP dossier						
Amphibia											
Xenopus laevi			28d-NOEC	10	PPP dossier						

Remark F.Balk: The most sensitive organisms for this substance are nitrifying bacteria (threshold ≤ 1 mg/l). These have not been tested here.

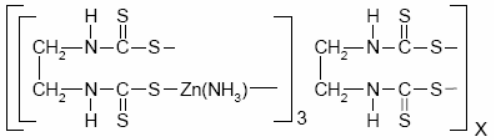
Summary report for Metiram

SUMMARY

Substance name	**Metiram**		**ETU***	
CAS-number	**9006-42-2**		**/**	
Proposed	**Freshwater**		**Freshwater**	
Quality Standard	**AA-QS**	**MAC-QS**	**AA-QS**	**MAC-QS**
Water **Sum of ethylene bisdithiocarbamates (metiram and mancozeb)**	0.063 µg/L **0.07 µg/L**	0.63 µg/L **0.7 µg/L**	**200 µg/L**	**325 µg/L**
Sediment	**/**	**/**	**/**	**/**
Remarks	**data from dossier;** **metiram and mancozeb has the same mode of action**			

*** QS for ETU is derived also in Summary report for Mancozeb**

1. IDENTITY

Substance name	Metiram
CAS-number	9006-42-2
Substance group	Fungicide-Dithiocarbamate, Inorganic-Zinc
Synonyms	/
Molecular formula	$(C_{16}H_{33}N_{11}S_{16}Zn_3)_x$
Structural formula	

Substance name	Ethylene-thiourea, EBIS and Carbimid*
CAS-number	/
Substance group	Metabolites
Synonyms	ETU
Molecular formula	/
Structural formula	/

*** Metabolitesis EBIS and Carbimid are not relevant due to the lack of toxicity data**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**		**ref.**
Substance	Metiram	ETU	
Molecular weight (g/mol)	1088.63	/	dossier
Vapour Pressure (Pa)	<1E-05	/	dossier
Water Solubility (mg/L)	<2.0	/	dossier
Log Kow	1.8	-0.82	dossier
Log Koc	No	1.53-2.16 → 1.85	dossier
Log K_{SED}	/	0.23-0.86 → 0.55	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	<0.0054	/	dossier
pKa	No	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic			**ref.**
Substance	Metiram	ETU	
BCF	No (log Kow<3)	/	dossier
(Aerobic bio)degradation	Not biodegradable, hydrolytic degradation (days-weeks)	/	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity Metiram

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Pseudokirchneriella subcapitata	3d-EC50	**0.063**	(3d-NOEC extrapolated)	(NOEC→ 0.063/3=0.021)	PPP dossier	MS	F	100	1000	**0.63**	**0.063**
Invertebrates											
Daphnia magna	2d-LC50	0.110	21d-NOEC	0.0043	PPP dossier	MS	F		10		0.43*
Chironomus riparius			28d-NOEC	0.22	PPP dossier	MS	F				
Fish											
Rainbow trout	96h-LC50	0.333	28d-NOEC	0.022	PPP dossier	MS	F				

*** Acute/chronic ration for Daphnia magna is 26, and for trout 15 → AF of 10 for A/C seems insufficient. Thus EC50 with AF 1000 is applied**

4.1.2 Aquatic toxicity metabolite ETU

Species	Endpoint-chronic	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Pseudokirchneriella subcapitata	3d-EC50	93.8	(3d-NOECextrapolated)	(NOEC→ 93.8/3= 31.3)	PPP dossier						
Pseudokirchneriella subcapitata	4d-EC50	>119	4d-NOEC	119	PPP dossier						
Daphnids											
Daphnia magna	2d-EC50	**32.5**	21d-NOEC	**2.0**	PPP dossier			100	10	**325**	**200**
Fish											
Rainbow trout	4d-LC50 4d-NOEC	>122 122			PPP dossier						
Amphibia											
Xenopus laevi			28d-NOEC	10	PPP dossier						

Remark F.Balk: The most sensitive organisms for this substance are nitrifying bacteria (threshold ≤ 1 mg/l). These have not been tested here.

Summary report for Molybdenum

SUMMARY

Substance name	**Molybdenum**	
CAS-number	**7439-98-7**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	**24 µg/L**	**200 µg/L**
Sediment EP	**14 mg/kg dw**	**110 mg/kg dw**
Remarks	**Total RA for water. Total RA for sediment.**	

*** data for fresh and marine water**

1. IDENTITY

Substance name	Molybdenum
CAS-number	7439-98-7
Substance group	metals
Synonyms	/
Molecular formula	Mo
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	95.94	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	2.93 (10% OC) → 2.754 (5% OC)	a
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

4.1 Aquatic toxicity data from RIVM database[a] and EPA Ecotox database[b]

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Glenodinium halli (Dinoflagellate)			2d-NOEC	4.5	EPA Ecotox	3	M				
Gymnodinium splendens (Dinoflagellate)			2d-NOEC	5.5-300	EPA Ecotox	>2	M				
Thalassiosira pseudonana (Diatom)			2d-NOEC	6.3-100	EPA Ecotox	>2	M				
Gymnodinium splendens (Dinoflagellate)	2d-LC50	**20**			EPA Ecotox	8	M	100		**200**	
Thalassiosira pseudonana (Diatom)	2d-LC50	82			EPA Ecotox	>6	M				
Invertebrates											
Daphnia magna (cru)			28d-NOEC	**1.2**	EPA Ecotox	2	F		50		**24**
Americamysis bahia (cru)	4d-LC50	149			EPA Ecotox	2	M				
Daphnia magna (cru)	4d-LC50	34.3			EPA Ecotox	2	F				
Fish											
Oncorhynchus mykiss	4d-LOEC/3 = NOEC	707/3 = 236[c]			EPA Ecotox	2	F				
Pimephales promelas	4d-LC50	70[d]			EPA Ecotox	4	F				
Oncorhynchus mykiss	4d-LC50	1028			EPA Ecotox	2	F				
Other											
/											

a RIVM e-toxBase, Bilthoven, 2004
b http://www.epa.gov/ecotox/
c additional data
d pH dependent

4.2 Sediment toxicity

Equilibrium partitioning method-calculated with log Ksed = 2.754
AA-QS sed = 567 L/kg*0.024 mg/L = 13.6 mg/ kg dw
MAC-QS sed = 567 L/kg*0.200 mg/L = 113 mg/kg dw

Summary report for n-Hexane

SUMMARY

Substance name	**n-Hexane**	
CAS-number	**110-54-3**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	**0.12 µg/L**	**1.2 µg/L**
Remarks	AA-QS determined from acute EC50 due to the lack of long term NOEC data	

*** marine and freshwater data**

1. IDENTITY

Substance name	n-Hexane
CAS-number	110-54-3
Substance group	Organics
Synonyms	/
Molecular formula	C_6H_{14}
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	86.1766	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	2.01E+04	SRC exp.
Water Solubility (mg/L)	9.5	SRC exp.
Log Kow	3.9	SRC exp.
Log Koc	2.2	SRC est.
Log K_{SED}	0.9	est. from Koc - 5% OC
Henry-coefficient (Pa-m3/mol)	182340	SRC exp.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	201	SRC est.
(Aerobic bio)degradation	Biodegradable	HSDB, SRC

4. ECOTOXICITY

4.1.1 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	REMARKS	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae										
Chlamydomonas angulosa (alg)	3h-EC50	8.1	1980. S, N, 19˚C short duration	RIVM database	1	F				
Chlorella vulgaris (alg)	3h-EC50	12.8	1980. S, N, 19˚C short duration	RIVM database	1	F				
Skeletonema costatum (alg)	8h-EC50	0.3	1977. S, N short duration	RIVM database	1	M				
Plankton (photosyntesis)	4h-EC50	**0.12**	1993. S, N short duration	RIVM database	1	F	100	1000	**1.2**	**0.12**
Invertebrates										
Branchiura sowerbyi (ann)	4d-LC50	3287 *	1988. S, N, 28˚C, >>Sol.	RIVM database	1	F				
Artemia salina (cru)	1d-LC50	1.6	1985, measured, 19˚C	RIVM database	2	M				
Cyclops viridis (cru)	4d-LC50	733 *	1989. S, N, >>Sol.	RIVM database	1	F				
Daphnia magna (cru)	2d-LC50	3.9	1983. S,N, 23˚C	RIVM database	3	F				
Melanoides tuberculata (mol)	4d-LC50	1900 *	1989. N, 27˚C, >>Sol.	RIVM database	1	F				
Brachionus plicatilis (rot)	1d-LC50	154 *	1988. S, N, 25˚C, >>Sol.	RIVM database	1	M				
Brachionus calyciflorus (rot)	1d-LC50	68 *	1992. S, N, 25˚C, >>Sol.	RIVM database	1	F				
Chironomidae (ins)	4d-LC50	595 *	1989. S, N, 27˚C, >>Sol.	RIVM database	1	F				
Fish										
Leuciscus idus melanotus (pis)	2d-LC50	970 *	1978. S, N, >>Sol.	RIVM database	2	F				
Oryzias latipes (pis)	2d-LC50	1000 *	1986. no data, >>Sol.	RIVM database	3	F				
Pimephales promelas (pis)	4d-LC50	2.5	1990. flow-through, 25˚C	RIVM database	1	F				
Tilapia mossambica (pis)	4d-LC50	113 *	1988. S, N, 28˚C, >>Sol.	RIVM database	1	F				

*** rejected:** Water Solubility =9.5 mg/L

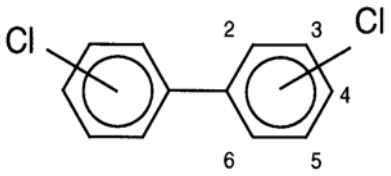
Summary report for Polychlorinated biphenyls

SUMMARY

Substance name	**Polychlorinated biphenyls**	
CAS-number	**1336-36-3**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**/**	**/**
Sediment PCB 118	**0.50 mg/kg ds ***	**/**
PCB 153	**3.0 mg/kg ds ***	**/**
Remarks	**Alternative: integrated measurement of AhR-mediated toxicity in CALUX assay** **No water QS proposed due to extremely low water solubilities. No MAC-QS (short term) for sediment proposed, as the concern in this groups is long-term presence and long-term effects**	

*RIVM report601501 006: Maximum permissible concentrations for polychlorinated biphenyls (Van Wezel et al, 1999)

1. IDENTITY (example)

Substance name	Polychlorinated Biphenyls
CAS-number	1336-36-3
Substance group	Organics
Synonyms	PCBs
Molecular formula	$C_{12}H_6Cl_4$
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES (example)

Property	**values**	**ref.**
Molecular weight (g/mol)	291.99	SRC
Vapour Pressure (Pa)	0.0115	SRC exp.
Water Solubility (mg/L)	0.7	SRC exp.
Log Kow	6.3	SRC exp.
Log Koc	4.65	SRC est.
Log K_{SED}	3.35	est. from Koc - 5% OC
Henry-coefficient (Pa-m3/mol)	19	SRC exp.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT (example)

Characteristic		**ref.**
BCF	57980	SRC est.
(Aerobic bio)degradation	Not degradable	HSDB

4. DERIVATION OF RISK LIMITS FOR PCBs

(RIVM report601501 006: Maximum permissible concentrations for polychlorinated biphenyls (Van Wezel et al, 1999).

PCB	Type of substitution	Routine analysis	Relevant toxicity	Proposed MPC	Remark
#18		yes2			
#28		yes7			
#44		yes2			
#49		yes2			
#52		yes7			
#77	non-ortho	no	AhR-mediated	+	
#101		yes7			
#105	mono-ortho		AhR-mediated	+	
#118	mono-ortho	yes7	AhR-mediated	+	Standard meas. and toxic
#126	non-ortho		AhR-mediated	+	
#138		yes7			
#153	di-ortho	yes7	other	+	Standard meas., persistent, relatively low toxicity
#156	mono-ortho		AhR-mediated		
#157	mono-ortho		AhR-mediated	+	
#169	non-ortho		AhR-mediated	+	
#179		yes2			
#180		yes7			
#187		yes2			

Yes7: included in the package of 7 PCBs analysed traditionally
Yes2: included in a more extended package

Non-ortho and to a lesser extent the mono-ortho PCBs may adopt a coplanar configuration. They are thought to work via the aryl hydrocarbon receptor (AhR), similar to the mechanism of dioxins.
TEFs (Toxic equivalency factors) relate the toxicity of an individual dioxine-like PCB congener to the toxicity of 2,3,7,8-TCDD. TEFs apply to AhR-mediated responses. Thus the concept cannot be applied to toxicity by other mechanisms (e.g., reprotox). TEFs are based upon multiple in vivo and in vitro studies with toxic as well as biochemical's endpoints.
Thus the toxicity of a mixture can be expressed as TEQ by multiplying the concentration of each individual congener with its TEF and summing these products. (This assumes that the combined effects are additive).

For the MPC derivation, TEFs were **not** used. MPCs were derived based on toxicity tests for each specific congener, taking **food chain effects** into account: biomagnification factors and biota-sediment accumulation factors. The environmental fate processes of these substances was taken into account by probabilistic modeling.

- Data were used from direct dose toxicity studies with mammals, bird, bird eggs, fish, fish eggs (diet, gavage, injection).
- The most sensitive tox test was selected.
- Using bioconcentration factors (BCF), biota-to-sediment concentration factors (BSAF) and biomagnification factors (BMF), the results were recalculated to equivalent toxic concentrations in sediment or soil.
- Using probabilistic modeling, the variability in these parameters (BCF, BSAF, BMF, lipid content) was taken into account en used to estimate the 5th percentile of the combined distribution of bird and mammal toxicity data (=MPC per substance)

A so-called '**mixture-MPC**' was derived which is assumed to be protective for the whole mixture of **planar** PCBs. This mixture MPC is expressed on the basis of PCB#118. The toxic potency of each planar congener is expressed as a fraction of the toxicity of PCB#118.
The congener pattern observed in the Netherlands was analyzed and normalized to the concentration of PCB#153 (:high concentrations, analyzed with precision and not metabolized). It was concluded that the PCB patterns are similar for different Dutch locations. However, it should be realized that this pattern is for only one sedimentation area (all of NL) with high atmospheric input.

The procedure is explained in the table which is an extension of Table 6.1 in the RIVM report.

<see table next page>.

The MPC for #118 (25 μg/kg o.c.) is multiplied with the fraction of the total toxicity that is explained by #118 (0.21), this yields the mixture-MPC (5 μg/kg o.c.). Thus 5 μg PCB#188 per kg o.c. in the mixture is thought to be protective for the total mixture of PCB congeners.
So:
If the concentration of PCB#118 in a field sample is below 5 μg/kg o.c., the ecosystem is assumed to be protected for the whole mixture of planar PCBs. Effects of other congeners, or of other types of halogenated aromatics that may act via concentration addition to the planar PCBs (e.g., dioxins), are not incorporated in this mixture MPC.

If the congener pattern deviates from the one listed in the second column of the table above (6.2), the mixture MPC for that location can be calculated in a similar way.

Current status of this approach in The Netherlands
Through contact between Froukje Balk & Theo Traas we learned that:
This approach has been reviewed by the Dutch Health Council. Their main comment was related to the probability distributions (uncertainty), which supposedly resulted in relatively conservative values. No revision was made and no decision for change of the WQS was taken.
Currently the analyses for PCBs is more directed towards the CALUX essay.

Alternative:
This test uses a cell that produces luciferase (the enzyme that makes fireflies light up) when the test substance interact with the cells' aryl-hydrocarbon receptors (AhR) - this type of assay is also referred to as a CALUX® (Chemically-Activated LUciferase gene eXpression cell bioassay system) assay. Unlike normal cells that produce a wide variety of responses when exposed to PCDH's, these cells light up. The amount of light generated is related to the quantity of the chemicals present in the test sample. These measurements are highly correlated to the 2,3,7,8-tetrachlorodibenzo-p-dioxin equivalents (TEQ's) that are typically used to express the concentration of dioxine-like substances.

The price of this bioassay compares well to the costs of the chemical analyses (reported to be 50% of PCB analyses).

Table 6.1 of the RIVM report:
Different steps to derive a mixture-MPC that accounts for the total toxicity of the toxic PCBs

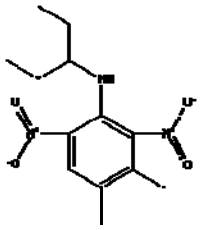
	Environmental Fingerprint		Toxicity					Mixture-MPC
PCB congener	Fraction in pattern ($C_{sed}/C_{sed\text{-}153}$ * 1000) Col.1	Fraction in pattern (% of concentration of planar PCBs) Col.2	MPC (ug/kg o.c.) ≈HC5 Col.4	Distribution, Mean ±sd of log data Col.5	Scaling factor for toxicity Col.6	Fraction/ Scaling Col.7	Fraction/ scaling as % Col.8	MPC (ug/kg o.c.)
77	28±13	4.73	7.2	4.04±1.93	11,000	0.0004	0.06	
105	124±54	21.4	26	1.87±0.28	74	0.29	41	
118	327±94	56.2	25	2.57±0.72	370	0.15	21	Col.8*Col.4 = **5**
126	1.6±0.6	0.28	0.042	0.07±0.88	1.2	0.233	34	
153	*1000*		*151*	*3.86±1.03*				
156	87±43	15.0	55	2.87±0.69	740	0.02	2.8	
157	13±8.0	2.29	2	3.00±0.923	1000	0.0023	0.32	
169	0.33±0.07	0.057	0.83	0.98±0.65	9.5	0.006	0.85	
	(total 585)	*Fraction (100%)*	*HC5 of distribution*		*10(exp.Col.5)*	*Col.2/Col.6 (total 0.70)*	*100%*	

Summary report for Pendimethalin

SUMMARY

Substance name	**Pendimethalin**	
CAS-number	**40487-42-1**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**0.3 µg/L**	**3.0 µg/L**
Sediment EP	**0.21mg/kg dw**	**2.1 mg/kg dw**
Remarks	**data from dossier**	

1. IDENTITY

Substance name	Pendimethalin
CAS-number	40487-42-1
Substance group	Herbicide-2,6-Dinitroaniline
Synonyms	/
Molecular formula	$C_{13}H_{19}N_3O_4$
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	281.3	dossier
Vapour Pressure (Pa)	1.94E-03	dossier
Water Solubility (mg/L)	0.33	dossier
Log Kow	5.2	dossier
Log Koc	3.83-4.47 → 4.15	dossier
Log K_{SED}	2.53-3.17 → **2.85**	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	2.728	dossier
pKa	2.8	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	1000 (daphnia, fish mesocosm study)	dossier
(Aerobic bio)degradation	Not readily biodegradable (degradation in weeks)	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum	5d-EC50	0.006	5d-NOEC	**0.003**	PPP dossier	MS	F	1	10	**3***	**0.3**
Invertebrates											
Daphnia magna	2d-EC50	0.28			PPP dossier	MS	F				
Daphnia magna			21d-NOEC	0.0145	PPP dossier	MS	F				
Chironomidus riparius (sediment organism)			NOEC	0.138		MS	F				
Fish											
Oncorhynchus mykiss	4d-LC50	0.138			PPP dossier	MS	F				
Pimephales promelas			life cycle NOEC	0.006	PPP dossier	MS	F				
Other											
Lemna gibba	14d-EC50	0.012	14d- NOEC	0.006	PPP dossier	MS	F				

*** MAC-QS derived from AA-QS with a factor of 10**

4.2 Sediment toxicity

Equilibrium partitioning (EP) method-calculated with log Ksed = 2.85
AA-QS sed = 708 L/kg*0.0003 mg/L = 0.21 mg/ kg dw
MAC-QS sed = 708L/kg*0.0003 mg/L = 2.1 mg/kg dw

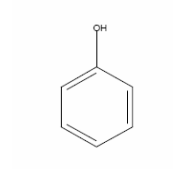
Summary report for Phenol

SUMMARY

Substance name	**Phenol**	
CAS-number	**108-95-2**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water PNEC AF 10	**7.7 µg/L**	**77 µg/L**
Sediment	**/**	**/**
Remarks	**EU RAR* data: AA-QS=PNEC MAC-QS=PNEC*10**	

***** EU RISK ASSESSMENT Report, **Draft** Report, PHENOL, 2002, Germany

1. IDENTITY

Substance name	Phenol
CAS-number	108-95-2
Substance group	Organics
Synonyms	/
Molecular formula	C_6H_6O
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	94.11	RAR
Vapour Pressure (Pa)	200	RAR
Water Solubility (mg/L)	84000	RAR
Log Kow	1.47	RAR
Log Koc	1.92	RAR
Log K_{SED}	0.62	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	0.022	RAR
pKa	9.89	RAR

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	17.5 (fish)	RAR
(Aerobic bio)degradation	Readily biodegradable, hydrolytically stable	RAR

Summary report for Propylene urea

SUMMARY

Substance name	**Propylene urea**	
CAS-number	**/**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**≥10 µg/L (low toxicity)***	**≥100 µg/L (low toxicity)***
Sediment	**/**	**/**
Remarks	**data from dossier**	

*** Due to rapid degradation it is unlikely for the Propylene urea to occur in water**

1. IDENTITY

Substance name	Propylene urea
CAS-number	/
Substance group	Metabolite of Propineb
Synonyms	PU
Molecular formula	/
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	/	dossier
Vapour Pressure (Pa)	/	dossier
Water Solubility (mg/L)	/	dossier
Log Kow	/	dossier
Log Koc	1.30	dossier
Log K_{SED}	0.0	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	/	dossier
pKa	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	No	dossier
(Aerobic bio)degradation	Degradation in days-weeks	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity PU

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Unknown species			4d-EC50	>1000	PPP dossier	MS	F				
Invertebrates											
Daphnia magna			NOEC	≥100	PPP dossier	MS	F				
Chironomus riparius			NOEC	**≥ 0.1**	PPP dossier	MS	F	1	10	**≥100***	**≥10**
Fish											
Rainbow trout	LC50	>100	63d-NOEC	≥2	PPP dossier	MS	F				

*** MAC-QS derived from NOEC (AF =1) is protective for sediment dwelling organisms, which are the most sensitive species**

Summary report for Selenium

SUMMARY

Substance name	**Selenium**	
CAS-number	**7782-49-2**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF	0.8 µg/L	0.9 µg/L
SSD	**6 µg/L**	**72 µg/L**
Sediment	**1.7 mg/kg dw + BC**	**20 mg/kg dw + BC**
Remarks	**Total RA for water. Added RA for sediment.**	

*** data for fresh and marine water**

1. IDENTITY

Substance name	Selenium
CAS-number	7782-49-2
Substance group	metals
Synonyms	/
Molecular formula	Se
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	78.96	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	2.62 (10% OC) → 2.444 (5% OC)	a
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

4.1 Aquatic toxicity data from RIVM database* and EPA Ecotox database**

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum	6d-EC50	65			RIVM database	2	F				
Invertebrates											
Brachionus calyciflorus (rot)	1d-EC50	16.1			RIVM database	3	F				
Chironomus thummi (ins)	2d-EC50	1.8***			RIVM database	2	F				
Daphnia magna (cru)	4d-EC50	0.43			RIVM database	>5	F				
Hyalella azteca (cru)	2d-EC50	0.34			RIVM database	1	F				
Scylla serrata (cru)	4d-EC50	39			RIVM database	1	F				
Chironomus thummi (ins)			30d-NOEC	0.303	RIVM database	1	F				
Daphnia magna (cru)			21d-NOEC	0.085	RIVM database	1	F				
Acartia clause – Copepoda (cru)	4d-EC50	2.1			RIVM database	1	M				
Acartia tonsa – Copepoda (cru)	4d-EC50	0.85			RIVM database	1	M				
Americamysis bahia (cru)	4d-EC50	0.60			RIVM database	1	M				
Brachionus plicatilis (rot)	1d-EC50	17			RIVM database	2	M				
Fish											
Oncorhynchus kisutch	4d-EC50	22.3			RIVM database	4	F				
Oncorhynchus mykiss	16d-EC50	5.0			RIVM database	5	F				
Oncorhynchus tshawytscha	4d-EC50	62.5			RIVM database	4	F				
Pimephales promelas	14d-EC50	0.60			RIVM database	1	F				
Lepomis macrochirus			60d-NOEC	0.46	RIVM database	>2	F				
Oncorhynchus mykiss			336d-NOEC	**0.040**	RIVM database	>2	F		50		**0.80**
Cyprinodon variegatus	4d-EC50	6.7			RIVM database	2	M				
Oncorhynchus kisutch	4d-EC50	29.3			RIVM database	4	M				
Oncorhynchus tshawytscha	4d-EC50	71.3			RIVM database	4	M				
Lepomis macrochirus			60d-NOEC	0.46	RIVM database	1	F/M				
Other											
Gastrophryne carolinensis – Anura (amp)	7d-EC50	**0.090**			RIVM database	1	F	100		**0.90**	
Lemna minor (mac)	4d-EC50	2.4			RIVM database	1	F				
Lemna minor (mac)			14d-NOEC	1.02	RIVM database	4	F				

a RIVM e-toxBase, Bilthoven, 2004 b http://www.epa.gov/ecotox/ c hardness dependent

Deriving MAC-QS: HC5 = 0.144 mg/L → AF = 2 (19 species from 8 major taxonomic groups from 3 trophic levels) → 72 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	65	alg-RIVM
2	16,1	rot-RIVM
3	1,8	ins-RIVM
4	0,43	cru-RIVM
5	0,34	cru-RIVM
6	39	cru-RIVM
7	2,1	cru-RIVM
8	0,85	cru-RIVM
9	0,6	cru-RIVM
10	17	rot-RIVM
11	22,3	pis-RIVM
12	5	pis-RIVM
13	62,5	pis-RIVM
14	0,6	pis-RIVM
15	6,7	pis-RIVM
16	29,3	pis-RIVM
17	71,3	pis-RIVM
18	0,09	amp-RIVM
19	2,4	mac-RIVM
20		
21		
22		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	6,52E-1	mean of the log toxicity values
s.d.	8,93E-1	sample standard deviation
n	1,90E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	3,072E-2	-1,513E0	lower estimate of the HC5
HC5	1,438E-1	-8,422E-1	median estimate of the HC5
UL HC5	4,093E-1	-3,879E-1	upper estimate of the HC5
sprHC5	1,333E1	1,125E0	spread of the HC5 estimate

FA At HC5 results

Name	Value	Description
FA lower	1,22	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	14,39	95% confidence limit of the FA at standardised median logHC5

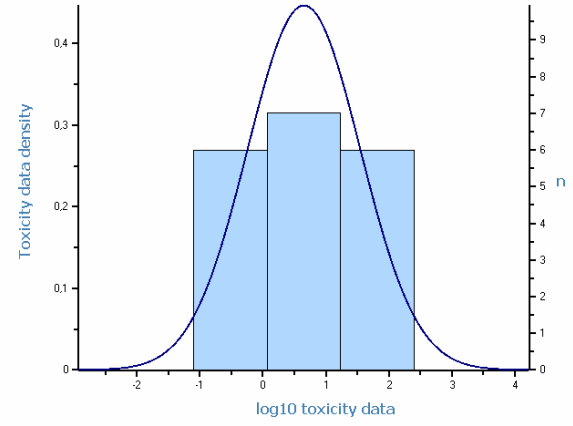
HC50 results

Name	Value	log10(Value)	Description
LL HC50	1,981E0	2,968E-1	lower estimate of the HC50
HC50	4,490E0	6,523E-1	median estimate of the HC50
UL HC50	1,018E1	1,008E0	upper estimate of the HC50
sprHC50	5,139E0	7,109E-1	spread of the HC50 estimate

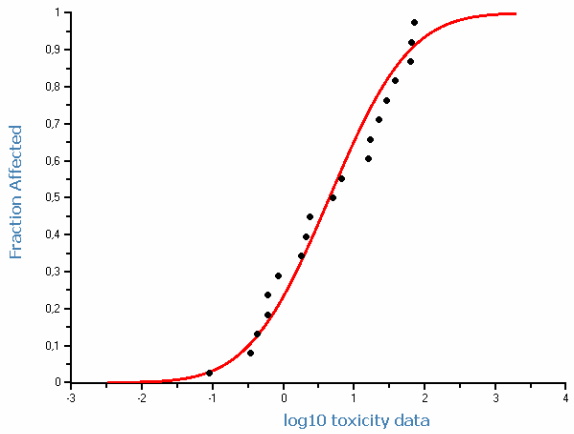
SSD Histogram and PDF

SSD graph

SSD Histogram and PDF



SSD Graph



Deriving AA-QS: HC5 = 0.030mg/L → AF = 5 (6 species from 4 major taxonomic groups from 3 trophic levels) → 6 µg/L

Input toxicity data

Data no.	Toxicity data	Label
1	0,303	ins-RIVM
2	0,085	cru-RIVM
3	0,46	pis-RIVM
4	0,04	pis-RIVM
5	0,46	pis-RIVM
6	1,02	mac-RIVM
7		
8		
9		
10		
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: NOEC

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	-6,09E-1	mean of the log toxicity values
s.d.	5,24E-1	sample standard deviation
n	6,00E0	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	2,808E-3	-2,552E0	lower estimate of the HC5
HC5	2,978E-2	-1,526E0	median estimate of the HC5
UL HC5	8,567E-2	-1,067E0	upper estimate of the HC5
sprHC5	3,051E1	1,484E0	spread of the HC5 estimate

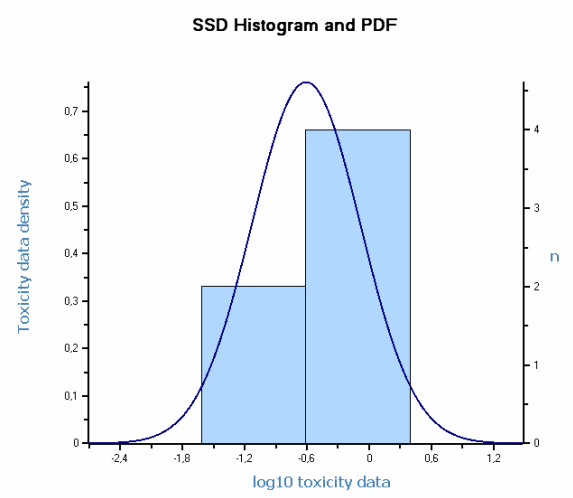
FA At HC5 results

Name	Value	Description
FA lower	0,25	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	27,74	95% confidence limit of the FA at standardised median logHC5

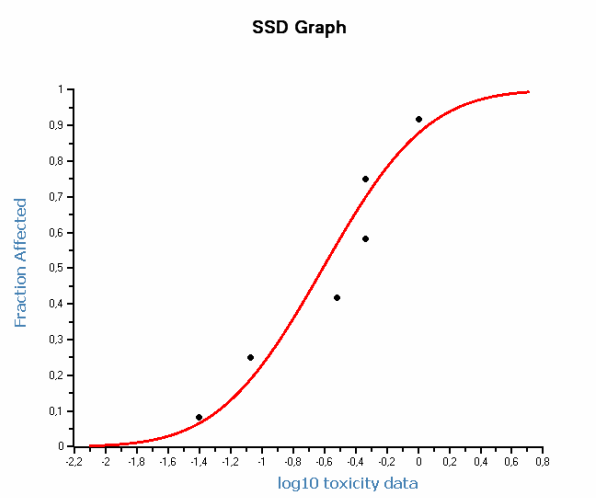
HC50 results

Name	Value	log10(Value)	Description
LL HC50	9,123E-2	-1,040E0	lower estimate of the HC50
HC50	2,461E-1	-6,088E-1	median estimate of the HC50
UL HC50	6,641E-1	-1,778E-1	upper estimate of the HC50
sprHC50	7,279E0	8,621E-1	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph



4.2 Sediment toxicity

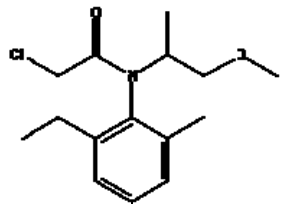
Equilibrium partitioning method-calculated with log Ksed = 2.444
AA-QS sed = 278 L/kg*0.006 mg/L = 1.7 mg/ kg dw
MAC-QS sed = 278 L/kg*0.072 mg/L = 20 mg/kg dw

Summary report for S-metolachlor

SUMMARY

Substance name	**S-metolachlor**	
CAS-number	**87392-12-9**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**0.27 µg/L**	**2.7 µg/L**
Sediment	**/**	**/**
Remarks	**data from dossier**	

1. IDENTITY

Substance name	S-metolachlor
CAS-number	87392-12-9
Substance group	Herbicide-Chloroacetanilide
Synonyms	/
Molecular formula	$C_{15}H_{22}ClNO_2$
Structural formula	

Substance name	CGA 51202*
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

Substance name	CGA 351916**
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

Substance name	CGA 354743**
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

Substance name	CGA 380168**
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

*** Metabolite is not relevant due to the low toxicity**
*** Metabolite is not relevant due to the lack of toxicity data**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**					**ref.**
Substance	S-metolachlor	CGA 51202	CGA 351916	CGA 354743	CGA 380168	
Molecular weight (g/mol)	283.8	/	/	/	/	dossier
Vapour Pressure (Pa)	3.7E-03	/	/	/	/	dossier
Water Solubility (mg/L)	480	/	/	/	/	dossier
Log Kow	3.1	/	/	/	/	dossier
Log Koc	2.04-2.57 → 2.35	/				dossier
Log K_{SED}	0.74-1.27 → 1.05	/				/
Henry-coefficient (Pa-m3/mol)	2.2E-03	/	/	/	/	dossier
pKa	No	/	/	/	/	dossier

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic						**ref.**
Substance	S-metolachlor	CGA 51202	CGA 351916	CGA 354743	CGA 380168	
BCF	69 (fish)	/	/	/	/	dossier
(Aerobic bio) degradation	Not degradable (degradation in weeks-months)	/	/	/	/	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity S-Metolachlor

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Selenastrum capricornutum	5d-EC50	**0.008**	(5d-NOEC extrapolated)	(NOEC→0.008/3= **0.0027)**	PPP dossier	MS	F	1	10	**2.7**	**0.27**
Aquatic invertebrates											
Mysidopsis bahia	4d-EC50	1.4			PPP dossier	MS	F				
Daphnia magna			21d-NOEC*	5.9*							
*Sediment dwelling organisms***			62d-NOEC*	0.54*	PPP dossier	MS					
Fish											
Oncorhynchus mykiss	4d-LC50	1.23			PPP dossier	MS	F				
Pimephales promelas			35d-NOEC*	0.78*	PPP dossier	MS	F				
Higher plants											
Lemna gibba	14d-EC50		(14d-NOEC extrapolated)	(NOEC→0.023/3= 0.008)	PPP dossier	MS	F				

*** data for Metolachlor**
**** benthic estuarine community-26 species of annelids, arthropods and molluscs**

4.1.2 Aquatic toxicity metabolite CGA 51202

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/ M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Unknown species	3d-EC50	77.6				MS	F				
Aquatic invertebrates											
Unknown species	2d-LC50	16.6				MS	F				
Fish											
Unknown species	4d-LC50	>100				MS	F				

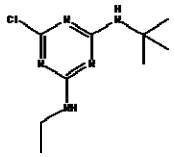
Aquatic toxicity of the metabolite CGA 51202 is between 10-100 mg/L → metabolite is not relevant due to the low toxicity

Summary report for Terbutylazine

SUMMARY

Substance name	**Terbutylazine**	
CAS-number	**5915-41-3**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	**0.53 µg/L**	**5.3 µg/L**
Sediment	**/**	**/**
Remarks	**data from dossier**	

1. IDENTITY

Substance name	Terbutylazine
CAS-number	5915-41-3
Substance group	Algaecide, Herbicide, Microbiocide-Triazine
Synonyms	/
Molecular formula	$C_9H_{16}ClN_5$
Structural formula	

Substance name	Diethyl-Terbutylazine
CAS-number	/
Substance group	Metabolite
Synonyms	/
Molecular formula	/
Structural formula	/

*** Metabolite is not relevant due to the lack of toxicity data**

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	229.7	dossier
Vapour Pressure (Pa)	1.49E-04	SRC exp.
Water Solubility (mg/L)	8.5	HSDB
Log Kow	3.2	HSDB
Log Koc	2.21-2.35 → 2.28	dossier
Log K_{SED}	0.91-1.05 → 0.98	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	0.0038	HSDB
pKa	/	/

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	33.7 (fish)	dossier
(Aerobic bio)degradation	Not biodegradable (degradation in weeks-monthes), hydrolytically stable	dossier

4. ECOTOXICITY (MS: most sensitive species of each group)

4.1.1 Aquatic toxicity Terbutylazine

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Scenedesmus subspicatus	3d-EC50	0.016	(3d-NOEC extrapolated)	(0.016/3 =**0.0053)**	dossier	MS	F	1	10	**5.3***	**0.53**
Daphnids											
Daphnia magna	2d-EC50	69.3	21d-NOEC	0.21	dossier	MS	F				
Fish											
Oncorhynchus mykiss	4d-EC50	3.8	90d-NOEC	0.09	dossier	MS	F				
Other											
Lemna gibba	14d-EC50	0.017	(14d-NOEC extrapolated)	(0.017/3 =0.0057)	dossier	MS	F				

*** MAC-QS derived from AA-QS with a factor of 10**

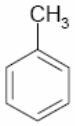
Summary report for Toluene

SUMMARY

Substance name	**Toluene**	
CAS-number	**108-88-3**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water PNEC AF 10	**74 µg/L**	**740 µg/L**
Sediment	**/**	**/**
Remarks	**EU RAR data: AA-QS=PNEC MAC-QS=PNEC*10**	

* EU RISK ASSESSMENT Report, Final Report, TOLUENE, 2003, Denmark (last literature search: 2000)

1. IDENTITY

Substance name	Toluene
CAS-number	108-88-3
Substance group	Organics
Synonyms	/
Molecular formula	C_7H_8
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	92.15	RAR
Vapour Pressure (Pa)	3.8E+03	RAR
Water Solubility (mg/L)	515	RAR
Log Kow	2.65	RAR
Log Koc	2.25	RAR
Log K_{SED}	0.95	est. from Koc-5% OC
Henry-coefficient (Pa-m3/mol)	673	SRC exp.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	13-90 (fish)	RAR
(Aerobic bio)degradation	Readily biodegradable, hydrolytically stable	RAR

Summary report for Total Petroleum Hydrocarbons

SUMMARY		
Substance name	**Total Petroleum Hydrocarbons**	
CAS-number	/	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water	*	*
Sediment	*	*
Remarks	**Data from RIVM Report** **AA-QS=MPC** **MAC-QS=MPC*10**	

*** MPC data in appendix**

**** Verbruggen, E.M.J., Environmental Risk Limits for Mineral Oil (Total Petroleum Hydrocarbons), 2004**

In this report maximum permissible concentrations and serious risk concentrations are derived for mineral oil (total petroleum hydrocarbons). The used method is based on a fraction analysis approach, in which aliphatic and aromatic compounds are regarded separately and are both further divided into different fractions. For each fraction or block separate risk limits are derived. The toxic unit approach must be applied to these blocks to calculate the environmental risk limits for the total (sum) toxicity of a specific oil type.

1. IDENTITY

Substance name	Total Petroleum Hydrocarbons
CAS-number	/
Substance group	Mineral oil is a complex mixture of aromatic and aliphatic hydrocarbons, which are divided in blocks of equivalent carbon numbers (EC) within the groups. Mineral oil is defined as the TPH fraction between EC number 10 and 40, the part that falls between *n*-decane and *n*-tetracontane in the GC.
Synonyms	Mineral oil
Molecular formula	Mw = 14.07*EC+3.51 (Aliphatic) Mw = 6.36*EC+60.86 (Aromatic)
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	EC number 10 to 40	RIVM Report
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	Log S = -1.144*log K_{OW} + 0.723 (Aliphatic) Log S = -0.171*log K_{OW}^2 – 0.231*log Kow – 0.436 (Aromatic)	RIVM Report
Log Kow	Log K_{OW} = 0.53*EC + 0.55 (Aliphatic) Log K_{OW} = 0.15*EC + 1.76 (Aromatic)	RIVM Report
Log Koc	Log K_{OC} = 0.81*log K_{OW} + 0.1 (Aliphatic) Log K_{OC} = log K_{OW} - 0.21 (Aromatic)	RIVM Report
Log K_{SED}	/	/
Henry-coefficient (Pa-m3/mol)	/	/
pKa	/	/

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	/
(Aerobic bio)degradation	/	/

4. APPENDIX : AA-QS(MPC) for TPH in water and sediment from RIVM Report

Table 1: Derived QS for mineral oil in water categorised according to the TPHCWG method (Gustafson et al., 1997)

Compounds	EC fraction	AA-QS* (µg/L)	MAC-QS** (µg/L)
Aliphatic	>5-6	12	120
	>6-8	2.6	26
	>8-10	0.33	3.3
	>10-12	0.084	0.84
	>12-16	0.047	0.47
	>16-21	-[a]	-[a]
Aromatic	>5-7 (benzene)	81	810
	>7-8 (toluene)	55	550
	>8-10	36	360
	>10-12	21	210
	>12-16	9.0	90
	>16-21	2.5	25
	>21-35	0.21	2.1

* AA-QS = MPC

** Calculated from AA-QS (MAC-QS = AA-QS*10)

[a] If no block of compound with a lower ERL are present, these values may be neglected, because solubility is so low that internal concentration corresponding to the ERL will not be reached

Table 2: Derived QS for mineral oil in standard soil and sediment (5% of organic carbon) categorised according to the TPHCWG method (Gustafson et al., 1997)

Compounds	EC fraction	AA-QS*(mg/kg_{dw})	MAC-QS** (mg/kg_{dw})
Aliphatic	>5-6	0.28	2.8
	>6-8	0.27	2.7
	>8-10	0.25	2.5
	>10-12	0.46	4.6
	>12-16	4.95	49.5
	>16-21	-[a]	-[a]
Aromatic	>5-7 (benzene)	0.65	6.5
	>7-8 (toluene)	0.75	7.5
	>8-10	0.85	8.5
	>10-12	1.0	10
	>12-16	1.2	12
	>16-21	1.55	15.5
	>21-35	3.5	35

* AA-QS = MPC/2 (the content of organic carbon is 5% instead of 10%)

** Calculated from AA-QS (MAC-QS = AA-QS*10)

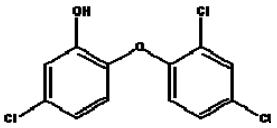
[a] If no block of compound with a lower ERL are present, these values may be neglected, because solubility is so low that internal concentration corresponding to the ERL will be reached

Summary report for Triclosane (2,4,4'-Trichloro-2-hydroxydiphenyl ether)

SUMMARY

Substance name	**2,4,4'-Trichloro-2-hydroxydiphenyl ether**	
CAS-number	**3380-34-5**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water AF	**0.29 µg/L**	**2.9 µg/L**
Sediment EP	**0.29 mg/kg**	**2.9 mg/kg**
Remarks	**/**	**/**

1. IDENTITY

Substance name	2,4,4'-Trichloro-2-hydroxydiphenyl ether
CAS-number	3380-34-5
Substance group	Biocid
Synonyms	Triclosane
Molecular formula	$C_{12}H_7Cl_3O_2$
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	289.5451	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	6.2E-04	SRC est.
Water Solubility (mg/L)	10	SRC exp.
Log Kow	4.8	SRC exp.
Log Koc	4.3	SRC est.
Log K_{SED}	3.0	est. from Koc - 5% OC
Henry-coefficient (Pa-m3/mol)	0.038	SRC est.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	368	SRC est.
(Aerobic bio)degradation	Probably biodegradable	HSDB

4. ECOTOXICITY

4.1.2 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
/											
Invertebrates											
Daphnia magna (cru)	2d-LC50	0.39			RIVM database	1	F				
Fish											
Oncorhynchus mykiss (pis)	4d-LC50	**0.29**			RIVM database	1	F	100	1000	**2.9**	**0.29**
Oryzias latipes (pis)	2d-LC50	0.35			RIVM database	1	F				
Pimephales promelas (pis)	4d-LC50	0.30			RIVM database	2	F				

4.2 Sediment toxicity

Equilibrium partitioning method-calculated with log Koc =4.3 (SRC) → log Ksed = 3.0 (5% OC)
AA-QS sed = 1000*0.00029 = 0.29 mg/ kg dw
MAC-QS sed = 1000*0.0029 = 2.9 mg/kg dw

Summary report for Xylenes

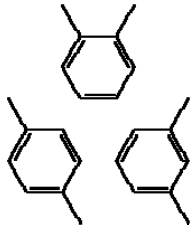
SUMMARY

Substance name	**Xylenes**	
CAS-number	**1330-20-7**	
Proposed Quality Standard	**Freshwater***	
	AA-QS	**MAC-QS**
Water AF **SSD****	3 µg/L **185 µg/L**	30 µg/L **1850 µg/L**
Sediment	**/**	**/**
Remarks	**MPC = 380µg/L** **MPC =14mg/kg**	**/**

*** marine and freshwater data**

**** AA-QS and MAC-QS derived with SSD are protective**

1. IDENTITY

Substance name	Xylenes
CAS-number	1330-20-7
Substance group	Organics
Synonyms	/
Molecular formula	$C_{24}H_{30}$
Structural formula	

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	318.501	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	1070	SRC exp.
Water Solubility (mg/L)	178	SRC exp.
Log Kow	3.1	SRC exp.
Log Koc	2.6	SRC est.
Log K_{SED}	1.3	est. from Koc - 5% OC
Henry-coefficient (Pa-m3/mol)	669	SRC exp.
pKa		

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	50	SRC est.
(Aerobic bio)degradation	Readily biodegradable	HSDB

4. ECOTOXICITY

4.1 Aquatic acute and chronic toxicity

Species	Endpoint-acute	Value – (mg/l)	Endpoint-chronic	Value – (mg/l)	ref.	Number of tests for species	F/M	AF MAC-QS	AF AA-QS	MAC-QS (µg/l)	AA-QS (µg/l)
Algae											
Algae (alg)	1d-EC50	3			RIVM database	1	M	100	1000	**30**	**3**
Chlorococcales (alg)	1d-EC50	100			RIVM database	1	F				
Invertebrates											
Artemia salina (cru)	1d-LC50	*583**			RIVM database	1	M				
Daphnia magna (cru)	1d-LC50	*218**			RIVM database	3	F				
Diaptomus forbesi (cru)	4d-LC50	99.5			RIVM database	1	F				
Palaemonetes pugio (cru)	4d-LC50	7.4			RIVM database	3	M				
Streptocephalus proboscideus (cru)	1d-LC50	*263**			RIVM database	1	F				
Brachionus calyciflorus (rot)	2d-LC50	*253**			RIVM database	5	F				
			2d-NOEC	20	RIVM database	2	F				
Brachionus plicatilis (rot)	1d-LC50	*496**			RIVM database	2	M				
Katelysia opima (mol)	4d-LC50	190			RIVM database	1	M				
Aedes aegypti (ins)	1d-EC50	13.9			RIVM database	1	F				
Fish											
Carassius auratus (pis)	3d-LC50	20.7			RIVM database	3	F				
Cyprinus carpio (pis)	4d-LC50	*780**			RIVM database	1	F				
Danio rerio (pis)	2d-LC50	20			RIVM database	2	F				
Lepomis macrochirus (pis)	16h-LC50	11			RIVM database	18	F				
Oncorhynchus mykiss (pis)	4d-LC50	10.3			RIVM database	6	F				
Pimephales promelas (pis)	4d-LC50	25.6			RIVM database	4	F				
Poecilia reticulata (pis)	4d-LC50	34.7			RIVM database	1	F				
Therapon jarbua (pis)	4d-LC50	89			RIVM database	1	M				
Other											
Xenopus sp (amp)	4d-LC50	77.9			RIVM database	9	F				
			(4d-LOEC) → extrapolated NOEC = LOEC/2	(68.2) → 68.2/2 = 34.1	EPA	18	F				

*** rejected: Water Solubilility = 178 mg/L**

Deriving MAC-QS: 3.70 mg/L (AF=2; 14 species from 6 major taxonomic groups from 3 trophic levels) → 1.85 mg/L
Deriving AA-QS: 1.85/10 = 0.185 mg/L

Input toxicity data

Data no.	Toxicity data	Label
1	3	alg-RIVM
2	100	alg-RIVM
3	99,5	cru-RIVM
4	7,4	cru-RIVM
5	190	mol-RIVM
6	13,9	ins-RIVM
7	20,7	pis-RIVM
8	20	pis-RIVM
9	11	pis-RIVM
10	10,3	pis-RIVM
11	25,6	pis-RIVM
12	34,7	pis-RIVM
13	89	pis-RIVM
14	77,9	amp-RIVM
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		
25		
26		

Enter non-transformed toxicity data in the first column. The second column can be used optionally to assign labels to the data. A maximum of 20 different labels can be used.

Specifics

Enter custom values, or make a choice from the lists

Unit: mg/l

Type: EC50

Small sample

Use small sample method

Pre-defined standard deviations:

Standard deviation:

Parameters of the normal distribution

Name	Value	Description
mean	1,44E0	mean of the log toxicity values
s.d.	5,20E-1	sample standard deviation
n	1,40E1	sample size

HC5 results

Name	Value	log10(Value)	Description
LL HC5	1,215E0	8,441E-2	lower estimate of the HC5
HC5	3,704E0	5,687E-1	median estimate of the HC5
UL HC5	7,468E0	8,732E-1	upper estimate of the HC5
sprHC5	6,149E0	7,888E-1	spread of the HC5 estimate

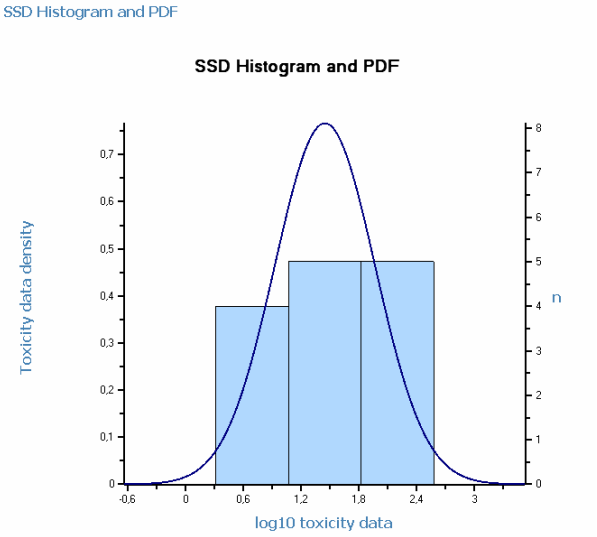
FA At HC5 results

Name	Value	Description
FA lower	0,92	5% confidence limit of the FA at standardised median logHC5
FA median	5,00	50% confidence limit of the FA at standardised median logHC5
FA upper	16,63	95% confidence limit of the FA at standardised median logHC5

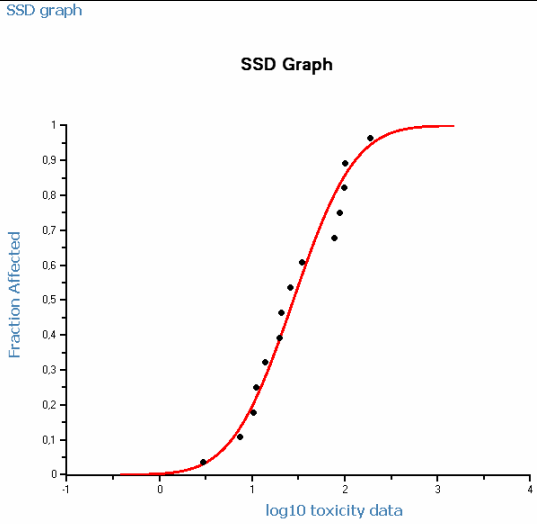
HC50 results

Name	Value	log10(Value)	Description
LL HC50	1,579E1	1,198E0	lower estimate of the HC50
HC50	2,785E1	1,445E0	median estimate of the HC50
UL HC50	4,909E1	1,691E0	upper estimate of the HC50
sprHC50	3,108E0	4,925E-1	spread of the HC50 estimate

SSD Histogram and PDF



SSD graph



Summary report for Zinc

SUMMARY

Substance name	**Zinc**	
CAS-number	**7440-66-6**	
Proposed Quality Standard	**Freshwater**	
	AA-QS	**MAC-QS**
Water* **RAR general** **RAR soft waters (<24mg/L$CaCO_3$)**	**7.8 µg/L+ BC** **3.1 µg/L + BC**	**78 µg/L + BC** **31 µg/L + BC**
Sediment *	**37 mg/kg + BC**	**370 mg/kg +BC**
Remarks	**Added RA for water (BC = 4.8).** **Added RA for sediment (BC = 180 mg/kg)**	

* **EU RAR Zn**

1. IDENTITY

Substance name	Zinc
CAS-number	7440-66-6
Substance group	metals
Synonyms	/
Molecular formula	Zn
Structural formula	/

2. PHYSICO-CHEMICAL PROPERTIES

Property	**values**	**ref.**
Molecular weight (g/mol)	65.39	http://chemfinder.cambridgesoft.com/
Vapour Pressure (Pa)	/	
Water Solubility (mg/L)	/	
Log K_{OW}	/	
Log K_{OC}	/	
Log K_{SED}	4.86 (10% OC) → 4.684 (5% OC)	a
Henry-coefficient (Pa-m3/mol)	/	
pKa	/	

a Crommentuijn T., Polder M.D., van der Plassche E., Maximum Permissible Concentration and Negligible Concentration for metals, taking background concentrations into account, RIVM Bilthoven, 1997

3. FATE AND BEHAVIOUR IN THE ENVIRONMENT

Characteristic		**ref.**
BCF	/	
(Aerobic bio)degradation	/	

4. ECOTOXICITY

An environmental risk assessment report (RAR) was produced by the Netherlands Organization for Applied Scientific Research (TNO) and the National Institute of Public Health and Environment (RIVM) [1]. The "added risk approach" has been used in this risk assessment report on zinc both in the exposure assessment and effect assessment.
The method for deriving the PNEC is the same as the method for the derivation of the AA-QS. Therefore it is proposed to use the PNECs presented in this report without any additional studies.

Background levels of Zinc

It can be concluded that there are several estimates available for a natural background value of zinc in fresh waters in a number of EU countries. Most data fall within the range of 2.5 to 12 µg total-Zn/l. In the present report on zinc a pragmatic approach is followed rather than selecting one particular natural background value by using both the lower limit of 3 µg total-Zn/l and the upper limit of 12 µg total-Zn/l for correcting the available EU monitoring data in the risk characterisation. The rapporteur is aware that some of the current sources refer to lower mean natural background values (around or below1 µg/l). Higher (> 12 µg/l) natural levels may be relevant as well in some cases. In general, if available monitoring data can unequivocally be linked with a particular natural background value in an area, preference should be given to that specific background value. An example of this is the Meuse river. There are indications that for this river, at least the part entering the Netherlands, the natural background is slightly higher than for other major surface waters in the Netherlands (pers. comm. RIZA, 2001). Therefore, rather than using the range 3-12 µg/l, a range of 6-12 µg/l is considered more appropriate for the Meuse in the current risk characterisation.

In conclusion, all currently available natural background data for sediment are more or less in the same order of magnitude (range 70-175 mg/kg dwt). Based on the data from several EU-regions (see above) the value of 140 mg/kg dwt will be used as a natural background for correcting the EU sediment monitoring data. If available monitoring data can unequivocally be linked with a particular natural background value in an area, preference should be given to that specific background value.

Variablity of the data, factors influencing Zinc toxicity

Background concentrations:
Increased tolerance of *Daphnia magna* towards zinc of a factor 2-3, optimum zinc concentration between 300 and 450 µg/L.
2 algae species increased tolerance towards zinc: culture between 1.4 and 65 µg Zn /L, by a factor of 2-3.
Yet not sufficient data to derive background dependent PNEC values for freshwater.

[1] The Netherlands Organization for Applied Scientific Research (TNO) and the National Institute of Public Health and Environment (RIVM), Risk assessment Zinc metal CAS-No: 7440-66-6, Final draft of December 2004, Part 1 Environment

pH:
Chronic toxicity of zinc between pH 5.5 and 8.5: modifying effect of pH was a factor 2 to 3 for the rainbow trout, a factor 3 to 4 for the *D. magna*, and a factor >20 for the algae.
Yet not sufficient data to derive pH-dependant PNEC.

Hardness:
Only small effects of hardness on zinc toxicity were shown.
The (assumed) inverse relationship between water hardness and aquatic toxicity of *various metals*:
Based mainly on acute toxicity tests with relatively high metal concentrations. And then the inverse relation between hardness and toxicity is unequivocal, although (Crommentuijn et al., 1997) (EU-RAR, p. 172):

- Mostly **fish** were used as test organisms; data for species with different uptake mechanisms are scarce.
- Hardness is related to other factors (alkalinity, ionic strength, pH). In most studies hard water was diluted with distilled or otherwise de-ionised water to reduce hardness, resulting in a simultaneous reduction in the other factors. This may influence the toxicity of metals: (1) through chemical speciation of the metal in water (affecting the bioavailability) and (2) influence of uptake and binding of available metal by biological tissues.
- Chronic toxicity tests with relatively low metal concentrations showed that the **relationship between water hardness and chronic toxicity of metals is less consistent** than that between hardness and acute toxicity. Furthermore, the influence can be relatively small, especially in the range of hardness between around 50 and 200 mg/l (as $CaCO_3$): studies with zinc, cadmium, copper and chromium usually showed a **2- to 3-fold decrease** in toxicity with increasing hardness, with **a maximum of around 5-fold**. Also examples exist with no effect or even an increase of toxicity with increasing hardness.

Conclusion: too small basis for correction of PNEC solely on one of the water chemistry properties.

The Biotic Ligand Model:
This model provides a mechanistic basis for understanding the bioavailability by integrating the chemical parameters (pH, hardness, DOC) and biologocal parameters (receptor sites on organism, mode of action). The chemical activity of Zn^{2+} is reduced by binding to organic (dissolved organic carbon, DOC) and inorganic ligands that reduce the bioavailability and thus reduce the toxicity. Inorganic ligands include OH^- and CO_3^{2-}. The concentrations of these ligands are increased at increased pH and increased alkalinity of the test medium, respectively. Cations in solution can compete with zinc for the biotic ligand, which also reduces bioavailability to the biotic ligand and thus reduces toxicity.
Application of the BLM model reduced the variability in the alga test results from a factor of 100 to a factor of 2, for trout and *Daphnia* from a factor of 20 to 2.
For this correction, BLM constants to describe the influence of the various variables per site should be known (see EU-RAR p. 180).
Reference water chemistry conditions have been formulated:
For all organisms: 10^{th} percentile of DOC.
For *D. magna* and *O. mykiss*: 10^{th}-percentile of inorganic parameters (including pH and hardness).

For *P. subcapitata*: 90th-percentile of inorganic parameters (including pH and hardness).

Unlike the approach in the RAR for Copper, in the RAR for zinc the PECs are corrected for bioavailability (see p. 180).

For the derivation of the WQS this implies that the AA-QS and MAC-QS for zinc are presenting a value assuming full bioavailability. For assessing compliance to the WQS, **the environmental concentration should be corrected for the bioavailability of zinc using the BLM constants, based on the local water characteristics (DOC, pH, hardness).**

$PNEC_{add}$ for surface water ($PNEC_{add, aquatic}$) - Generic

NOEC values were extracted from scientific publications and research activities. The "added risk approach" has been used in this risk assessment report on zinc both in the exposure assessment and effect assessment. With respect to the effect assessment the added risk approach implies that the PNEC is derived from toxicity data that are based on the added zinc concentration in the tests. This results in an "*added* Predicted No Effect Concentration" ($PNEC_{add}$).

The calculation of the $PNEC_{add}$ values is in agreement with the calculation of PNEC values (for substances with no background concentration) as described in the TGD, i.e. the $PNEC_{add}$ values are derived from toxicity data (either NOEC values or LC50 and EC50 values from laboratory tests), using assessment factors or statistical extrapolation.
These species represent different trophic levels (primary producers, primary consumers and secondary consumers).

The "species mean" NOEC values for freshwater organisms (n = 18) listed in Table 1 were used in the calculations using statistical extrapolation. For the species sensitivity distributions, see Figures 1 (freshwater organisms).

Table 1 "Species mean" NOEC values that are used as input values for deriving the 5th percentile values as a basis for the freshwater $PNEC_{add, aquatic}$.

Taxonomic groups	**"Species mean" NOEC values (µg/l)**
Algae (unicellular)	17
Algae (multicellular)	60
Poriferans	43; 43; 43; 65
Molluscs	75; 400
Crustaceans	37; 42; 88
Insects	137
Fish	44; 50; 78; 189; 530; 660

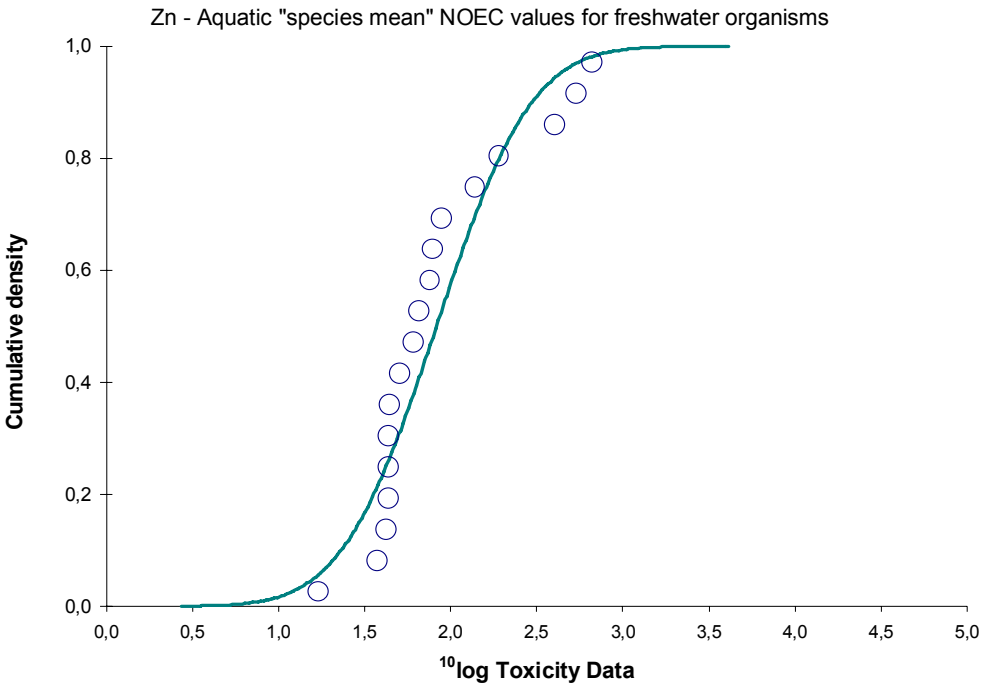


Figure 1 Freshwater organisms: species sensitivity distribution based on "species mean" chronic NOEC values.

The above procedure results in a median 5th-percentile value of 15.6 µg/l and justifies the use of an assessment factor of 2. Arguments for the factor 2 are provided in RAR[1] and result in a $PNEC_{add,\ aquatic}$ that is sufficiently protective for the most sensitive species and for the field situation. Thus, a **$PNEC_{add,\ aquatic}$ of 7.8 µg/l for dissolved zinc in freshwater** is proposed. This value is used in the risk assessment, which is aimed at freshwater. For pragmatic reasons it will also be used for a number of local marine scenarios.

The fraction of zinc that is dissolved in surface water depends on abiotic factors, especially the suspended matter concentration (C_{susp}). Hence, no single value can be given for the $PNEC_{add,\ aquatic}$ expressed as total zinc. In the TGD a C_{susp} of 15 mg/l is used for "standard" surface water (freshwater). From this C_{susp} and a Kp_{susp} of 110,000 l/kg (median partition coefficient for the distribution between solid particulate matter and water, see section 3.2.1) and the $PNEC_{add,\ aquatic}$ for dissolved zinc in freshwater (7.8 µg/l), a $PNEC_{add,\ aquatic}$ of 21 µg/l is calculated for total zinc in freshwater. When a C_{susp} of 30 mg/l is used, a $PNEC_{add,\ aquatic}$ of 34 µg/l is calculated for total zinc in freshwater.

PNEC for soft water – specific

A WER (Water effect ratio) was derived by comparing the results of toxicity tests in soft water (6 and 8 mg CaCO3/l) with the same tests in medium hard water (100 mg/l). The arithmatic mean WER was 2.5 is thoufht to be a conservative factor to derive a'soft water' PNECadd. As a result, the **$PNEC_{add,\ aquatic}$ is 3.1 µg/l for dissolved zinc for freshwater with low hardness, i.e. < 24 mg $CaCO_3$/l.**

Predicted no effect concentration for sediment ($PNEC_{add,\ sediment}$)

Chronic sediment toxicity data from single-species tests in Zn-spiked freshwater sediments are available (although limited to three freshwater species, viz. the worm *Tubifex tubifex,* the midge *Chironomus tentans* and the amphipod *Hyalella azteca*; these species are among the benthic organisms most frequently used for assessing sediment toxicity) and thus have been used to derive the $PNEC_{add}$ for freshwater sediment.

For benthic organisms there are only four chronic NOEC values, viz. one for the oligochaete *Tubifex tubifex* (1100 mg/kg d.w.), two for the insect *Chironomus tentans* (610 and 800 mg/kg d.w.) and one for the crustacean *Hyalella azteca* (74 mg/kg d.w.), see earlier and Table 3.3.2.e – Part I in Annex 3.3.2.D. These NOEC values are expressed as the added concentration (Cn, being actual-Cb). Both with respect to the number of chronic NOEC values and the number of different species, these data are too limited to apply statistical extrapolation (see section 3.3.1.3). Thus, the $PNEC_{add,\ sediment}$ has been derived from the lowest chronic NOEC, i.e. the NOEC of 74 mg/kg d.w for *H. azteca* (from Farrar & Bridges, 2002, 2003).

The above data indicate that *H. azteca* is (one of the) most sensitive benthic species and field or mesocosm related studies do not show toxicity at concentrations below the NOEC for this species. This and the comparison with the terrestrial toxicity data for species (including invertebrates) justifies the use of an assessment factor of 2 on the lowest NOEC for benthic species.

The risk characterisation for sediments is though based on a **$PNEC_{add,\ sediment}$ of 37 mg/kg <u>dry</u> weight,** equivalent to a $PNEC_{add,\ sediment}$ of 8 mg/kg <u>wet</u> weight.