

Sammanställning av protokoll om riktvärden för växtskyddsmedel i ytvatten

År 2004 tog Kemikalieinspektionen fram riktvärden för 100 verksamma ämnen i godkända växtskyddsmedel och i vissa fall även för ämnenas nedbrytningsprodukter.

För varje enskilt ämne finns ett protokoll över ämnets egenskaper samt vilka beräkningar som gjorts för att ta fram riktvärdet.

År 2007 gjorde Kemi på uppdrag av Naturvårdsverket en revidering av vissa riktvärden från 2004. I de fall protokollet reviderades under 2007 framgår det i dokumentets huvud.

I följande dokument finns beskrivningar av metoderna för framtagning av riktvärdena vid respektive tillfälle:

[Beskrivning av riktvärden år 2004 \(PDF, 144 kB\)](#)

[Beskrivning av riktvärden år 2007 \(PDF, 82 kB\)](#)

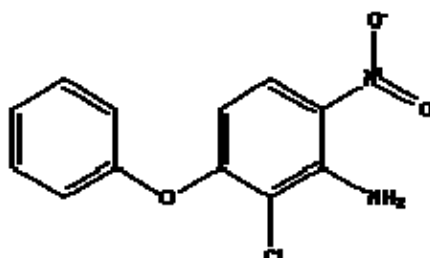
Riktvärdena ska ses som ett verktyg vid bedömning av miljökvaliteten i svenska vattendrag. På [Naturvårdsverkets webbplats](#) finns en vägledning för hur de kan användas.

I [bekämpningsmedelsregistret](#) finns information om enskilda medel, hur de får användas med mera.

[Sveriges lantbruksuniversitet \(SLU\)](#) har en pesticiddatabas som innehåller resultat från provtagningar av svenska yt- och grundvatten.

1. Aclonifen

Aclonifen is member of the group of diphenyl ether herbicides, and works by inhibiting the protoporphyrinogen oxidase. The herbicide is intended for use in peas, carrots and potatoes.



1.1 Physico-chemical properties

Physico-chemical properties of *aclonifen* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *aclonifen*.

		Reference
CAS-No.	74070-46-5	2
Empirical formula	C ₁₂ H ₉ ClN ₂ O ₃	2
Molecular weight [g/mol]	264.7	2
Solubility in water [mg/kg]	1.4	1
pKa	Not relevant	
Vapour pressure [Pa]	1.6 × 10 ⁻⁵	1
Log P _{ow}	4.37	1
Henry's law constant [Pa×m ³ /mol]	0.003	1

1.2 Toxicity to aquatic organisms

The toxicity of *aclonifen* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *aclonifen*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scendesmus subspicatus</i>	growth rate	24h, static 96h, static	E _r C ₅₀ 0.0069 NOEC 0.0025	1
<i>Scendesmus subspicatus</i>	growth rate	96h, static	E _r C ₅₀ 0.029 ²⁾ NOEC 0.0032	1
<i>Selenastrum capricornutum</i>	growth rate	96h, static	E _r C ₅₀ 0.028 ¹⁾ NOEC 0.0049 ¹⁾	1
Crustaceans				

<i>Daphnia magna</i>	immobility/ mortality	48h, static	EC ₅₀ 1.2	1
<i>Daphnia magna</i>	immobility/ mortality	48h, static	EC ₅₀ 1.1 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.016	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.054 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.67	1
<i>Cyprinus caprio</i>	mortality	96h, flow-through	LC ₅₀ 1.3	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.61 ¹⁾	1
<i>Cyprinus caprio</i>	mortality	96h, semi-static	LC ₅₀ 0.87 ¹⁾	1
<i>Onchorhynchus mykiss</i>		21d, semi-static	NOEC 0.01 (nominal)	1
<i>Cyprinus carpio</i>		21d, flow-through	NOEC 0.009	1
<i>Onchorhynchus mykiss</i>		21d, flow-through	NOEC 0.01 ¹⁾	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 91.3%

Former water quality objective calculation

The most sensitive of the tested species was *Scendesmus subspicatus*, with a NOEC of 0.0025 mg/L, different tests. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *aclonifen* is calculated to 0.00025 mg/L.

Revised EQS calculation according to harmonised methodology (3)

The PNEC of 0.00025 mg/L for *aclonifen* is still valid.

1.3 Bioaccumulation and persistence

Aclonifen is expected to bioaccumulate. BCF is 840 in *Onchorhynchus mykiss*, whole fish. *Alconifen* is stable towards hydrolysis at pH 5.7 and 9. However the photochemical transformation has a DT₅₀ of 9 days during summer. Two water/sediment tests have been performed at pH 7.3 and 9.1. The primary degradation of *aclonifen* was DT₅₀ 15.4-16.1 days. No major metabolites have been detected.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.00025 mg/L, the proposed EQS/water quality standard for *aclonifen* is 2×10^{-4} mg/L.

1.5 Comments

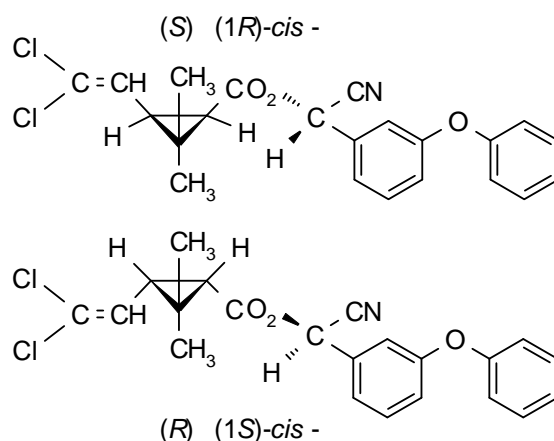
No distribution studies are available, however due to high partition coefficient and low water solubility, *alconifen* is expected to partition into sediment. Therefore additional quality objective for sediment is recommended.

1.6 Literature

- (1) Andersson L, Andersson Y, 1994. *Ecotoxicological evaluation of the herbicide acetonifin*. National Chemical Inspectorate, Solna, Sweden.
- (2) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (3) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Alpha-cypermethrin

Alpha-cypermethrin is a synthetic pyrethroid insecticide intended for use in, among other crops, oleiferous plants, cereals, potatoes and fruit. The substance consists of the two insecticidally active isomers of *cypermethrin* (the cis-2 pair). *Alpha-cypermethrin* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *alpha-cypermethrin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *alpha-cypermethrin*.

		Reference
CAS-No.	67375-30-8	1
Empirical formula	C ₂₂ H ₁₉ Cl ₂ NO ₃	1
Molecular weight [g/mol]	416.3	1
Solubility in water [mg/kg]	6.7 × 10 ⁻⁴ at pH 4 3.97 × 10 ⁻³ at pH 7 4.54 × 10 ⁻³ at pH 9	2
Vapour pressure [Pa]	3.4 × 10 ⁻⁷ at 25°C	2
Log P _{ow}	5.5 at 20°C	1
Henry's law constant [Pa×m ³ /mol]	0.069 at 20°C	2

1.2 Toxicity to aquatic organisms

The toxicity of *alpha-cypermethrin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *alpha-cypermethrin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
		96h	EC ₅₀ >100	3
Crustaceans				

<i>Daphnia magna</i>		48 h, semi-static	EC ₅₀ 0.0003	1
<i>Daphnia magna</i>		21 d, semi-static	NOEC 0.00003 ¹⁾	1
<i>Chaoborus crystallinus</i> , 4 th instar		24h	EC50 0.07 ²⁾ NOEC 0.001 ²⁾	4
Fish				
<i>Oncorhynchus mykiss</i>		96 h, semi-static	LC ₅₀ 0.0028	1
<i>Pimephales promelas</i>		34 d, early life stage, flow-through	NOEC 0.00003	1
<i>Mesocosm</i>				
	community structure	126 d	EAC 0.000015	3

¹⁾ Corresponding to ~0.000012 mg/l dissolved in the water-phase (40 % of nominal value).

²⁾ Test performed on preparation (OESC 100g ai/l). Value expressed as active substance.

³⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98.2-98.9 %.

The most sensitive of the tested species was the aquatic invertebrate *Chaoborus crystallinus*, with an EC₅₀ of 0.00007 mg/L and NOEC 0.000001 mg/L. Since the most sensitive life stage was included, this study is regarded as a long term study.

The microcosm study, addresses long term effects and potential for recovery under more realistic exposure conditions. According to the microcosm studie, is crustacea the most sensitive group of organisms, for alpha-cypermethrin. Although the results could not be directly compared with those from laboratory, it can be anticipated that the *Chaoborus crystallinus* NOEC would cover possible effects in the field. Therefore, an assessment factor of 1 is used, together with the NOEC, resulting in a PNEC of 1.0×10^{-6} mg/L.

1.3 Bioaccumulation and persistence

Alpha-cypermethrin has bioaccumulation potential. BCF is 1204 in fish. Photolysis in water is very slow. Hydrolysis is pH-dependent with rapid degradation at higher pH and very slow degradation at low pH. In water/sediment systems, *alpha-cypermethrin* was rapidly partitioned to the sediment, with a DT₅₀ in the water phase of 0.4-2.1 days. Major metabolites were *phenoxybenzoic acid* and *cyclopropane carboxylic acid*, both significantly less toxic than the parent compound (3).

1.4 Proposed water quality objective

Since PNEC is 1.2×10^{-6} mg/L, the proposed water quality objective for *alpha-cypermethrin* is 1×10^{-6} mg/L.

1.5 Comments

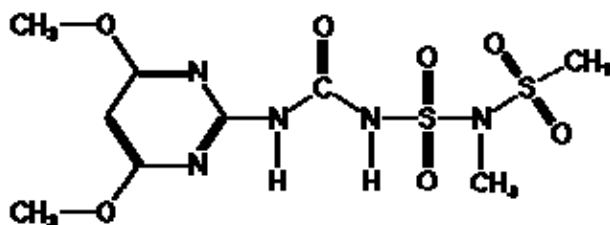
Alpha-cypermethrin is practically immobile in soil. In water-sediment systems the active substance is strongly bound to the sediment; therefore a quality objective for sediment may be relevant. The major metabolites are shared between the water and the sediment. Because of bioaccumulation potential of *alpha-cypermethrin*, a quality objective for biota may be considered.

1.6 Literature

- (1) European Commission Peer Review Programme. *Alpha-cypermethrin* Monograph, 1999. Rapporteur Member State: Belgium.
- (2) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (3) European Commission Peer Review Programme. *Alpha-cypermethrin* List of end points, 2003. Rapporteur Member State: Belgium.
- (4) European Commission Peer Review Programme. *Alpha-cypermethrin* Addendum to the monograph, Annex B, Ecotoxicology, 2003 Rapporteur Member State: Belgium.

1. Amidosulfuron

Amidosulfuron is a selective sulfonylurea herbicide intended for use in cereals and pasture. The mode of action is by inhibition of acetolactate synthesis and thereby plant growth is inhibited.



1.1 Physico-chemical properties

Physico-chemical properties of *amidosulfuron* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *amidosulfuron*.

		Reference
CAS-No.	120923-37-7	2
Empirical formula	C ₉ H ₁₅ N ₅ O ₇ S ₂	2
Molecular weight [g/mol]	369	2
Solubility in water [mg/kg]	3.3 at pH 3 13500 at pH 10	2
pKa	3.58	2
Vapour pressure [Pa]	1.3 × 10 ⁻⁵ at 20°	2
Log K _{ow}	1.63	2
Henry's law constant [Pa×m ³ /mol]	5.34 × 10 ⁻⁴ at 20°	2

1.2 Toxicity to aquatic organisms

The toxicity of *amidosulfuron* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *amidosulfuron*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth	72h	E _b C ₅₀ 93 ¹⁾ NOEC 1.4 ¹⁾	1
Aquatic organism				
<i>Lemna gibba</i>	frond number	14d, semi-static	IC ₅₀ 0.018 ²⁾ NOEC 0.0087	2

Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 36	2
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 55	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 142 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 1	3
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 24 ¹⁾	1
Mollusc				
<i>Mysidopsis bahia</i>		96h, static	EC ₅₀ 75	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h	LC ₅₀ >320	1
<i>Lepomis macrochirus</i>	mortality	96h	LC ₅₀ >100	1
<i>Cyprinodon variegates</i>	mortality	96h	LC ₅₀ >94	1
<i>Onchorhynchus mykiss</i>	mortality	96h	LC ₅₀ 114 ¹⁾	1
<i>Cyprinodon variegates</i>	mortality	96h	LC ₅₀ 340 ¹⁾	1
<i>Onchorhynchus mykiss</i>	behaviour	21d	NOEC 10	1
<i>Onchorhynchus mykiss</i>	behaviour	21d	NOEC 0.76 ¹⁾	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an IC₅₀ of 0.018 mg/L and a NOEC of 0.0087 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest IC₅₀ of 0.018 mg/L is divided by a factor of 100, which results in a PNEC of 0.00018 mg/L.

1.3 Bioaccumulation and persistence

Amidosulfuron is not expected to bioaccumulate. In environmental pH, hydrolysis of *amidosulfuron* is very slow. In sediment/water systems the primary degradation occurs with a DT₅₀ of 57-121 days. *Amidosulfuron* is transformed into two metabolites: *2-amino-4,6-dihydroxypyrimidine (HOE 094206)* and *4,6-dimethylpyrimidine-2-ylcarbamoil-amidosulfuric acid (HOE 101630)*. The parent compound and metabolites remain in the water phase with only small fraction found in the sediment extracts. Based on available studies (4) the metabolites are not toxic to aquatic organisms.

1.4 Proposed water quality objective

Since PNEC is 0.00018 mg/L, the proposed water quality standard for *amidosulfuron* is 2×10^{-4} mg/L.

1.5 *Comments*

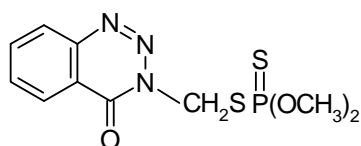
Amidosulfuron and its metabolites show high mobility in soil and have potential to leach through the soil profile.

1.6 *Literature*

- (1) Morka H., 1995, *Ecotoxicological evaluation of amidosulfuron*, Norwegian Agricultural Inspection Service.
- (2) *Evaluation of Amidosulfuron*, Food and Environment Protection Act 1985, Part III, Control of Pesticides Regulations 1986, Ministry of Agriculture, Fisheries and Food, Pesticides Safety Directorate, No 91, 1994.
- (3) Bogers et al., 1996 GRATIL/Amidosulfuron, Summary of environmental fate, path H. File no 96/5578.
- (4) Elzvik A., 1996. *Ecotoxicological Evaluation of the Herbicide Amidosulfuron-Supplementary Documentation*. The National Chemicals Inspectorate.

1. Azinphos-methyl

Azinphos-methyl is an organophosphorous insecticide/acaricide intended for use in fruit cultivation. *Azinphos-methyl* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *azinphos-methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *azinphos-methyl*.

		Reference
CAS-No.	86-50-0	1
Empirical formula	C ₁₀ H ₁₂ N ₃ O ₃ PS ₂	1
Molecular weight [g/mol]	317.1	1
Solubility in water [mg/kg]	27.9±1,6	1
Vapour pressure [Pa]	1.8×10 ⁻⁴ at 20°C 3.1×10 ⁻⁴ at 25°C	1
Log P _{ow}	2.87≤P _{ow} ≤3.02 mean=2.96	1
Henry's law constant [Pa×m ³ /mol]	2.0×10 ⁻³ at 20°C	1

1.2 Toxicity to aquatic organisms

The toxicity of *azinphos-methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *azinphos-methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth	96 h, static	EC ₅₀ 3.61 NOEC 1.8	1
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48 h, flow-through	EC ₅₀ 4.4 ¹⁾	1
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 6.7 ¹⁾	1
<i>Daphnia magna</i>	immobilisation	48h, static	EC ₅₀ 0.0011 (nominal)	
<i>Mysidopsis bahia</i>	mortality	96 h	LC ₅₀ 0.00021 ²⁾	2
<i>Daphnia magna</i>	reproduction	21 d, flow-trough	NOEC 0.00025	1
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 5.3 ¹⁾	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 6.2 ¹⁾	1
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 8.8 ¹⁾	1
<i>Oncorhynchus mykiss</i>	sublethal effects	21 d, flow-trough	NOEC 0.00039	1
<i>Oncorhynchus</i>		85 d, flow-through	NOEC 0.00044	1

<i>mykiss</i>				
<i>Oncorhynchus mykiss</i>	behaviour	85 d, flow-through	NOEC 0.00023	1
Mesocosm				
		10 weeks, out doors	NOEC _{community} 0.00032 ¹⁾ EAC 0.001 ¹⁾	3
<i>Long term fish Water/sediment</i>		21 d	NOEC 0.00064 ¹⁾	3

¹⁾ Test performed on preparation (Guthion 50 WP, 50%as, Guthion 2S 22%, Guthion 2E, 23.8% and Gusathion M WP 25). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 88.8%.

The most sensitive (acute effects) of the tested species was *Mysidopsis bahia*, with a LC₅₀ of 0.00021 mg/L. Since the acute/chronic ratio is low, a PNEC based on long term effect does not guarantee appropriate protection against acute effects. Hence, the PNEC is based on acute toxicity data. The lowest LC₅₀ of 0.00021 mg/L is divided by a factor of 100, which results in a PNEC of 0.0000021 mg/L.

1.3 Bioaccumulation and persistence

Bioaccumulation is not considered to be important because of rapid transformation of *azinphos-methyl* in water. Photolysis markedly accelerates in the presence of light and hydrolytic half-lives range between 4 and 87 days. The degradation rate is pH dependent, with decreasing half-lives with increasing pH.

1.4 Proposed water quality objective

Since PNEC is 2.1×10^{-6} mg/L, the proposed water quality objective for substance is 2×10^{-6} mg/L.

1.5 Comments

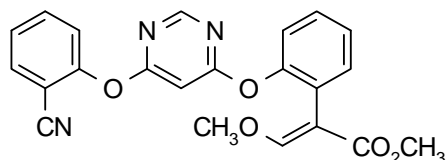
Mobility of *azinphos-methyl* in soil is low. The high K_{oc}-value indicates that a quality objective for sediment may be relevant.

1.6 Literature

- (1) European Commission Peer Review Programme. *Azinphos-methyl* Monograph (draft), 1996. Rapporteur Member State: Germany.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *Azinphos-methyl* Review Report, 2003. Rapporteur Member State: Germany.

1. Azoxystrobin

The strobilurin *azoxystrobin* is a systemic fungicide, intended for use in cereals, oleiferous plants and potatoes. *Azoxystrobin* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *azoxystrobin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *azoxystrobin*.

		Reference
CAS-No.	131860-33-8	1
Empirical formula	C ₂₂ H ₁₇ N ₃ O ₅	1
Molecular weight [g/mol]	403.4	1
Solubility in water [mg/kg]	6.7 at pH 5.2, 20°C 6.7 at pH 7.0, 20°C 5.9 at pH 9.2, 20°C	1
Vapour pressure [Pa]	1.1×10 ⁻¹⁰ (extrapolated)	1
Log P _{ow}	2.5 at 20°C	1
Henry's law constant [Pa×m ³ /mol]	7.3×10 ⁻⁹	1

1.2 Toxicity to aquatic organisms

The toxicity of *azoxystrobin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *azoxystrobin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	96 h, static	E _r C ₅₀ 2.0 NOEC 0.038	1
Higher aquatic plants				
<i>Lemna gibba</i>	not specified	14 d, static	EC ₅₀ 3.4 NOEC 0.8	2
Crustaceans				

<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.28	1
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.27	1
<i>Daphnia pulex</i>	immobilisation	48 h, static	EC ₅₀ 0.2	1
<i>Macrocyclus fuscus</i>	immobilisation	48 h, static	EC ₅₀ 0.13	1
<i>Chaoborus crystallinus</i>	immobilisation	48 h, static	EC ₅₀ 1.6	1
<i>Gammarus pulex</i>	immobilisation	48 h, static	EC ₅₀ 0.35	1
<i>Asellus aquaticus</i>	immobilisation	48 h, static	EC ₅₀ >4.00	1
<i>Daphnia magna</i>	growth, reproduction, survival	21 d, semi-static	NOEC 0.044	1, 2
<i>Mysidopsis bahia</i>		28 d, flow-through	NOEC 0.0095 ¹⁾	2
<i>Mysidopsis bahia</i>		96 h, static	EC ₅₀ 0.056	2
<i>Daphnia magna</i>		48 h, static	EC ₅₀ 0.259	2
Insecta				
<i>Chironimus riparius</i>	immobilisation	48 h, static	EC ₅₀ 0.21	1
<i>Ischnura elegans</i>	immobilisation	48 h, static	EC ₅₀ >4.0	1
<i>Cloeon dipterum</i>	immobilisation	48 h, static	EC ₅₀ 3.2	1
<i>Notonecta glauca</i>	immobilisation	48 h, static	EC ₅₀ >4.0	1
Molluscs				
<i>Crassostrea gigas</i>		48 h, static	EC ₅₀ 1.3	2
<i>Lymnea stagnalis</i>	immobilisation	48 h, static	EC ₅₀ >4.0	1
Rotifera				
<i>Brachionus calyciflorus</i>	immobilisation	48 h, static	EC ₅₀ >4.0	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96 h, flow-through	LC ₅₀ 0.47	1,2
<i>Cyprinus carpio</i>	mortality	96 h, flow-through	LC ₅₀ 1.6	1
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ 1.1	1,2
<i>Onchorhynchus mykiss</i>	mortality	28 d, flow-through	NOEC 0.16	1
<i>Pimephales promelas</i>	mortality and growth effects	28 d, flow-through	NOEC 0.147	1,2
<i>Cyprinodon variegatus</i>		96 h, flow-through	LC ₅₀ 0.671	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96.2%.

The most sensitive of the tested species was *Mysidopsis bahia*, with a NOEC of 0.0095 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *azoxystrobin* is calculated to 0.00095 mg/L.

1.3 Bioaccumulation and persistence

Azoxystrobin is not expected to bioaccumulate, the log P_{ow}- value of *azoxystrobin* is 2.5. Bioaccumulation studies are not relevant. *Azoxystrobin* is persistent, both in soil, sediment and water. In water/sediment systems degradation occurs with in a DT₅₀ of 34-57 days in water and 170-294 days in the whole system. *Azoxystrobin* is mainly partitioned into the sediment. One major metabolite is formed in water/sediment system: 2- (6-(2-cyanophenoxy)

pyrimidin-4-yloxy) phenyl)-3-methoxyacrylic acid. The metabolite is less toxic than *azoxystrobin* but persistent (1).

1.4 Proposed water quality objective

Since PNEC is 0.00095 mg/L, the proposed water quality objective for *azoxystrobin* is 0.0009 mg/L.

1.5 Comments

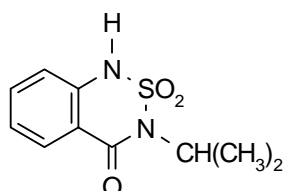
Azoxystrobin has a low to medium mobility in soil and may leach through the soil profile and reach surface- and ground water. Because the substance partition into the sediment additional quality objective for sediment should be established.

1.6 Literature

- (1) European Commission Peer Review Programme. *Azoxystrobin Monograph, 1997*. Rapporteur Member State: Germany.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA. Washington, D.C.

1. Bentazone

Bentazone is a weak acid working as a selective contact herbicide, intended for use in pasture and legumes *Bentazone* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *bentazone* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *bentazone*.

		Reference
CAS-No.	25057-89-0	1
Empirical formula	C ₁₀ H ₁₂ N ₂ O ₃ S	1
Molecular weight [g/mol]	240.3	1
Solubility in water [mg/kg]	490 at 20°C, pH 3 570 at 20°C, ~pH 7	1
pKa	3.3	3
Vapour pressure [Pa]	1.7×10 ⁻⁴ at 20 °C	1
Log P _{ow}	0.77 at pH 5, 22°C -0.46 at pH 7, 22°C -0.55 at pH 9, 22°C	1
Henry`s law constant [Pa×m ³ /mol]	7.2×10 ⁻⁵	1

1.2 Toxicity to aquatic organisms

The toxicity of *bentazone* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *bentazone*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Ankistrodesmus bibrainus</i>	not specified	72 h	EC ₅₀ 62 NOEC 5.0	1
<i>Ankistrodesmus bibrainus</i>	not specified	96 h	EC ₅₀ 47	1
<i>Ankistrodesmus bibrainus</i>	not specified	72 h	EC ₅₀ 69 ¹⁾ NOEC 4.7 ¹⁾	1
<i>Chlorinella fusca</i>	not specified	96 h	EC ₅₀ 236 ¹⁾	1
Higher aquatic plants				
<i>Lemna gibba</i>	not specified	14 d	EC ₅₀ 3.6 ^{1,2)} NOEC 2.7 ^{1,3)}	1, 2
Crustaceans				

<i>Daphnia magna</i>	immobility	96 h	EC ₅₀ 64	2
<i>Daphnia magna</i>	immobility	48 h	EC ₅₀ 58 ¹⁾	1
<i>Daphnia magna</i>	immobility	48 h	EC ₅₀ 125	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96 h	LC ₅₀ >100	1, 2
<i>Lepomis macrochirus</i>	mortality	96 h	LC ₅₀ >100	1
<i>Cyprinus carpio</i>	mortality	96 h	LC ₅₀ >910 ¹⁾	1

¹⁾ Test performed on two different salt compounds (67% ai and 91% ai). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of former PNEC. Test substance purity 67.27%.

³⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 3.6 mg/L and a NOEC of 2.7 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 3.6 mg/L is divided by a factor of 100, which results in a PNEC of 0.036 mg/L.

Revised EQS calculation according to EU-harmonised methodology (4)

There is only chronic data for algae and higher aquatic plants. The lowest of these is the NOEC for *Lemna gibba* of 2.7 mg/l. Aquatic plants seem to be the most sensitive trophic level. Bentazone is a selective herbicide, inhibiting the photosynthetic electron transfer, but short-term data for crustaceans indicates similar sensitivity as for algae. Short-term data for fish does not indicate that a long term study would result in a lower NOEC than that for plants. An assessment factor of 100 is proposed to be used on the lowest NOEC of 2.7 mg/L (even though it is not generated from fish or *Daphnia*) which results in a PNEC of 0.027 mg/L.

1.3 Bioaccumulation and persistence

Bentazone is not expected to bioaccumulate. Log Pow is lower than 3, therefore bioaccumulation study is not relevant. In water/sediment systems *bentazone* degrades very slowly. The substance is stable towards hydrolysis. In water phase the substance is degraded 62 -69% after 100 days. Degradation in the whole system varies with in a DT₅₀ of 500 to 900 days (1).

1.4 Proposed EQS/water quality objective

Since PNEC is 0.027 mg/L, the proposed EQS/water quality objective for *bentazone* is 0.027 mg/L.

1.5 Comments

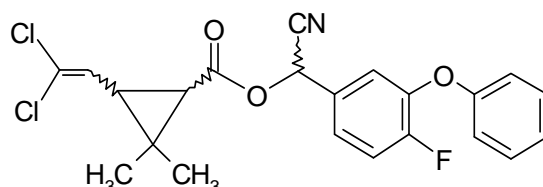
Bentazone is very mobile and may leach through the soil profile and therefore reach surface- and groundwater. In water/sediment systems the main portion of *bentazone* is located in the water phase (1).

1.6 Literature

- (1) European Commission Peer Review Programme. *Bentazone Monograph, 1996*. Rapporteur Member State: Germany.
- (2) European Commission Peer Review Programme. *Bentazone Review report. Appendix II -Endpoints and related information, 2000*. Rapporteur Member State: Germany.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (4) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. *beta*-Cyfluthrin

The pyrethroid *beta-cyfluthrin* is an insecticide, acting as a contact and stomach poison and exert neurotoxic effects. The insecticide is intended for use in fruit cultivation, potatoes and beets. *beta-Cyfluthrin* like *cyfluthrin* consists of four diastereomers, which are presenting in both active substances but in different percentages. *beta-Cyfluthrin* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *beta-cyfluthrin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *beta-cyfluthrin*.

		Reference
CAS-No.	68359-37-5	1
Empirical formula	C ₂₂ H ₁₈ Cl ₂ FNO ₃	1
Molecular weight [g/mol]	434.3	1
Solubility in water [mg/kg]	Isomer II 2.1 × 10 ⁻³ Isomer IV 1.2 × 10 ⁻³	1
pKa	No dissociation	1
Vapour pressure [Pa]	Isomer II 1.4 × 10 ⁻⁸ Isomer IV 8.5 × 10 ⁻⁸	1
Log P _{ow}	Isomer II 5.9 Isomer IV 5.9	1
Henry's law constant [Pa×m ³ /mol]	Isomer II 3.2 × 10 ⁻³ Isomer IV 1.3 × 10 ⁻²	1

1.2 Toxicity to aquatic organisms

The toxicity of *beta-cyfluthrin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *beta-cyfluthrin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scendesmus subspicatus</i>		96h, static	EC ₅₀ >0.01	1

Crustaceans				
<i>Daphnia magna</i>		48h, flow-through	EC ₅₀ 0.00029	1
<i>Ceriodaphnia dubia</i>	mortality	48h, static	EC ₅₀ 0.000014 ^{1,2)}	1
<i>Daphnia magna</i>		48h, static	EC ₅₀ 0.002 (nominal)	1
<i>Daphnia magna</i>	immobility	21d, flow-through	NOEC 0.00004 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, flow-through	NOEC 0.00002 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.0001 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.0001 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.000089	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.000068	1
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 0.00028	1
<i>Onchorhynchus mykiss</i>	mortality	58d, flow-through	NOEC 0.00001 ¹⁾	1
Mesocosm studie				
			EAC 50×10 ⁻⁶ NOEC _{community} 10×10 ⁻⁶	2

¹⁾ Studies using cyfluthrin as test compound.

²⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Ceriodaphnia dubia*, with a LC₅₀ of 0.000014 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest LC₅₀ of 0.000014 mg/L is divided by a factor of 100, which results in a PNEC of 1.4×10^{-7} mg/L.

1.3 Bioaccumulation and persistence

beta-Cyfluthrin has potential to bioaccumulate, BCF 506. *beta-Cyfluthrin* rapidly partitions into sediment from water phase. In neutral water the substance is stable, but hydrolyses within a DT₅₀ of <2 days in water with alkaline pH-value. In water/sediment systems DT₅₀ for the whole system varies between 0.22-3.5 days. Major metabolites in water are mainly DCVA (permetrin acid) and FPBacid. The metabolites show much lower toxicity to aquatic organisms than the parent compound.

1.4 Proposed water quality objective

Since PNEC is 1.4×10^{-7} mg/L, the proposed water quality standard for *beta-cyfluthrin* is 1×10^{-7} mg/L.

1.5 Comments

beta-Cyfluthrin binds strongly to organic material and is therefore not expected to leach through the soil profile. The substance is primarily degraded with a DT₅₀ of 48-54 days. Volatilisation from water surface may occur. Because the compound participates to sediment

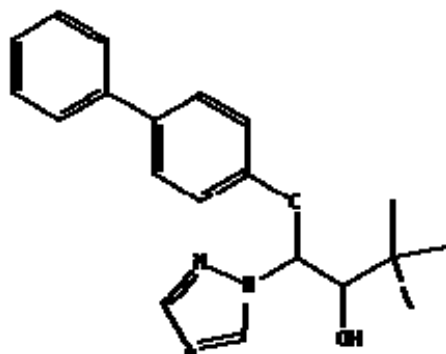
and soil further quality objectives are needed.

1.6 Literature

- (1) European Commission Peer Review Programme. *Beta-cyfluthrin Monograph, 1996.*
Rapporteur Member State: Germany.
- (2) European Commission Peer Review Programme. *Beta-cyfluthrin Review report, 2002.*
Rapporteur Member State: Germany.

1. Bitertanol

Bitertanol is a fungicide with both protective and curative effect. The mode of action is an inhibition of the sterol biosynthesis. The fungicide is intended for use in cultivation of fruit, winter cereals and as seed treatment. The substance consists of two diastereoisomers A and B.



1.1 Physico-chemical properties

Physico-chemical properties of *bitertanol* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *bitertanol*.

		Reference
CAS-No.	55179-31-2	1
Empirical formula	C ₂₀ H ₂₃ N ₃ O ₂	1
Molecular weight [g/mol]	337.4	1
Solubility in water [mg/kg]	1.6-2.9	1
pKa	Not relevant	1
Vapour pressure [Pa]	0.2-2.5 ×10 ⁻⁹ at 20°C	1
Log P _{ow}	4.1-4.4 at 20°C	1
Henry's law constant [Pa×m ³ /mol]	ca 10 ⁻⁸	1

1.2 Toxicity to aquatic organisms

The toxicity of *bitertanol* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *bitertanol*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth inhibition	96h, static	EC ₅₀ 0.31 ¹⁾	1
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 2.8	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 7.0	1
<i>Daphnia magna</i>	reproduction mortality	21d, flow-through	NOEC <0.15 NOEC 0.89	1
Fish				
<i>Leuciscus idus melanotus</i>	mortality	96h	LC ₅₀ 3.0	1
<i>Onchorhynchus mykiss</i>	mortality	96h	LC ₅₀ 2.7	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96%

The most sensitive of the tested species was *Scenedesmus subspicarius*, with an EC₅₀ of 0.31 mg/L. Only short term studies are reliable. NOEC derived from *Daphnia magna* is lower than 0.15 mg/L. A water quality objective based on NOEC will not guarantee appropriate protection against chronic effects. PNEC is therefore based on acute toxicity data, applied with an assessment factor of 1000 to protect from chronic effects. Hence, the lowest EC₅₀ of 0.31 mg/L is divided by a factor of 1000, which results in a PNEC of 0.00031 mg/L.

1.3 Bioaccumulation and persistence

Bitertanol is expected to bioaccumulate, BCF 175. *Biteranol* is stable towards hydrolysis at pH 4,7 and 9. Degradation in water/sediment systems occurs with a DT₅₀ of 24-27 days. The substance partitions into the sediment. No major metabolites, exceeding 10%, were found.

1.4 Proposed water quality objective

Since PNEC is 0.00031 mg/L, the proposed water quality standard for *bitertanol* is 3×10^{-4} mg/L.

1.5 Comments

The substance is strongly absorbed to particles. However the metabolites may reach surface- and ground water through the soil profile. A complementary quality objective for sediment is recommended.

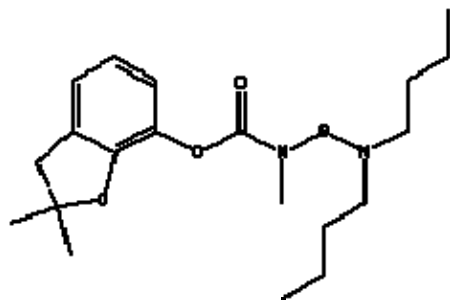
1.6 Literature

- (1) Lundberg I., 1991. *Ekotoxikologisk utvärdering av fungiciden bitertanol*. Kemikalieinspektionen, Sverige.

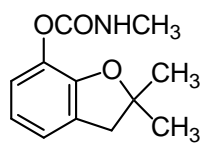
1. Carbosulfan and carbofuran

Carbosulfan is a systemic carbamate insecticide, chlorinesterase inhibitor, with contact and stomach action. It is intended for use as seed dressing in sugar beets and oleiferous plants.

Carbofuran is the main metabolite, with insecticidal activity. *Carbosulfan* and *carbofuran* are under evaluation within the framework of EU Dir. 91/414.



Carbosulfan



Carbofuran

1.1 Physico-chemical properties

Physico-chemical properties of *carbosulfan* are summarised in table 1.1.1.

Table 1.1.1: Physico-chemical properties of *carbosulfan*.

		Reference
CAS-No.	55285-14-8	1
Empirical formula	C ₂₀ H ₃₂ N ₂ O ₃ S	1
Molecular weight [g/mol]	380.6	1
Solubility in water [mg/kg]	0.3 at 25°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	0.021 at 20°C	1
Log P _{ow}	1.2-1.5	1
Henry's law constant [Pa×m ³ /mol]	5.2 × 10 ⁻² at 25°C	1

Physico-chemical properties of *carbofuran* are summarised in table 1.1.2.

Table 1.1.2: Physico-chemical properties of *carbofuran*.

		Reference
CAS-No.	1563-66-2	1
Empirical formula	C ₁₂ H ₁₅ NO ₃	1
Molecular weight [g/mol]	221.3	1
Solubility in water [mg/kg]	260-700 at 25°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	6.9 at 25°C	1
Log P _{ow}	1.2-1.5	1
Henry's law constant [Pa×m ³ /mol]	2.2-5.9 × 10 ⁻³ at 25°C	1

1.2 Toxicity to aquatic organisms

The toxicity of *carbosulfan* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *carbosulfan*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scendesmus subspicatus</i>	Growth rate	96h, static	EC ₅₀ >17.3 NOEC 17.3	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.0015 ¹⁾	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.0024	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.0032	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	EC ₅₀ 0.015	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ 0.042	1
<i>Lepomis macrochirus</i>	mortality	96h, static	EC ₅₀ 0.015	1
<i>Onchorhynchus mykiss</i>	growth	21d, flow-through	NOEC 0.016	1

¹⁾ Effect concentration basis for calculation of PNEC. Carbosulfan technical, no purity reported.

The most sensitive (acute effects) of the tested species was *Daphnia magna*, with an EC₅₀ of 0.0015 mg/L and. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.0015 mg/L is divided by a factor of 100, which results in a PNEC of 0.000015 mg/L.

The toxicity of *carbofuran* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *carbofuran*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Daphnia magna</i>		48h, static	EC ₅₀ 0.039	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.029	2
<i>Daphnia magna</i>		21d, flow-through	NOEC 0.0098	2
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.13	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.36	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.38	2
<i>Ictalurus punctatus</i>	mortality	96h, static	LC ₅₀ 0.25	2
<i>Salmo trutta</i>	mortality	96h, static	LC ₅₀ 0.28	2
<i>Salvelinus namaychirus</i>	mortality	96h, flow-through	LC ₅₀ 0.16	2
<i>Menidia menidia</i>	mortality	96h, flow-through	LC ₅₀ 0.033	2
<i>Onchorhynchus mykiss (ErlyLf)</i>	mortality	14d, flow-through	NOEC 0.025	2
<i>Cyprinidon variegates (ErlyLf)</i>	growth	32d, flow-through	NOEC 0.0026 ¹⁾	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98%

The most sensitive of the tested species was *Cyprinodon variegatus*, with a NOEC 0.0026 mg/L. Since both short and long term studies are available, and two trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *carbofuran* is calculated to 0.00026 mg/L.

1.3 Bioaccumulation and persistence

The potential for bioaccumulation appears to be low for both *carbosulfan* and *carbofuran*. *Carbosulfan* is hydrolysed under acid conditions, DT₅₀ <1h at pH 4, and more slowly transformed at higher pH, DT₅₀ 14d at pH 8. Hydrolysis of *carbofuran* is the opposite, stable under acid conditions and rapidly degraded under basic conditions. At neutral pH, the transformation rate is moderate. Anaerobic degradation of *carbofuran* has been studied in two water/sediment and water/soil systems at pH 6.8-6.9, DT₅₀ were 48 and 38 days respectively, based on whole system. No major metabolites, exceeding 10%, were found.

1.4 Proposed water quality objective

Carbosulfan

Since PNEC is 0.000015 mg/L, the proposed water quality standard for *carbosulfan* is 0.00001 mg/L.

Carbofuran

Since PNEC is 0.00026 mg/L, the proposed water quality standard for *carbofuran* is 0.0003 mg/L.

1.5 Comments

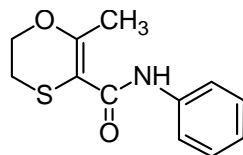
Carbosulfan is strongly bound to soil. However *carbofuran* may leach through the soil profile and reach surface- and groundwater.

1.6 Literature

- (1) Dryselius, Hagelin, Sandberg, 1995. *Ecotoxicological evaluation of carbosulfan supplementary documentation*. Kemikalieinspektionen, Sverige
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Carboxin/ carboxin sulfoxide

Carboxin is a systemic fungicide, chemically classified as an anilide. The fungicide is used for seed dressing of cereals.



1.1 Physico-chemical properties

Physico-chemical properties of *carboxin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *carboxin*.

	carboxin	Carboxin sulfoxide	Reference
CAS-No.	5234-68-4		1
Empirical formula	C ₁₂ H ₁₃ O ₂ S ₁ N ₁	C ₁₂ H ₁₃ O ₃ S ₁ N ₁	1
Molecular weight [g/mol]	235	251	1
Solubility in water [mg/kg]	170 at 25°C		1
pKa	<0.5		3
Vapour pressure [Pa]	2 × 10 ⁻⁵		3
Log P _{ow}	2.1		1
Henry's law constant [Pa×m ³ /mol]	3.24 × 10 ⁻⁵		3

1.2 Toxicity to aquatic organisms

The toxicity of *carboxin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *carboxin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Chlorella pyrenoidosa</i>	growth rate	72h, static	E _r C ₅₀ 5.5 NOEC 1.0	1
Higher aquatic plants				
<i>Lemna gibba</i>	growth rate	14d, static	E _r C ₅₀ 0.67 NOEC 0.15 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	mortality	48h, static	EC ₅₀ 84.4	1
<i>Daphnia magna</i>	reproduction	17d, semi-static	NOEC 0.32	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 1.2	2
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 2.0	2
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 3.6	2

<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 2.3	2
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¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97.5%

The most sensitive of the tested species was *Lemna gibba*, with a NOEC of 0.15 mg/L. Short term studies for three trophic levels and long term studies for two trophic levels are available. Hence, an assessment factor of 50 is used for calculation of the predicted no effect concentration and, the PNEC for *carboxin* is calculated to 0.003 mg/L.

1.3 Bioaccumulation and persistence

Carboxin has a moderate potential for bioaccumulation, log P_{ow} 2.1. *Carboxin* is stable towards hydrolysis at environmental pH, 5-9. The transformation in soil of *carboxin* to the more persistent *carboxin-sulfoxide* is fast (DT₅₀<1day). This indicates that the substance reaching the recipient would mainly be *carboxin-sulfoxide* and only a smaller amount of *carboxin* (1). Adequate studies for degradation of *carboxin* in water are not available.

1.4 Proposed water quality objective

Since PNEC is 0.003 mg/L, the proposed water quality standard for *carboxin* is 0.003 mg/L. Since the parent compound will probably not reach surface water, the corresponding value for *carboxin-sulfoxide* is more relevant.

1.5 Comments

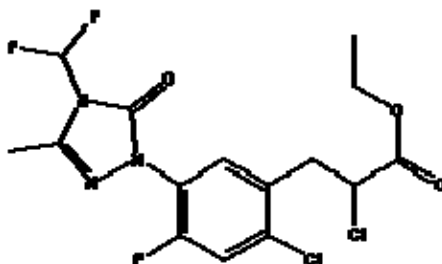
Carboxin has potential for mobility, and may reach ground and surface water via transport through the soil profile. In monitoring studies it is more likely to find *carboxin* as the metabolite *carboxin sulfoxide*.

1.6 Literature

- (1) Pedersen A., 1992. *Ecotoxicological evaluation of carboxin*. Scientific documentation and research. National Chemical Inspectorate. Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Carfentrazone-ethyl and its metabolites: F8426-chloropropionic acid & F8426-cinnamic acid

Carfentrazone-ethyl is an herbicide. Treatment of weeds causes a rapid destruction of sensitive tissues leading to necrosis. The herbicide is intended for use in cereals and potatoes. *Carfentrazone-ethyl* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *carfentrazone-ethyl* are summarised in table 1.1.

Table 1.1.1: Physico-chemical properties of *carfentrazone-ethyl*.

		Reference
CAS-No.	128639-02-1	1
Empirical formula	C ₁₅ H ₁₄ Cl ₂ N ₃ O ₃ F ₃	1
Molecular weight [g/mol]	412.19	1
Solubility in water [mg/kg]	12 at pH7 and 20°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	7.2 × 10 ⁻⁶	1
Log P _{ow}	3.36	1
Henry's law constant [Pa×m ³ /mol]	2.5 × 10 ⁻⁴	1

Physico-chemical properties of *chloropropionic acid* and *cinnamic acid* are summarised in table 1.1.2.

Table 1.1.2: Physico-chemical properties of relevant metabolites.

	Chloropropionic acid	Cinnamic acid	Reference
CAS-No.	128621-72-7		3
Empirical formula	C ₁₃ H ₁₀ Cl ₂ N ₃ O ₃ F ₃	C ₁₃ H ₁₀ ClN ₃ O ₃ F ₃	3
Molecular weight [g/mol]	384.14	ca 350	3
Solubility in water [mg/kg]	2382 at pH 4 488 at pH 6.3 17 at pH 10	18.3 at pH 4 34.6 at pH 6.3 267 at pH 267	3
pKa	2.66	4.83	3

Vapour pressure [Pa]	1.07×10^{-7}	3.13×10^{-10}	3
Log P _{ow}	8.6 at pH 4 and 25°C 5.71 at pH 6 0.06 at pH 10	129 at pH 4 8.21 at pH 6.3 0.04 at pH 10	3
Henry's law constant [Pa×m ³ /mol]	2.92×10^{-7}		3

1.2 Toxicity to aquatic organisms

The toxicity of *carfentrazone-ethyl* to aquatic organisms is summarised in table 1.2.

Table 1.2.1: Aquatic ecotoxicity data of *carfentrazone-ethyl*.

Species	End-point	Exposure duration and formulation	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	72h, static	ErC ₅₀ 0.017 NOEC 0.008	1
<i>Anabaena flos-aquae</i>	growth rate	72h, static	ErC ₅₀ 0.012 NOEC 0.002	1
Aquatic plants				
<i>Lemna gibba</i>	growth	14d, static	EC ₅₀ 0.0057 ¹⁾ NOEC 0.0022	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, flow-through	EC ₅₀ >9.8	1
<i>Daphnia magna</i>	immobility	21d, flow-through	EC ₅₀ 0.22	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.6	1
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 2	1
<i>Onchorhynchus mykiss</i>	mortality	28d, flow-through	NOEC 0.11	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 91.7%

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0057 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.0057 mg/L is divided by a factor of 100, which results in a PNEC of 0.000057 mg/L.

The toxicity of F8426-*chloropropionic acid* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of F8426-*chloropropionic acid*.

Species	End-point	Exposure duration and formulation	Result [mg/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	72h, static	ErC ₅₀ 0.787 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ >101	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ >92.2	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 0.79 mg/L. Since only short-term studies are available, and three trophic levels are tested, an assessment factor of 1000 is used for calculation of the predicted no effect concentration. Hence, the PNEC for F8426-chloropropionic acid is calculated to 0.0007 mg/L.

The toxicity of *F8426-cinnamic acid* to aquatic organisms is summarised in table 1.2.3.

Table 1.2.3: Aquatic ecotoxicity data of *F8426-cinnamic acid*.

Species	End-point	Exposure duration and formulation	Result [mg/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	Growth rate	72h, static	ErC ₅₀ 0.0372 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	Immobility	48h, static	EC ₅₀ >10.7	1
Fish				
<i>Onchorhynchus mykiss</i>	Mortality	96h, flow-through	LC ₅₀ >25.4	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 0.0372 mg/L. Since only short-term studies are available, and three trophic levels are tested, an assessment factor of 1000 is used for calculation of the predicted no effect concentration. Hence, the PNEC for F8426-chloropropionic acid is calculated to 0.0000372 mg/L.

1.4 Bioaccumulation and persistence

Carfentrazone-ethyl is expected to bioaccumulate. Although Log P_{ow} is high, BCF values in fish were moderate. *Carfentrazone-ethyl* is hydrolytically stable in water at pH 5. Degradation occurs at pH 7 and 9 with DT₅₀ 13.7 and 5.1 respectively. In a water/sediment study performed at pH 7.85-8.07 in water phase, the substance was rapidly degraded, with DT₅₀ of < 0.4 days in the water phase as well as whole system. *F8426-chloropropionic acid* is the main degradation product and is transformed with in a DT₅₀ of 67 days. Other metabolites are *F8426-cinnamic* and *benzoic acids*. The metabolites, with exception for benzoic acid show high toxicity towards algae. Separate water quality objectives for the metabolites are therefore established.

1.3 Proposed water quality objective

Carfentrazone-ethyl:

Since PNEC is 0.000057 mg/L, the proposed water quality standard for *carfentrazone-ethyl* is 6×10⁻⁵ mg/L.

F8426-chloropropionic acid:

Since PNEC is 0.00079 mg/L, the proposed water quality standard for *F8426-chloropropionic acid* is 8×10⁻⁴ mg/L.

F8426-cinnamid acid:

Since PNEC is 0.000037 mg/L, the proposed water quality standard for *F8426-cinnamid acid* is 4×10^{-5} mg/L.

1.4 *Comments*

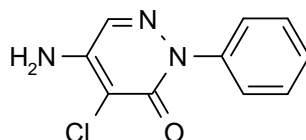
Carfentrazone-ethyl is rapidly transformed in soil. Route of degradation results in the same transformation products as in water. The metabolites are mobile in soil and may have a potential to leach through the soil profile. *Carfentrazone-ethyl* is not expected to volatilise.

1.5 *Literature*

- (1) European Commission Peer Review Programme. *Carfentrazone-ethyl Monograph*, 1998. Rapporteur Member State: France.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *Carfentrazone-ethyl Addendum Physical and chemical properties of the carfentrazone-chloropropionic acid*. Rapporteur Member State: France.

1. Chloridazon

Chloridazon is a selective systemic herbicide used against dicotyledonous weeds in beets and vegetables. The substance has not been evaluated within the EU Review Programme.



1.1 Physico-chemical properties

Physico-chemical properties of *chloridazon* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *chloridazon*.

		Reference
CAS-No.	1698-60-8	4
Empirical formula	C ₁₀ H ₈ ClN ₃ O	4
Molecular weight [g/mol]	221.6	4
Solubility in water [mg/kg]	340 at 20°C	5
Vapour pressure [Pa]	<10 at 20°C	5
Log P _{ow}	1.19 at pH 7	5
Henry's law constant [Pa×m ³ ×mol]	<6.52×10 ⁻⁶ at 20°C	5

1.2 Toxicity to aquatic organisms

The toxicity of *chloridazon* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *chloridazon*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Ankistrodesmus bibrainus</i>	biomass	72 h	EC ₅₀ 0.6 NOEC 0.03 ³⁾	1
<i>Ankistrodesmus bibrainus</i>	growth rate	72 h	EC ₅₀ > 3.0 NOEC 0.42	6
Aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ >4.6 NOEC 2.9	3
<i>Lemna gibba</i>	growth	7 d	EC ₅₀ > 3.16 NOEC 0.1 ⁴⁾	6
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 132	1
<i>Daphnia magna</i>	immobilisation	48 h	EC ₅₀ 0.15 ²⁾	2
<i>Daphnia magna</i>	reproduction	21 d	NOEC 10	1
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ 30-66 ¹⁾	4

<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ 29 ²⁾	2
<i>Lebistes reticulatus</i>	mortality	96 h	LC ₅₀ 66 ²⁾	2
<i>Carassius auratus</i>	mortality	96 h	LC ₅₀ 129 ²⁾	2
<i>Cyprinus carpio</i>	mortality	96 h	LC ₅₀ 109 ²⁾	2
<i>Oncorhynchus mykiss</i>	growth	28 d, flow-trough	NOEC 3.2	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Test performed on technical substance >84% purity. Value recalculated on basis of 84% active substance.

³⁾ Effect concentration basis for calculation of former PNEC. Test substance purity >84%.

⁴⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The lowest EC₅₀ in short-term tests was *Daphnia magna*, with an LC₅₀-value of 0.15 mg/L in one study. However, this value is considered to be an outlier, since it is much lower than in a corresponding test on the same species, and than the long term NOEC for the same species. Hence, it is concluded that algae are the most sensitive group, showing an EC₅₀ of 0.6 mg/L and a NOEC of 0.03 mg/L from *Ankistrodesmus bibraianus*. Since both short- and long-term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for chloridazon is calculated to 0.003 mg/L.

Revised EQS calculation according to EU-harmonised methodology (7)

Growth rate should be preferred as end-point in toxicity tests with algae, and as the NOEC_{growth} for *Pseudokirchneriella subcapitata* (syn. *Ankistrodesmus bibraianus*) is 0.42 mg/L, the most sensitive species is instead *Lemna gibba* with a NOEC_{growth} of 0.1 mg/L. Since both short- and long-term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for chloridazon is calculated to 0.01 mg/L.

1.3 Bioaccumulation and persistence

Based on the low log P_{ow} value, the substance is not expected to bioaccumulate. The degradation is mainly a microbial process and breakdown in water is very slow. Degradation is retarded at low pH. *Chloridazon* is stable to hydrolysis. Photolysis in water is relatively slow with 50% breakdown in one month.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.01 mg/L, the proposed EQS/water quality objective for the substance is 0.01 mg/L.

1.5 Comments

Adsorption to soil may be medium to weak, and therefore *chloridazon* is expected to be mobile in soil. The high mobility together with the slow breakdown indicates possible

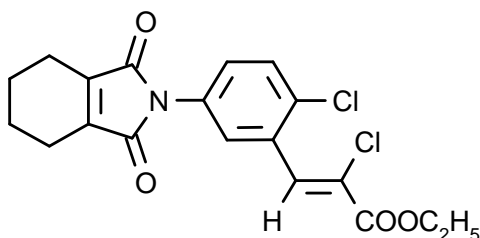
findings of *chloridazon* in aquatic systems. The metabolite *4-amino-5-chlor-6-pyridazon* is very persistent and may be of concern.

1.6 Literature

- (1) Bogers, M. et. al., 1996, *Summary of environmental fate and environmental risk assessment*, Notox proj. No. 183419, RIVM, The Netherlands.
- (2) Plassche, E.V.D and Linders, J., 1990, *Adviesrapport 88/678801/042, Chloridazon (definitieve versie: M 73)*, RIVM, The Netherlands.
- (3) Pesticide Ecotoxicity Database, 2001, Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (4) Stenström, J. & Torstensson, L., 1994, *Ecotoxicological evaluation of chloridazon*, Swedish University of Agricultural Sciences, Department of Microbiology, Uppsala.
- (5) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (6) European Commission Peer Review Programme. *Chloridazon* Draft Assessment Report vol 1, 2005. Rapporteur Member State: Germany.
- (7) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Cinidon-ethyl

Cinidon-ethyl is a selective contact acting herbicide belonging to the isoindoldione class of compounds. The herbicide is intended for use in winter cereals. *Cinidon-ethyl* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *cinidon-ethyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *cinidon-ethyl*.

		Reference
CAS-No.	142891-20-1	1
Empirical formula	C ₁₉ H ₁₇ Cl ₂ NO ₄	1
Molecular weight [g/mol]	394.3	1
Solubility in water [mg/kg]	0.057 at 20°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	<1 × 10 ⁻⁵	1
Log P _{ow}	4.5	1
Henry's law constant [Pa×m ³ /mol]	6.91 × 10 ⁻²	1

1.2 Toxicity to aquatic organisms

The toxicity of *cinidon-ethyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *cinidon-ethyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudo-krichneriella subcapitata</i>	growth rate	72h, static	E _r C ₅₀ 0.098 nominal NOEC _r 0.007 ²⁾	1
<i>Anabaena flos-aquae</i>	growth rate	72h, static	E _r C ₅₀ 1.53 nominal	1
Aquatic plants				
<i>Lemna gibba</i>	growth rate	7d, static	E _r C ₅₀ 0.602 nominal NOEC _r 0.122 nominal	1

Crustaceans				
<i>Daphnia magna</i>		48h, static	EC ₅₀ 59 nominal	1
<i>Daphnia magna</i>		48h, static	EC ₅₀ 0.63 nominal ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.11	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.012 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 1 ¹⁾	1
<i>Onchorhynchus mykiss</i>	mortality	28d, flow-through	NOEC 1.0 nominal	1
<i>Onchorhynchus mykiss</i>	growth	28d, flow-through	NOEC 0.25 ¹⁾	1

¹⁾ Test performed on preparation (Lotus 20% as). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96.5%

The most sensitive of the tested species was *Pseudo-kirchneriella subcapitata*, with a NOEC of 0.007 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for cinidon-ethyl is calculated to 0.0007 mg/L.

1.3 Bioaccumulation and persistence

Although log P_{ow} is high, due to rapid metabolism and depuration, *cinidon-ethyl* is not expected to bioaccumulate. *Cinidon-ethyl* is rapidly transformed in water, mainly by hydrolysis. The DT₅₀ varies from 54 minutes to 5 days, depending on the pH. In available water/sediment degradation studies the half time in the whole system is 5 hours at pH 5.9-6.4 in sediment and pH ca 6-8 in water phase. Following metabolites are formed: 615M10, 615M16, 615M01 and 615M45. However only 615M01 and 615M10 are considered as major metabolites; exceed 10% and not transient. Studies performed on metabolite 615M10 showed low toxic toward aquatic organisms.

1.4 Proposed water quality objective

Since PNEC is 0.0007 mg/L, the proposed water quality standard for *cinidon-ethyl* is 7×10⁻⁴ mg/L.

1.5 Comments

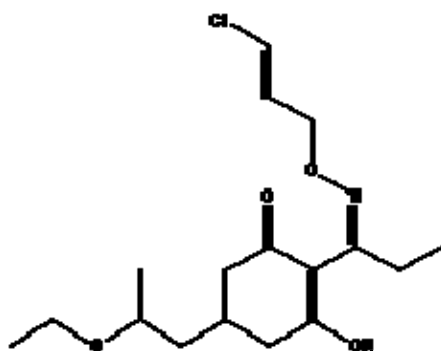
Cinidon-ethyl and its metabolites are mainly kept in water phase. Degradation in soil is similar to water. *Cinidon-ethyl* is rapidly transformed, DT₅₀ 6 days, into metabolites. The metabolites are more persistent than their parent compound, DT₅₀ 25-27 days but less toxic. *Cinidon-ethyl* is not mobile in soil. Metabolites show higher mobility than the parent compound, however the risk for leaching through the soil profile is considered low.

1.6 Literature

- (1) European Commission Peer Review Programme. *Cinidon-ethyl Monograph, 1998.*
Rapporteur Member State: United Kingdom.

1. Clethodim

Clethodim is a member of the 1,3 cyclohexodine group of herbicides and an organic acid. The herbicide is systemic, rapidly absorbed and readily translocated from treated foliage to the root system and growing parts of the plant. Intended for use in cultivation of strawberries, beets, potatoes and oleiferous crops.



1.1 Physico-chemical properties

Physico-chemical properties of *clethodim* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *clethodim*.

		Reference
CAS-No.	99129-21-2	1
Empirical formula	C ₁₇ H ₂₆ ClNO ₃ S	1
Molecular weight [g/mol]	359	1
Solubility in water [mg/kg]	100 at pH 5 5000 at pH 7 10000 at pH 8	1
pKa	4.5	1
Vapour pressure [Pa]	<1×10 ⁻²	3
Log P _{ow}	4.1-4.2	1
Henry's law constant [Pa×m ³ /mol]	1.3 × 10 ⁻¹⁰	4

1.2 Toxicity to aquatic organisms

The toxicity of *clethodim* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *clethodim*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scendesmus subspicatus</i>	growth rate	96h, static	EC ₅₀ 48	5
Aquatic plant				
<i>Lemna gibba</i>	growth rate	14d, static	EC ₅₀ 1.0 ^{1,2)} NOEC 0.3 ¹⁾	2
Crustaceans				

<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ >100	3,5
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 54	5
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 16 ¹⁾	2
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 27 ¹⁾	2
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 46 ¹⁾	3
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ >100 ¹⁾	3

¹⁾ Test performed on substance with purity <90%. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 82.4%

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 1.0 mg/L and (chronic effects) NOEC 0.3 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Long term studies have been performed on two trophic levels, crustaceans and aquatic plants. Herbicide is expected to be most toxic towards plants. It is therefore likely that the most sensitive organism group have been tested for acute- and chronic toxicity. Hence, the lowest EC₅₀ of 1.0 mg/L is divided by a factor of 100, which results in a PNEC of 0.01 mg/L.

1.3 Bioaccumulation and persistence

Log P_{ow} is high indicates potential for bioaccumulation. However BCF is very low, 0.5-4 in fish. Hence *clethodim* is not expected to bioaccumulate. *Clethodim* is degraded with in a DT₅₀ of 5 and 23 days in water/sediment systems. *Clethodim* is mainly distributed to water phase. Major metabolite in aquatic phase was *clethodim sulfoxide* (4).

1.4 Proposed water quality objective

Since PNEC is 0.01 mg/L, the proposed water quality standard for *clethodim* is 0.01 mg/L.

1.5 Comments

Weak adsorption of *clethodim* and metabolites to soil indicates a potential for leaching. Therefore the herbicide may reach ground and surface waters through the soil profile

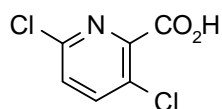
1.6 Literature

- (1) *Environmental assessment report Clethodim*, 1990. National Registration Authority or Agricultural and Veterinary Chemicals.

- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (4) *Review of data in support of the registration for Select herbicide and the active ingredient clethodim*, 1990. Environment Canada, Conservation and Protection, Canada.
- (5) *Sagens oplysninger og miljøsyrelsens vurdering af Select indeholdende aktivstoffet cletodim, økotoxikologi*, 2000, Miljøsyrelsen, bekaepelsesmiddelkontoret.

1. Clopyralid

Clopyralid is a systemic herbicide, intended for use in cereals and pasture.



1.1 Physico-chemical properties

Physico-chemical properties of *clopyralid* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *clopyralid*.

		Reference
CAS-No.	1702-17-6	1
Empirical formula	C ₆ H ₃ Cl ₂ NO ₂	1
Molecular weight [g/mol]	192	1
Solubility in water [mg/kg]	7850 in distilled water 118000 at pH 5, 20 °C 143000 at pH 7, 20 °C 157000 at pH 9, 20 °C	3
pKa	2.3	1
Vapour pressure [Pa]	1.5 × 10 ⁻³ at 25 °C	3
Log P _{ow}	-1.8 at pH 5, 20 °C -2.6 at pH 7, 20 °C -2.6 at pH 9, 20 °C 1.07 unionised, 25 °C	3
Henry's law constant [Pa×m ³ /mol]	1.8 × 10 ⁻⁶ (calc)	

1.2 Toxicity to aquatic organisms

The toxicity of *clopyralid* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *clopyralid*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth	96 h, static	E _r C ₅₀ 5.4 ¹⁾ NOEC <4	1
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ 89 NOEC 7.2	1
Crustaceans				

<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 225	1, 2
<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 233	1
<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 318	1
<i>Daphnia magna</i>	reproduction	21 d, semi-static	NOEC 17	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, static	EC ₅₀ 125.4	1, 2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	EC ₅₀ 103.5	1, 2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 95%

The most sensitive of the tested species was *Selenastrum capricornutum*, with an E_rC₅₀ of 5.4 mg/L and a NOEC of <4 mg/L. Since a PNEC based on chronic values includes uncertainty due to the unsure NOEC, PNEC is based on acute toxicity data. The lowest EC₅₀ of 5.4 mg/L is divided by a factor of 100, which results in a PNEC of 0.054 mg/L.

1.3 Bioaccumulation and persistence

Clopyralid is not expected to bioaccumulate. Log P_{ow} is low, therefore bioaccumulation study is not considered as relevant. *Clopyralid* is readily soluble in water and has low hydrolysis and photodegradation. The substance is slightly degradable in water/sediment systems (1).

1.4 Proposed water quality objective

Since PNEC is 0.054 mg/l, the proposed water quality standard for *clopyralid* is 0.05 mg/L.

1.5 Comments

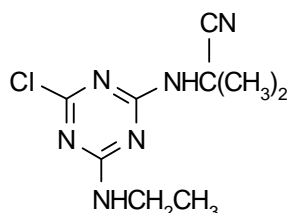
Clopyralid is fairly degradable in soil, but mobile (mean Koc 4) and can therefore leach through soil and reach surface- and groundwater. Since transformation in water is low, no metabolites of concern are known (1, 3).

1.6 Literature

- (1) Montforts, M. & Linders, J., 1989. *Clopyralid*. Toxicology advisory center, National Institute of Public Health and Environmental Protection (RIVM). Holland.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Cyanazine

Cyanazine is an herbicide, intended for use in rapeseed.



1.1 Physico-chemical properties

Physico-chemical properties of *cyanazine* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *cyanazine*.

		Reference
CAS-No.	21725-46-2	4
Empirical formula	C ₉ H ₁₃ ClN ₆	4
Molecular weight [g/mol]	240.7	4
Solubility in water [mg/kg]	171 at 25 °C	4
pKa	0.63	4
Vapour pressure [Pa]	2 × 10 ⁻⁷	4
Log P _{ow}	2.1	4
Henry's law constant [Pa×m ³ /mol]	2.9 × 10 ⁻⁷	4

1.2 Toxicity to aquatic organisms

The toxicity of *cyanazine* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *cyanazine*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	biomass	96 h, static	E _b C ₅₀ 0.020 ¹⁾ NOE _b C 0.010 ²⁾	1, 5
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ 0.064 NOEC 0.030	3
Crustaceans				
<i>Daphnia magna</i>		48 h, static	EC ₅₀ 49	3
<i>Daphnia magna</i>		48 h, static	EC ₅₀ 42	1, 3, 5
Fish				
<i>Pimephales promelas</i>	mortality	96 h, static	LC ₅₀ 16.3	3
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ 17.4	3
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ 10	1

<i>Cyprinus carpio</i>	mortality	96 h	LC ₅₀ 30	1
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¹⁾ Effect concentration basis for calculation of former PNEC. Test substance purity 97.3%.

²⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 0.02 mg/L and. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.02 mg/L is divided by a factor of 100, which results in a PNEC of 0.0002 mg/L.

Revised EQS calculation according to EU-harmonised methodology (6)

There is only chronic data available for algae and plants, but given that cyanazine is a photosynthesis inhibitor and the EC₅₀-values for crustaceans and fish are much higher (150-500x) than the NOECs for algae and plants it is unlikely that long term tests with fish and crustacea would generate lower NOEC values, and thus an assessment factor of 10 is proposed to be used for the lowest NOEC. The lowest NOEC is 0.01 mg/l for *Selenastrum capricornutum*. Thus, the lowest NOEC of 0.01 mg/L is divided by a factor of 10, which results in a PNEC of 0.001 mg/L.

1.3 Bioaccumulation and persistence

Cyanazine is not expected to bioaccumulate (log P_{ow} 2.1). The rate of hydrolysis of *cyanazine* is pH dependent, (DT₅₀ at pH 5.6: 28 weeks, DT₅₀ at pH 3.9: 20 hours, DT₅₀ at pH 9.5: 5 days).

1.4 Proposed EQS/water quality objective

Since PNEC is 0.001 mg/L, the proposed EQS/water quality objective for *cyanazine* is 0.001 mg/L.

1.5 Comments

Cyanazine has several transformation products. Initially *cyanazine* is metabolised into *cyanazine* amide and then to *cyanazine* acid, after that several other transformation products are formed. *Cyanazine* has medium to low adsorption ability (K_{oc} 73-413) and thus a medium to high mobility potential. The metabolites have high potential to leach through the soil profile (*cyanazine* amide; K_{oc} 6.4-6.6) (2).

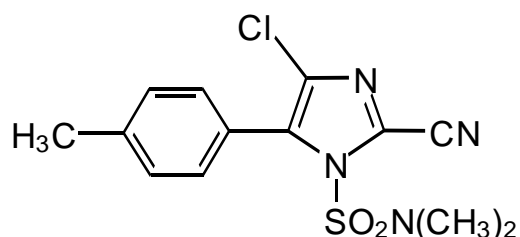
1.6 Literature

- (1) Henning, I., & Clausen, S. *Cyanazin Økotoksikologisk baggrundsrapport*. Miljøministeriet, Miljøstyrelsen, Bekæmpningsmiddelkontoret. København, Danmark.
- (2) National Chemicals Inspectorate, 1994. *PM -Bladex 500 SC*. Solna, Stockholm.

- (3) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (5) Tuinstra, J., & Linders, J., 1989. *Cyanazin*. Adviescentrum toxicologie, National Institute of Public Health and Environmental Protection (RIVM). Holland.
- (6) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Cyazofamid

Cyazofamid is a contact fungicide, which is used against fungus from the class of Oomycetes. The fungicide is intended for use in potatoes. *Cyazofamid* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *cyazofamid* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *cyazofamid*.

		Reference
CAS-No.	120116-88-3	1
Empirical formula	C ₁₃ H ₁₃ CIN ₄ O ₂ S	1
Molecular weight [g/mol]	324.8	1
Solubility in water [mg/kg]	0.107-0.121 at 20°C and pH 5-9	1
pKa	No dissociation	1
Vapour pressure [Pa]	<1.33 × 10 ⁻⁵	1
Log P _{ow}	3.2	1
Henry's law constant [Pa×m ³ /mol]	<4.03 × 10 ⁻²	1

1.2 Toxicity to aquatic organisms

The toxicity of *cyazofamid* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *cyazofamid*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	96h, static	E _r C ₅₀ >0.1 NOE _r C 0.01 ¹⁾	1
<i>Selenastrum capricornutum</i>	growth rate biomass	72h, static	E _r C ₅₀ 60.9 NOE _b C 0.026	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, flow-through	EC ₅₀ >0.14	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.11	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ >0.14	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ >0.10	1
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ >0.14	1

<i>Cyprinus carpio</i>	mortality	96h, flow-through	LC ₅₀ >0.14	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.56	1
<i>Onchorhynchus mykiss</i>	mortality	28d, flow-through	NOEC 0.13	1

¹⁾ Test performed on preparation, Ranman IKF-916. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Selenastrum capricornutum*, with a NOEC of 0.01 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *Selenastrum capricornutum* is calculated to 0.001 mg/L.

1.3 Bioaccumulation and persistence

Cyazofamid is expected to bioaccumulate, which is indicated by Log P_{ow} 3.2 and BCF 286. *Cyazofamid* is to some extent partitioned into sediment, max 35% after 7 days. Primary degradation occurs by hydrolysis forming the metabolite *CCIM*, at pH 4-9. *CCIM* is further transformed into *CCIM-AM* and *CTCA*. Only *CCIM* is assessed as a major metabolite, exceeding 10% in water phase. Half-lives of *cyazofamid* in water/sediment-system are 8.7-9.9 days water phase and 10.8-16.5 days and in the sediment phase. *CCIM* is degraded within a DT₅₀ of 22.8-26.4 days in water.

1.4 Proposed water quality objective

Since PNEC is 0.001 mg/L, the proposed water quality standard for *cyazofamid* is 1×10⁻³ mg/L.

1.5 Comments

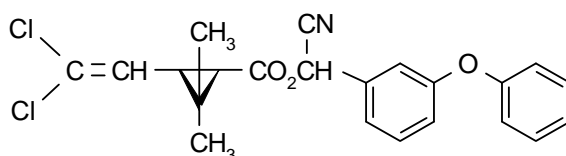
In soil the substance is primary degraded within a DT₅₀ of 10 days. Same metabolites as in water are formed, but to a higher extent. The metabolites do not show higher ecotoxicological effects than the parent compound.

1.6 Literature

- (1) European Commission Peer Review Programme. *Cyazofamid Monograph*, 2001. Rapporteur Member State: France.

1. Cypermethrin

Cypermethrin is a synthetic pyrethroid insecticide. The substance consists of eight optical isomers, four pairs of enantiomers. Only two of the isomers, one enantiomer pair (the *cis*-2 pair), have insecticidal activity. These two enantiomers are the components of the active substance *alpha-cypermethrin*. *Cypermethrin* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *cypermethrin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *cypermethrin*.

		Reference
CAS-No.	52315-07-8	1
Empirical formula	C ₂₂ H ₁₉ Cl ₂ NO ₃	1
Molecular weight [g/mol]	416.3	1
Solubility in water [mg/kg]	0.004 at pH 7	4
Vapour pressure [Pa]	2.3 × 10 ⁻⁷ at 20°C	3
Log P _{ow}	6.6	4
Henry's law constant [Pa×m ³ /mol]	2.0 × 10 ⁻²	4

1.2 Toxicity to aquatic organisms

The toxicity of *cypermethrin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *cypermethrin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>		96 h	EC ₅₀ 15	1
Crustaceans				
<i>Daphnia magna</i>	immobilisation	24 h, static	EC ₅₀ 0.0042	1
<i>Daphnia magna</i>	immobilisation	24 h, static	EC ₅₀ 0.001	2
<i>Daphnia magna</i>	immobilisation	48 h, semi-static	EC ₅₀ 0.0003	1
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.089	2
<i>Penaeus duorarum</i>	mortality	96 h, flow-through	LC ₅₀ 0.000036	2
<i>Orconectes nais</i>	mortality	96 h, flow-through	LC ₅₀ 0.000069	2
<i>Palaemonetes pugio</i>	mortality	96 h, flow-through	LC ₅₀ 0.000016 ²⁾	2
<i>Daphnia magna</i>	reproduction	21 d, semi-static	NOEC 0.0001 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21 d	NOEC 0.00004	1

Insecta				
<i>Cloeon dipterum</i>	mortality	96 h, flow-through	LC ₅₀ 0.00003	2
Mollusca				
<i>Crassostrea virginica</i>	shell deposition	96 h, flow-through	EC ₅₀ 0.37	2
Fish				
<i>Cyprinus carpio</i>	mortality	96 h, flow-through	LC ₅₀ 0.0005-0.0017	1
<i>Scardinius erythrophthalmus</i>	mortality	96 h, flow-through	LC ₅₀ 0.0004-0.0005	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow-through	LC ₅₀ 0.0007-0.0011	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, semi-static	LC ₅₀ 0.0028	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow-through	LC ₅₀ 0.00092	2
<i>Oncorhynchus mykiss</i>	mortality	101 h, flow-through	LC ₅₀ 0.00082	
<i>Cyprinodon variegatus</i>	mortality	96 h, flow-through	LC ₅₀ 0.00073	2
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ 0.00178	2
<i>Pimephales promelas</i>		30 d, early life stage, flow-through	NOEC 0.00014	2
<i>Pimephales promelas</i>		30 d, early life stage, flow-through	NOEC 0.00025	1
<i>Pimephales promelas</i>		34 d, early life stage, flow-through	NOEC <0.00003	1

¹⁾ Corresponding to ~0.0004 mg/l dissolved in the water-phase (40 % of nominal value).

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96 %.

The most sensitive of the tested species was *Palaemonetes pugio*, with an LC₅₀ of 0.000016 mg/L. Both short- and long-term studies are available, and three trophic levels have been tested. As the lowest effect concentration is an LC₅₀ an assessment factor of 100 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *cypermethrin* is calculated to 1.6×10^{-7} mg/L.

1.3 Bioaccumulation and persistence

Cypermethrin has bioaccumulation potential (BCF=1204). Photolysis in water is very slow. Hydrolysis is pH-dependent with rapid degradation at higher pH and very slow degradation at low pH. The main hydrolytic metabolites are (*RS*)- α -carbamoyl-3-phenoxybenzyl-(*1R*)-*cis*, *trans*-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropane carboxylate; (*1R*)-*cis*, *trans*-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylic acid and 3-phenoxybenzoic acid.

1.4 Proposed water quality objective

Since PNEC is 1.6×10^{-7} mg/L, the proposed water quality objective for *cypermethrin* is 2×10^{-7} mg/L.

1.5 Comments

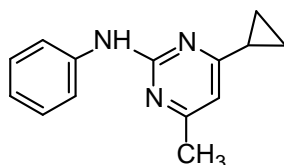
Cypermethrin is practically immobile in soil. In water-sediment systems the active substance is rapidly partitioned to the sediment; therefore a quality objective for sediment may be relevant. Also the metabolite 3-phenoxybenzaldehyde is distributed to the sediment while 3-phenoxybenzoic acids and dichlorovinyl cyclopropane acids are shared between water and sediment phase. Because of bioaccumulation potential a quality objective for biota may be considered.

1.6 Literature

- (1) European Commission Peer Review Programme. Cypermethrin Monograph, 1999. Rapporteur Member State: Belgium.
- (2) Pesticide Ecotoxicity Database, 2001, Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Report from ECCO 101 Peer Review Meeting, 16 February 2001, Rapporteur Member State: Belgium.
- (4) Tomlin, C., 2000. *The Pesticide Manual*, 12th edition. British Crop Protection Council.

1. Cyprodinil

Cyprodinil is a systemic pyrimidine fungicide for foliar applications on cereals and strawberries against plant pathogenic fungi. *Cyprodinil* is acting by inhibiting both the penetration of the fungi into the plant and their mycelial growth on the surface of and inside leaves. *Cyprodinil* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *cyprodinil* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *cyprodinil*.

		Reference
CAS-No.	121552-61-2	1
Empirical formula	C ₁₄ H ₁₅ N ₃	1
Molecular weight [g/mol]	225.3	1
Solubility in water [mg/kg]	16 at 25°C and pH 7.6	1
pKa	4.44	1
Vapour pressure [Pa]	4.7-5.1 × 10 ⁻⁴ at 25°C	1
Log P _{ow}	3.9 - 4.0 at 25°C	1
Henry's law constant [Pa×m ³ /mol]	6.6 - 7.2 × 10 ⁻³	1

1.2 Toxicity to aquatic organisms

The toxicity of *cyprodinil* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *cyprodinil*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudokirchneriella subcapitata</i>	growth rate	72 h static	E _r C ₅₀ 5.2 NOE _r C 0.4	1
Higher Aquatic Plants				
<i>Lemna gibba</i>	frond numbers, presence of flowers	14 d	EC ₅₀ 7.71 NOEC 4.42	1
Crustaceans				
<i>Daphnia magna</i>	mortality	48 h flow-through	LC ₅₀ 0.033	1
<i>Daphnia longispina</i>	immobility	48 h static	EC ₅₀ 0.22	1
<i>Daphniopsis sp.</i>	immobility	24 h static	EC ₅₀ 0.21	1
<i>Simocephalus vetulus</i>	immobility	48 h static	EC ₅₀ 0.15	1
<i>Gammarus sp.</i>	immobility	48 h static	EC ₅₀ 1.8	1
<i>Thamnocephalus</i>	immobility	24 h static	EC ₅₀ 0.12	1

<i>platyurus</i>				
<i>Ostracoda sp.</i>	immobility	48 h static	EC ₅₀ 1.1	1
<i>Brachionus calyciflorus</i>	immobility	24 h static	EC ₅₀ >9.5	1
<i>Cloeon sp.</i>	immobility	48 h static	EC ₅₀ 3.5	1
<i>Chaoborus sp.</i>	immobility	48 h static	EC ₅₀ 4.0	1
<i>Lymnea stagnalis</i>	immobility	48 h static	EC ₅₀ 2.9	1
<i>Daphnia magna</i>	survival, growth, reproduction	21 d flow-through	NOEC 0.0082	1
<i>Daphnia magna</i>	survival, growth, reproduction	21 d semi-static	NOEC (<24 h old) 0.0018 ¹⁾ NOEC (8-9 d old) 0.0088	1
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h static	LC ₅₀ 2.41	1
<i>Lepomis macrochirus</i>	mortality	96 h static	LC ₅₀ 2.17	1
<i>Lepomis macrochirus</i>	mortality	96 h flow-through	LC ₅₀ 3.20	1
<i>Oncorhynchus mykiss</i>	mortality	21 d flow-through	NOEC 0.083	1
<i>Pimephales promelas</i> (early-life-stage toxicity)	hatching success, growth, survival	36 d flow-through	NOEC 0.231	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.0018 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *cyprodinil* is calculated to 0.00018 mg/L.

1.3 Bioaccumulation and persistence

Cyprodinil is expected to bioaccumulate. Log P_{ow} indicates bioaccumulation 3.9 and is confirmed by studies, BCF (whole fish) is 387-399. *Cyprodinil* is hydrolytically stable. The substance dissipates from the water phase with a DT₅₀ of 2.1 – 5.4 days, while the degradation half-life is 106 – 178 days in the whole water/sediment. After 14 days 87.3 % of the substance has adsorbed to the sediment. One major metabolite is formed, CGA 249287. The metabolite is stable for hydrolysis and in sediment CGA 249287 is exceeding 10 %. The metabolite shows, however, lower toxicity towards aquatic organisms than the parent compound. (1)

1.4 Proposed water quality objective

Since PNEC is 0.00018 mg/L, the proposed water quality standard for *cyprodinil* is 0.0002 mg/L.

1.5 *Comments*

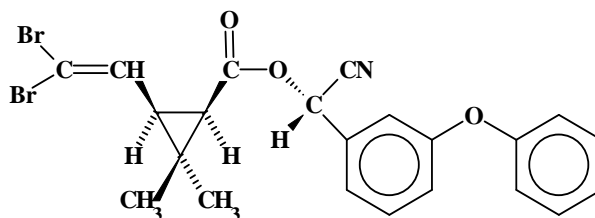
The metabolite is not mobile in soil and is therefore not presumed to leach through the soil profile and reach ground and surface water. *Cyprodinil* is rapidly partitioned into sediment; hence a complementary quality objective is needed for this compartment. (1)

1.6 *Literature*

- (1) European Commission Peer Review Programme. *Cyprodinil Monograph, 2003*.
Rapporteur Member State: France.

1. Deltamethrin

Deltamethrin is a pyrethroids insecticide, intended for use in oleiferous plants, beans, cereals and potatoes. It acts on the insects by contact and ingestion. *Deltamethrin* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *deltamethrin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *deltamethrin*.

		Reference
CAS-No.	52918-63-5	1
Empirical formula	C ₂₂ H ₁₉ Br ₂ NO ₃	1
Molecular weight [g/mol]	505.2	1
Solubility in water [mg/kg]	0.0002 at 25° C	1
pKa	Not relevant	1
Vapour pressure [Pa]	1.24×10 ⁻⁸	1
Log P _{ow}	4.6	1
Henry's law constant [Pa×m ³ /mol]	3.1×10 ⁻²	1

1.2 Toxicity to aquatic organisms

The toxicity of *deltamethrin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *deltamethrin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, semi-static	EC ₅₀ 1.1× 10 ^{-4 1)}	1
<i>Daphnia magna</i>		48h, static	EC ₅₀ 3.5× 10 ⁻³ (nominal)	1
<i>Daphnia magna</i>		48h, flow-through	EC ₅₀ 5.6× 10 ⁻⁴	1
<i>Asellus aquaticus</i>	immobility	96h, semi-static	EC ₅₀ 3.5× 10 ^{-7 1)} (nominal) NOEC 2.5× 10 ^{-7 1) 2)} (nominal)	3
<i>Gammarus fasciatus</i>		96h, flow-through	EC ₅₀ 3.1× 10 ^{-7 1)} NOEC <2.8× 10 ^{-7 1)}	3
<i>Daphnia magna</i>		21d, semi-static	NOEC 2.3× 10 ^{-5 1)}	1
<i>Daphnia magna</i>	growth	21d, flow-through	NOEC 4.1× 10 ⁻⁶	1
Molluscs				
<i>Crassostrea virginica</i>		96h, flow-through	EC ₅₀ 8.2	2
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 3.6× 10 ^{-7 41)}	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 2.6× 10 ^{-4 1)}	1
<i>Cyprinodon variegatus</i>	mortality	96h, flow-through	LC ₅₀ 5.8× 10 ⁻⁴	2
<i>Onchorhynchus mykiss</i>	mortality	48h, flow-through	LC ₅₀ 2.5× 10 ⁻⁴	2
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 1.4× 10 ⁻³	2
<i>Oncorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 9.1× 10 ⁻⁴	2
<i>Cypridon variegatus</i>	mortality	96h, static	LC ₅₀ 3.6× 10 ⁻⁴	2
<i>Onchorhynchus mykiss</i>	mortality	28d, flow-through	NOEC <3.2× 10 ⁻⁵	1
<i>Pimephales promelas</i>	early life stage	36d, flow-through	NOEC 2.2× 10 ⁻⁵	1
<i>Pimephales promelas</i>	life-cycle toxicity	260d, flow-through	NOEC 1.7× 10 ⁻⁵	1
Microcosm				
<i>Invertebrates including sediment living organisms</i>		Approx. 6 months	EAC 3.2× 10 ^{-6 1)}	3

¹⁾ Test performed on preparation (IS-002A, 25 g as/l, and Decis 25 EC, 25g as/l). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC.

The microcosm study, addresses long term effects and potential for recovery under more realistic exposure conditions. According to the microcosm studie, is crustacea the most sensitive group of organisms, for *deltamethrin*. Laboratory studies indicate *Gammarus fasciatus* to be the most sensitive species. Among present crustaceans in the microcosm *Asellus aquaticus* is the most responsive species, with an EC₅₀ of 3.5×10⁻⁷ mg/L and NOEC 2.5×10⁻⁷ mg/L. Since the most susceptible life stage was included, this study is regarded as a long term study. Although the results could not be directly compared with those from the laboratory, it can be anticipated that the NOEC derived from *Asellus aquaticus* would cover possible effects in the field. Therefore, an assessment factor of 1 is used, together with the NOEC, resulting in a PNEC of 2.5×10⁻⁷ mg/L.

1.3 Bioaccumulation and persistence

Deltamethrin is expected to bioaccumulate in aquatic organisms, BCF is 1400 in fish. *Deltamethrin* is hydrolysed in alkaline waters. In sediment/water system the half-life of the substance was 130-290 days with one major metabolite; α -R-*deltamethrin*. The metabolite is not toxic towards aquatic organisms. In aquatic environments *deltamethrin* will dissipate from water phase as it adsorbs rapidly to organic material, to biota and eventually to sediment. Volatilisation is also expected to contribute to disappearance from water.

1.4 Proposed water quality objective

Since PNEC is 2.5×10^{-7} mg/L, the proposed water quality standard for *deltamethrin* is 2×10^{-7} mg/L.

1.5 Comments

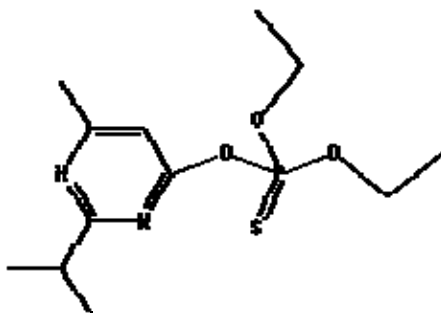
The parent compound is not mobile in soil, however the metabolite may leach through the soil profile and reach surface- and ground water. *Deltamethrin* has a tendency to volatilise from water. An additional quality objective for sediment is recommended.

1.6 Literature

- (1) European Commission Peer Review Programme. *Deltamethrin Monograph, 1998*. Rapporteur Member State: Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *Deltamethrin Review report, 2002*. Rapporteur Member State: Sweden.

1. Diazinon

Diazinon is a non-systemic organophosphorus insecticide and acaricide, intended for use in cultivation of leak and cabbage. The substance is primarily a contact insecticide which affects the nervous system (2). *Diazinon* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *diazinon* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *diazinon*.

		Reference
CAS-No.	333-41-5	1
Empirical formula	C ₁₂ H ₂₁ N ₂ O ₃ PS	1
Molecular weight [g/mol]	304.35	1
Solubility in water [mg/kg]	40 at 20°C	1
pKa	2.39 at 20°C	2
Vapour pressure [Pa]	1.9 × 10 ⁻²	2
Log P _{ow}	3.95	1
Henry's law constant [Pa×m ³ /mol]	0.05	4

1.2 Toxicity to aquatic organisms

The toxicity of *diazinon* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *diazinon*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ 0.00096	3,5
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.0011 ¹⁾	5
<i>Gammarus fasciatus</i>	mortality	96h, static	EC ₅₀ 0.00018 ^{2,3)}	3
<i>Daphnia magna</i>	immobility	21d, flow-through	NOEC 0.00017	5
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 1.8	5
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.21 ¹⁾	5
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 0.46	5

<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.08 ²⁾	5
<i>Cyprinodon variegatus</i>	mortality	96h, flow-through	LC ₅₀ 1.47	5
<i>Cyprinodon variegatus</i>		4 weeks, flow-through	LOEC 0.47	5

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Test performed on substance with purity <90%. Value expressed as active substance.

³⁾ Effect concentration basis for calculation of PNEC. Test substance purity 89%

The database set is not complete, algal studies are missing due to low quality. However supportive test indicates that *diazinon* is toxic towards primary producers although not the most sensitive trophic level. The most sensitive (acute effects) of the tested species was *Gammarus fasciatus*, with a LC₅₀ of 0.00018 mg/L. Long term studies have been performed but using *Daphnia magna* as test organism. *Daphnia magna* is less sensitive; therefore the NOEC-value is misleading. Also the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is therefore based on acute toxicity data. Hence, the lowest LC₅₀ of 0.00018 mg/L is divided by a factor of 100, which results in a PNEC of 0.0000018 mg/L.

1.3 **Bioaccumulation and persistence**

Diazinon is expected to bioaccumulate. The octanol/water coefficient Log P_{ow} indicates bioaccumulation. However laboratory studies show varying results, BCF 18-152 (1) and BCF 470-540 (5) in fish. Primary degradation occurs mainly by chemical reactions. Hydrolysis is an important degradation route, forming the metabolite 2-isopropyl-4-methyl-6-hydroxy pyrimidine (*IMPH*) and diethyl thiophosphoric acid. *Diazinon* is hydrolysed more rapidly in low pH and at high temperature, DT₅₀ 23d at pH 7 and DT₅₀ 42h, at pH 5. *Diazinon* may also be transformed into *IMPH* due to oxidation. Laboratory studies of degradation in natural waters show rapid initial adsorption into sediment, followed by degradation of diazinon with half-lives in the range 8 to 15 days. The degradation results in the metabolite pyrimidinol (2). The product is used as micro-capsules resulting in longer persistence (1).

1.4 **Proposed water quality objective**

Since PNEC is 0.0000018 mg/L, the proposed water quality standard for *diazinon* is 2×10^{-6} mg/L.

1.5 **Comments**

The insecticide *diazinone* is not mobile in soil and is therefore unlikely to leach through the soil profile. The substance is considered to have volatility potential, the first 24 hours after application 3-10% is evaporated (4). The substance partitions into the sediment, therefore additional quality objective for sediment should be established. Products of acid hydrolysis of formulations are toxic to fish (0.4-1.5µg/L), as is the impurity sulfotep. However these studies

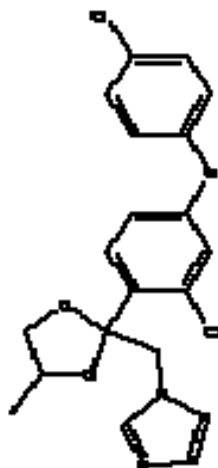
are considered as indicative due to variable quality and not reported to modern standard (2). Metabolites and impurities should be more studied.

1.6 Literature

- (1) Vaittinen, Sirkka-Liisa, Diazinon, 1988. *Upptredande och verkan i naturen*. Institutet för arbets- och industrihygien, Kuopio Universitet, Kuopio.
- (2) *Evaluation on DIAZINON*, 1991. Food and environment protection act 1985, Part III, Ministry of Agriculture, Fisheries and Food, Pesticides Safety Directorate, London.
- (3) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (4) Lindqvist et al., 1995. *BASUDIN 600 EW*. Kemikalieinspektionen, avdelningen för bekämpningsmedel. Sverige.
- (5) Matcher S., 1990. *Økotoxikologisk vurdering af DIAZINON viksom bestanddel i Basudin 25 Emulsion og Basudin 10 Granulat*. Dansk miljøanalyse. Danmark.

1. Difenoconazole

Difenoconazole is a slightly systemic fungicide, belonging to the azole group. The fungicide has a preventive and curative action against a broad range of fungal diseases. It inhibits the growth of the fungi by disturbing the ergosterol synthesis in the cell membrane. Intended for use in seed treatment.



1.1 Physico-chemical properties

Physico-chemical properties of *difenoconazole* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *difenoconazole*.

		Reference
CAS-No.	C ₁₉ H ₁₇ Cl ₂ N ₃ O ₃	1
Empirical formula	11944-68-3	4
Molecular weight [g/mol]	406.27	1
Solubility in water [mg/kg]	3.3	1
pKa	No dissociation	1
Vapour pressure [Pa]	3 × 10 ⁻⁸	1
Log P _{ow}	4.2	1
Henry's law constant [Pa×m ³ /mol]	4.1 × 10 ⁻⁶	1

1.2 Toxicity to aquatic organisms

The toxicity of *difenoconazole* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *difenoconazole*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass	72h, static	E _b C ₅₀ 1.2 NOEC _b 0.87	1,2,3
<i>Scenedesmus subspicatus</i>	biomass	72h, static	E _b C ₅₀ 0.032 NOEC _b 0.086	1

Aquatic plants				
<i>Lemna gibba</i>	Fronnd number	14d, semi-static	EC ₅₀ 18.5 NOEC 10	1,2
<i>Lemna gibba</i>		14d, semi-static	EC ₅₀ 9.9 NOEC 2.5	3
Crustaceans				
<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ 0.77	1,2,4
<i>Daphnia magna</i>	immobility	48h, static	LC ₅₀ 1.0 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.018	1
<i>Daphnia magna</i>	reproduction, survival, length	21d, flow-through	NOEC 0.0056	1,2,3
Molluscs				
<i>Crassostrea virginica</i>	shell deposition	96h, flow-through	EC ₅₀ 0.44	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 1.2	1,2,3
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.81	1,2,3
<i>Cyprinus variegatus</i>	mortality	96h, static	LC ₅₀ 0.82	1,4
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.1	1,2,3
<i>Pimephales promelas</i>	growth	34d, flow-through	NOEC 0.0076	1,2,3,4
<i>Pimephales promelas</i>	growth	68d, flow-through	NOEC 0.00087 ²⁾	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 94.8%

The most sensitive of the tested species was *Pimephales promelas*, with a NOEC of 0.00087 mg/L. Both short and long term studies are available, and three trophic levels have been tested. However the lowest NOEC does not generate from the level showing the lowest LC₅₀ in short-term tests. Therefore the NOEC derived from fish is not considered to protect the whole aquatic system. Hence, an assessment factor of 50 is used for calculation of the predicted no effect concentration. The PNEC for *difenoconazole* is calculated to 1.7×10^{-5} mg/L.

1.3 Bioaccumulation and persistence

Difenoconazole is expected to bioaccumulate, BCF 330-420 in fish. The substance has affinity for sediment where uptake to sediment- living organisms can occur. *Difenoconazole* is persistent in water, DT₅₀ <12 months. The substance is photolysed in artificial light, however due to rapid adsorption photolysis is not considered as a major degradation pathway. It is stable to hydrolysis. The degradation is low and no major metabolites are formed.

Difenoconazole is rapidly distributed into the sediment, where no further degradation has been demonstrated.

1.4 Proposed water quality objective

Since PNEC is 1.7×10^{-5} mg/L, the proposed water quality standard for *difenoconazole* is 2×10^{-5} mg/L.

1.5 Comments

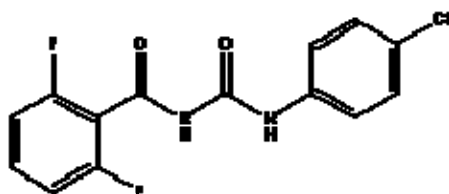
Difenoconazole partitions into the sediment, hence a supplementary quality objective for sediment should be established.

1.6 Literature

- (1) Anneli Sandberg, 1995. *Ecotoxicological evaluation of the fungicide difenoconazole*. National Chemical Inspectorate, Sweden.
- (2) Otermann et al., 1993. *Difenoconazool*. Adviesrapport 93/679101/003.
- (3) Montfarts, Verdam H., 1988. *Difenoconazool*. Adviesrapport 05554A00.
- (4) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (5) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Diflubenzuron

Diflubenzuron is a non-systemic insect growth regulator with uptake through food and contact. Mode of action is chitin synthesis inhibitor. *Diflubenzuron* is intended for use in fruit cultivation and cabbage.



1.1 Physico-chemical properties

Physico-chemical properties of *diflubenzuron* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *diflubenzuron*.

		Reference
CAS-No.	35367-38-5	3
Empirical formula	C ₁₄ H ₉ ClF ₂ N ₂ O ₂	3
Molecular weight [g/mol]	310.7	3
Solubility in water [mg/kg]	0.08	3
pKa	Not relevant	3
Vapour pressure [Pa]	1.2 × 10 ⁻⁴	3
Log P _{ow}	3.89	3
Henry's law constant [Pa×m ³ /mol]	4.7 × 10 ⁻³	3

1.2 Toxicity to aquatic organisms

The toxicity of *diflubenzuron* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *diflubenzuron*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	biomass	72h, static	NOEC 0.2	1
<i>Plectonema boryanum</i>	growth rate	72h, static	NOEC 6.25 ¹⁾	1
Crustaceans				

<i>Gammarus pseudolimnaeus</i>	not specified	96h, static	EC ₅₀ 0.045	2
<i>Daphnia magna</i>	not specified	48h, static	EC ₅₀ 0.0037	2
<i>Daphnia magna</i>	not specified	48h, static	EC ₅₀ 0.0057	1
<i>Daphnia magna</i>	not specified	48h, static	EC ₅₀ 0.0041 ¹⁾	1
<i>Hyallela azteca</i>	not specified	120h, flow-through	EC ₅₀ 0.0017 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, flow-through	NOEC 0.000036 ¹⁾	1
<i>Daphnia magna</i>	growth	21d, flow-through	NOEC 0.000036 ¹⁾	1
<i>Daphnia magna</i>	growth	21d, static	NOEC 0.056 ¹⁾	1
Mollusc				
<i>Mydopsis bahia</i>		28d, static	NOEC 0.000045	2
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 100	2
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 50	2
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 135	2
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 140	2
<i>Cyprinodon variegatus</i>	mortality	96h, static	LC ₅₀ 0.013	2
<i>Cyprinodon variegatus</i>	mortality	96h, static	LC ₅₀ 0.13	2
<i>Onchorhynchus mykiss</i>	not specified	28d, flow-through	NOEC 0.041 ¹⁾	2
<i>Pimpephales promelas</i>	not specified	30d, flow-through	NOEC 0.041 ¹⁾	2

¹⁾ Test performed on preparation, 90% *diflubenzuron*. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 90%

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.000036 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *diflubenzuron* is calculated to 3.6×10^{-6} mg/L.

1.3 Bioaccumulation and persistence

Diflubenzuron is expected to bioaccumulate, log K_{ow} is 3.89 and BCF 320. Hydrolysis of *diflubenzuron* is pH-dependent, DT₅₀ >150 days at pH 5 and DT₅₀ 7.5 days at pH 12. Degradation time has been studied in three different water/sediment systems, all in the range of pH 7-8, resulting in DT₅₀ of 2.8-3.2 days in water and DT₅₀ 3.7 to 5.7 days in the whole system. Two major metabolites were formed; *4-chlorophenylurea* and *2,3-difluorobenzoic acid* (5). *4-chlorophenylurea* is more persistent in water/sediment systems DT₅₀ is 18-32 days in water and 27-57 days in whole system and may be more likely to find in aquatic systems than the parent compound. The toxicity of the metabolites to aquatic organisms has not been studied. When such data is available this may indicate that additional water quality objectives need to be established.

1.4 Proposed water quality objective

Since PNEC is 3.6×10^{-6} mg/L, the proposed water quality standard for *diflubenzuron* is 4×10^{-6} mg/L.

1.5 Comments

Diflubenzuron adsorbes strongly to the soil particles (4). The compound is therefore not expected to reach ground- and surface water via leaching through the soil profile.

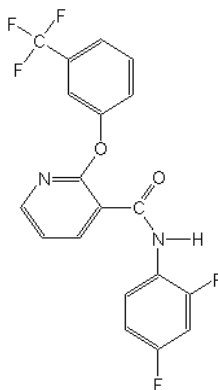
Diflubenzuron partitions into the sediment (5). However the substance is rapidly degraded. Therefore risk for accumulation in sediment is low.

1.6 Literature

- (1) Smith, Post and de Knecht, 1999. *Diflubenzuron*, Adviesrapport: 06323A00.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (4) Samuelsson M., 1990. *Ekotoxikologisk utvärdering av diflubenzuron*. Asteria
- (5) Vonk, 2001. Samenvattingen diflubenzuron. EPP Consultancy, Environmental Pollutants & Pesticide Fate.

1. Diflufenican

Diflufenican is an herbicide intended for use against mono- and dicotyledon weeds in autumn cereals. The modes of action consist of an inhibition of the carotenoid biosynthesis and indirect interference with plant photosynthesis.



1.1 Physico-chemical properties

Physico-chemical properties of *diflufenican* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *diflufenican*.

		Reference
CAS-No.	83164-33-4	1
Empirical formula	C ₁₉ H ₁₁ F ₅ N ₂ O ₂	1
Molecular weight [g/mol]	394	1
Solubility in water [mg/kg]	<0.05 at 25°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	3.07 × 10 ⁻⁵ at 25°C	1
Log P _{ow}	4.9	1
Henry's law constant [Pa×m ³ /mol]	>0.24	2

1.2 Toxicity to aquatic organisms

The toxicity of *diflufenican* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *diflufenican*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Chlorella vulgaris</i>	biomass	96h	EC ₅₀ >10 ¹⁾ NOEC 10	1
<i>Scenedesmus subspicatus</i>	growth	72 h	EC ₅₀ 0.00045 ²⁾	3
Crustaceans				
<i>Daphnia magna</i>	immobility	48h	EC ₅₀ >10	1
<i>Daphnia magna</i>	reproduction	21 d	NOEC 0.052	3
Fish				
<i>Cyprinus carpio</i>	mortality	96h, flow-through	LC ₅₀ 105	1

<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 75	1
<i>Pimephales promelas</i>	growth	35 d, early life stage	NOEC 0.015	3

- 1) Effect concentration basis for calculation of former PNEC.
- 2) Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

Apart from the algal growth inhibition study, no reliable long term data are available, and although a herbicide, it is not obvious that algae is the most sensitive taxonomic group. Therefore, the lowest EC₅₀ of 10 mg/L (both algae and *Daphnia*) is divided by a factor of 1000, which results in a PNEC of 0.01 mg/L.

Revised EQS calculation according to EU-harmonised methodology (4)

Results from additional long term studies with fish and crustacea are now available (3). The alga *Scenedesmus subspicatus* is the most sensitive of the tested species and as the EC₅₀ of 0.45 µg/L derived from this test is lower than all NOECs the PNEC is derived based on acute toxicity data. With an AF=100 the PNEC is 0.0045 µg/l.

1.3 Bioaccumulation and persistence

Diflufenican is expected to bioaccumulate, due to high log P_{ow}, 4.9, and BCF, 1100 in fish. The herbicide has low water solubility and is rapidly partitioned into sediment. *Diflufenican* is hydrolytically stable and only slowly degraded through photolysis in water. Studies made in water/sediment-systems showed a slow degradation rate, after 12 weeks, *diflufenican* was mineralised from 85% to 65%. Four non-identified metabolites were detected.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.0045 µg/L, the proposed EQS/water quality objective for *diflufenican* is 0.0045 µg/L.

1.5 Comments

Degradation in soil occurs slowly, with in a DT₅₀ of 168-460 days. Henry's constant is moderate, indicating a potential for atmospheric dispersion through volatilisation. According to calculation of fugacity, *diflufenican* concentrates to sediment and soil. Therefore a quality objective for sediment needs to be set, as well as quality objectives for biota due to risk for bioaccumulation.

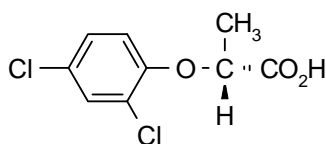
1.6 Literature

- (1) *Ekotoxikologisk utvärdering av diflufenikan*. Vej lens, E. Kemikalieinspektionen, Sverige 910417.

- (2) Supplementary ecotoxicological evaluation of the herbicide diflufenican. Lundbergh, I. Kemikalieinspektionen, Sverige 1992.
- (3) European Commission Peer Review Programme. *Diflufenican* Draft Assessment Report vol 1-3, 2006. Rapporteur Member State: UK
- (4) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Dichlorprop-p

Dichlorprop-p is an auxin type systemic herbicide, intended for use in cereals, pasture and fruit cultivation.



Dichlorprop-p

1.1 Physico-chemical properties

Physico-chemical properties of *dichlorprop-p* is summarised in table 1.1.

Table 1.1: Physico-chemical properties of *dichlorprop-p*.

		Reference
CAS-No.	15165-67-0	1
Empirical formula	C ₉ H ₈ Cl ₂ O ₃	1
Molecular weight [g/mol]	235.1	1
Solubility in water [mg/kg]	590 at 20°C	2
pKa	3.67 at 20°C	2
Vapour pressure [Pa]	6.510 ⁻⁵ at 20°C	2
Log P _{ow}	-0.25 at pH 7, 25°C	2
Henry's law constant [Pa×m ³ /mol]	2.471×10 ⁻⁵ (calc.)	2

1.2 Toxicity to aquatic organisms

The toxicity of *dichlorprop-p* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *dichlorprop-p*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	72h, static	EC ₅₀ >93.6 NOEC 39.3	1
<i>Anabaena flos aquae</i>	growth rate	72h, static	EC ₅₀ 26.5 NOEC 6.1	1
Higher aquatic plants				
<i>Lemna gibba</i>	frond number root formation	14d, semi-static	EC ₅₀ 2.5 ^{2,3)} NOEC 0.15 ^{2,3,4)}	1
<i>Lemna gibba</i>	frond number	7d	EC ₅₀ 21.1 ^{1,2,3)} NOEC 2.8 ^{1,2,3)}	1
Crustaceans				

<i>Daphnia magna struas</i>	immobility	48h, static	EC ₅₀ >100	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ >100	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ >63.2 ^{2,3)}	1
<i>Daphnia magna</i>	immobility reproduction	21d, semi-static	NOEC >100 NOEC >100	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >206	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ >109 ^{2,3)}	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >206 ^{2,3)}	1
<i>Onchorhynchus mykiss</i> (early life stage)	Mortality and sublethal effects	28d, flow-through	NOEC >100	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Test performed on salt compound. Value expressed as active substance.

³⁾ Test performed on substance with purity <90%. Value expressed as active substance.

⁴⁾ Effect concentration basis for calculation of PNEC.

Former water quality objective calculation

The most sensitive of the tested species was *Lemna gibba*, with a NOEC of 0.15 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *dichlorprop-p* is calculated to 0.015 mg/L.

Revised EQS calculation according to harmonised methodology (3)

The PNEC of 0.015 mg/L for *dichlorprop-p* is still valid.

1.3 Bioaccumulation and persistence

Dichlorprop and *dichlorprop-p* is not expected to bioaccumulate. Because Log P_{ow} is low <3, bioaccumulation studies are not required. *Dichlorprop-p* is stable towards hydrolysis in pH 5,7 and 9. Degradation has been studied in two water/sediment systems, resulting in DT₅₀ of 14.6-15.3 days. The substance, to some extent, partitions in to the sediment, 28.4% was found after 30 days. In one anaerobic eutrophic pond study, *dichlorprop-p* is degraded much slower, DT₅₀ 160 days. No major metabolites, exceeding 10%, has been found.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.015 mg/L, the proposed EQS/water quality objective for *dichlorprop-p* is 0.01 mg/L.

1.5 Comments

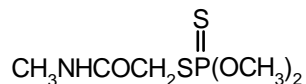
Dichlorprop-p is mobile in soil and may reach ground- and surface water via leakage through the soil profile.

1.6 Literature

- (1) European Commission Peer Review Programme. *Dichlorprop-p Monograph, 2003*. Rapporteur Member State: Denmark.
- (2) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (3) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Dimethoate

Dimethoate is an organophosphorus insecticide, intended for use in beets.



1.1 Physico-chemical properties

Physico-chemical properties of *dimethoate* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *dimethoate*.

		Reference
CAS-No.	60-51-5	5
Empirical formula	C ₅ H ₁₂ NO ₃ PS ₂	5
Molecular weight [g/mol]	229.3	5
Solubility in water [mg/kg]	23300 at pH 5, 20°C 23800 at pH 7, 20°C 25000 at pH 9, 20°C	5
Vapour pressure [Pa]	2.5×10 ⁻³ at 25°C	5
Log P _{ow}	0.704	5
Henry's law constant [Pa×m ³ /mol]	1.2×10 ⁻⁶	5

1.2 Toxicity to aquatic organisms

The toxicity of *dimethoate* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *dimethoate*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Insects				
<i>Baetis rhodani</i>	mortality	96 h, flow-through	LC ₅₀ 0.007 ²⁾	7, 8
Molluscs				
<i>Cassostrea virginica</i>		96 h, flow-through	EC ₅₀ 133	2
Crustaceans				
<i>Daphnia magna</i>	immobilisation	24 h, static	EC ₅₀ 4.7	1
<i>Daphnia magna</i>	mortality and growth	21 d, semi-static	NOEC 0.04 ¹⁾	2
<i>Mysidopsis bahia</i>	immobilisation	96 h, flow-through	EC ₅₀ 15	2
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 30.2	4
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 6.2	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 7.5	2
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 6.0	2
<i>Cyprinus carpio</i>	mortality	96 h, static	LC ₅₀ 690	3
<i>Cyprinodon</i>	mortality	96 h, static	LC ₅₀ >110	2

<i>variegatus</i>				
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- 1) Effect concentration basis for calculation of former PNEC. Technical substance.
- 2) Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.04 mg/L. Supplementary tests on algae, which is not represented in the table above, show that they are less sensitive than daphnia (6). Algae tests, together with the daphnia and fish tests in the table above, show that three trophic levels are available, but there are only two long-term studies together with the supplementary tests. An assessment factor of 50 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *dimethoate* is calculated to 0.0008 mg/L.

Revised EQS calculation according to EU-harmonised methodology (9)

Results from several other tests than those represented above are now available for dimethoate (8). There are chronic NOEC values representing three trophic levels (algae, crustacea and fish) available (Annex 1). Therefore, the use of an assessment factor of 10 is justified. The short term data indicate that insects are probably the most sensitive group. There are no results from long term tests available for this group. The lowest valid EC₅₀ value reported, 7 µg/l for *Baetis rhodani*, is lower than the chronic NOEC values reported. Therefore, the assessment factor of 10 is applied on this LC₅₀ value and a PNEC of 0.0007 mg/L is derived:

1.3 Bioaccumulation and persistence

Dimethoate is not expected to bioaccumulate. *Dimethoate* is relatively stable in water between pH 2-7. In water with pH 9, the substance is primarily degraded with a DT₅₀ of 12 days. Degradation products at pH 5 and 7 were *O-desmethyl-dimethoate* and *O,O-dimethyl-phosphorothioic acid*.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.0007 mg/L, the proposed EQS/water quality objective for *dimethoate* is 0.0007 mg/L.

1.5 Comments

Dimethoate is very mobile in soil. Both *dimethoate* and *O-desmethyl-dimethoate*, are microbially degradable in soil (pH dependent process). *O-desmethyl-dimethoate* is believed to be more toxic than the parent compound (6). Therefore an additional water quality objective for the metabolite is recommended.

1.6 Literature

- (1) H. Ellgehausen. (1983). *Acute toxicity of Dimethoate to Daphnia magna (24 hours OECD mobility test)*. Project No.: 020610; R.C.C – Research & Consulting Company Ltd.

- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of Office of Pesticide programs, U.S. EPA. Washington, D.C.
- (3) R. Bathe. (1982). *Acute toxicity to the carp of Dimethoate*. Project No.: 013702;R.C.C – Research & Consulting Company Ltd.
- (4) R. Bathe. (1982). *Acute toxicity to rainbow trout of Dimethoate*. Project No.: 013691; R.C.C– Research & Consulting Company Ltd.
- (5) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (6) Torstensson, L. *Ekotoxikologisk värdering av dimetoat*. Institutionen för mikrobiologi. Sveriges lantbruksuniversitet.
- (7) Baekken, T & Aanes, K.J. (1991). *Pesticides in Norwegian Agriculture. Their Effects on Benthic Fauna in Lotic Environments. Preliminary Results*. Int. Assoc. Theor. Appl. Limnol. Proc.(Int. Ver. Theor. Angew. Limnol.Verh.) 24(4):2277-2281.
- (8) Proposal for Environmental Water Quality Standards in Finland. Finnish Environment Institute, 2005. ISBN 952-11-1950-0.
- (9) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

Annex 1: Additional test results for dimethoate from Proposal for quality standards in Finland.

Table 1. Short term tests for dimethoate.

Scientific Name	Common Name	Endpoint	Effect	Test conditions etc.	Test Duration; hours	Concentration, µg/l	Master reference	Reference in master reference	Quality in master reference
Algae									
<i>Chlamydomonas noctigama</i>	Green algae	EC50	POP	TS: F; DIMETHOATE, ROGOR L20	3 d	5 500	AQ 16010	Kallqvist & Romstad 1994	M
<i>Microcystis aeruginosa</i>	Blue-green algae	EC50	POP	TS: F; DIMETHOATE, ROGOR L20	6 d	8 500	AQ 16010	Kallqvist & Romstad 1994	M
<i>Synechococcus leopoliensis</i>	Blue-green algae	EC50	POP	TS: F; DIMETHOATE, ROGOR L20	5 d	10 000	AQ 16010	Kallqvist & Romstad 1994	M
<i>Cyclotella</i>	Diatom	EC50	POP	TS: F; DIMETHOATE, ROGOR L20	6 d	14 000	AQ 16010	Kallqvist & Romstad 1994	M
<i>Cryptomonas pyrenoidifera</i>	Cryptomonad	EC50	POP	TS: F; DIMETHOATE, ROGOR L20	6 d	16 000	AQ 16010	Kallqvist & Romstad 1994	M
<i>Selenastrum capricornutum</i>	Green algae	EC50	POP	TS: F; DIMETHOATE, ROGOR L20	3 d	35 000	AQ 16010	Kallqvist & Romstad 1994	M
<i>Chlorella pyrenoidosa</i>	Green algae	EC50	GRO	TS: 98%	24	290 000	AQ 5180	Canton et al. 1980	C
<i>Chlorella pyrenoidosa</i>	Green algae	EC50	GRO	TS: 98%	48	300 000	AQ 5180	Canton et al. 1980	C
<i>Chlorella pyrenoidosa</i>	Green algae	EC50	GRO	TS: 98%	72	470 000	AQ 5180	Canton et al. 1980	C
<i>Scelenastrum capricornutum</i>	green algae	EC50	growth, rate	OECD guideline; GLP; TS: F; Roxion	72	477 000	Nurmi 1994		well done and reported
<i>Chlorella pyrenoidosa</i>	Green algae	EC50	GRO	TS: 98%	96	480 000	AQ 5180	Canton et al. 1980	C
Invertebrate									
<i>Baetis rhodani</i>	Mayfly	LC50	MOR	Flow-through system; TS: F; Rogor L20; 200 g/l dimethoate.	96	7		-	C
<i>Hydropsyche sitalai</i>	Caddisfly	LC50	MOR	Flow-through system; TS: F; Rogor L20; 200 g/l dimethoate.	96	23	Baekken & Aanes 1991 (cited in AQ 13409)	-	C
<i>Pteronarcys californicus</i>	Stonefly	LC50	MOR	TS: 97.4 % T	96	43	AQ 666	Johnson & Finley 1980	C
<i>Heptagenia sulphurea</i>	Mayfly	LC50	MOR	Flow-through system; TS: F; Rogor L20; 200 g/l dimethoate.	96	81	Baekken & Aanes 1991 (cited in AQ 13409)		C
<i>Gammarus lacustris</i>	Scud	LC50	MOR	Flow-through system; TS: F; Rogor L20; 200 g/l dimethoate.	96	180	Baekken & Aanes 1991 (cited in AQ 13409)		M
<i>Gammarus lacustris</i>	Scud	LC50	MOR	TS: 97.4 %	96	200	AQ 666	Johnson & Finley 1980	C
<i>Daphnia magna</i>	Water flea	EC50	REP	TS: 98%	20	310	AQ 5180	Canton et al. 1980	C
<i>Daphnia magna</i>	Water flea	LC50	MOR	TS: 98%	20	310	AQ 5180	Canton et al. 1980	C

Table 1. Short term tests for dimethoate. (Continued)

Scientific Name	Common Name	Endpoint	Effect	Test conditions etc.	Test Duration; hours	Concentration, µg/l	Master reference	Reference in master reference	Quality in master reference
<i>Daphnia magna</i>	Water flea	EC50	REP		16	310	AQ 5675	Hermens et al. 1984	M
<i>Daphnia magna</i>	Water flea	EC50	ITX; IMBL	TS: 98%	48	2900	AQ 5180	Canton et al. 1980	C
<i>Daphnia magna</i>	Water flea	LC50	MOR	TS: > 95% PU, CRY, CYGON	48	3120	AQ 18476	Song et al. 1997	C
<i>Daphnia magna</i>	Water flea	LC50	MOR	TS: > 95% PU, CRY, CYGON	48	3320	AQ 18476	Song et al. 1997	C
<i>Daphnia magna</i>	Water flea	EC50	immobilisation	OECD guidelines; TS: tech. dimethoate, 95 %, nom. conc.		4700	Nurmi 1994		
<i>Aedes aegypti</i>	Yellow fever mosquito	LC50	MOR	TS: F; > 95% PU, CRY, CYGON	48	5040	AQ 18476	Song et al. 1997	C
<i>Daphnia magna</i>	Water flea	LC50	MOR	TS: 98%	48	6400	AQ 5180	Canton et al. 1980	C
<i>Daphnia magna</i>	Water flea	LC50	MOR		48	6400	AQ 5675	Hermens et al. 1984	M
<i>Aedes aegypti</i>	Yellow fever mosquito	LC50	MOR	TS: F; > 95% CRY, CYGON	48	6410	AQ 18476	Song et al. 1997	C
<i>Daphnia magna</i>	Water flea	EC50	ITX; IMBL		24	3500 - 10000	AQ 17456	Devillers et al. 1985	C
<i>Daphnia magna</i>	Water flea	EC50	ITX; IMBL		2	35000 - 100000	AQ 17456	Devillers et al. 1985	C
<i>Daphnia magna</i>	Water flea	EC50	ITX; IMBL		4	10000 - 35000	AQ 17456	Devillers et al. 1985	C
<i>Daphnia magna</i>	Water flea	EC50	ITX; IMBL		6	10000 - 35000	AQ 17456	Devillers et al. 1985	C
Fish									
<i>Salmo trutta</i>	Brown trout	LC50	MOR		96	1400	AQ 19224	Aanes 1992	M
<i>Danio rerio</i>	Zebra danio	NOEC	MOR	TS: F, 10 % EC, DIMETHOATE, BAYER	7 d	3100	AQ 600	Beusen & Neven 1989	M
<i>Cyprinus carpio</i>	Common, mirror, colored, carp	LC50	MOR		72	3560	AQ 45084	Dutt & Guha, 1988.	M
<i>Cyprinus carpio</i>	Common, mirror, colored, carp	LC50	MOR		48	4000	AQ 45084	Dutt & Guha, 1988.	M
<i>Cyprinus carpio</i>	Common, mirror, colored, carp	LC50	MOR		72	4000	AQ 45084	Dutt & Guha, 1988.	M

Table 1. Short term tests for dimethoate. (Continued)

Scientific Name	Common Name	Endpoint	Effect	Test conditions etc.	Test Duration; hours	Concentration, µg/l	Master reference	Reference in master reference	Quality in master reference
<i>Cyprinus carpio</i>	Common, mirror, colored, carp	LC50	MOR		24	4230	AQ 45084	Dutt & Guha, 1988.	M
<i>Cyprinus carpio</i>	Common, mirror, colored, carp	LC50	MOR		48	4550	AQ 45084	Dutt & Guha, 1988.	M
<i>Cyprinus carpio</i>	Common, mirror, colored, carp	LC50	MOR		24	4620	AQ 45084	Dutt & Guha, 1988.	M
<i>Danio rerio</i>	Zebra danio	NOEC	MOR	TS: F, 10 % EC, DIMETHOATE, BAYER	7 d	5300	AQ 600	Beusen & Neven 1989	M
<i>Lepomis macrochirus</i>	Bluegill	LC50	MOR	TS: 97.4 % T	96	6000	AQ 666	Johnson & Finley 1980	C
<i>Oncorhynchus mykiss</i>	Rainbow trout, donaldson trout	LC50	MOR	TS: 97.4 % T	96	6200	AQ 666	Johnson & Finley 1980	C
<i>Oncorhynchus mykiss</i>	Rainbow trout, donaldson trout	EC50	BEH	TS: 98%	48	8600	AQ 5180	Canton et al. 1980	C
<i>Oncorhynchus mykiss</i>	Rainbow trout, donaldson trout	LC50	MOR	TS: 98%	48	10000	AQ 5180	Canton et al. 1980	C
<i>Heteropneustes fossilis</i>	Indian catfish	LC50	MOR	TS: F, 30 EC, ROGOR	96	10550	AQ 4366	Chaturvedi & Agrawal 1991	M
<i>Heteropneustes fossilis</i>	Indian catfish	LC50	MOR	TS: F; 30 EC, ROGOR	48	11400	AQ 4366	Chaturvedi & Agrawal 1991	M
<i>Heteropneustes fossilis</i>	Indian catfish	LC50	MOR	TS: F; 30 EC, ROGOR	24	12130	AQ 4366	Chaturvedi & Agrawal 1991	M
<i>Heteropneustes fossilis</i>	Indian catfish	LC50	MOR	TS: F; 30 EC, ROGOR	12	12880	AQ 4366	Chaturvedi & Agrawal 1991	M
<i>Tilapia mossambica</i>	Mozambique tilapia	LC50	MOR	TS: DIMETHOATE	72	49800	AQ 45084	Dutt & Guha, 1988.	M
<i>Clarias batrachus</i>	Walking catfish	LC50	MOR	TS: DIMETHOATE, > 94 %	96	50000	AQ 16180	Begum et al. 1994	M
<i>Tilapia mossambica</i>	Mozambique tilapia	LC50	MOR	TS: DIMETHOATE	72	50200	AQ 45084	Dutt & Guha, 1988.	M
<i>Tilapia mossambica</i>	Mozambique tilapia	LC50	MOR	TS: DIMETHOATE	48	50700	AQ 45084	Dutt & Guha, 1988.	M
<i>Tilapia mossambica</i>	Mozambique tilapia	LC50	MOR	TS: DIMETHOATE	48	51200	AQ 45084	Dutt & Guha, 1988.	M
<i>Tilapia mossambica</i>	Mozambique tilapia	LC50	MOR	TS: DIMETHOATE	24	53100	AQ 45084	Dutt & Guha, 1988.	M
<i>Tilapia mossambica</i>	Mozambique tilapia	LC50	MOR	TS: DIMETHOATE	24	60800	AQ 45084	Dutt & Guha, 1988.	M
<i>Danio rerio</i>	Zebra danio	LC50	MOR		2	100000	AQ 17456	Devillers et al. 1985	C
<i>Danio rerio</i>	Zebra danio	LC50	MOR		4	100000	AQ 17456	Devillers et al. 1985	C

Table 1. Short term tests for dimethoate. (Continued)

Scientific Name	Common Name	Endpoint	Effect	Test conditions etc.	Test Duration; hours	Concentration, µg/l	Master reference	Reference in master reference	Quality in master reference
<i>Danio rerio</i>	<i>Zebra danio</i>	LC50	MOR		6	100000	AQ 17456	Devillers et al. 1985	C
<i>Danio rerio</i>	<i>Zebra danio</i>	LC50	MOR		24	100000	AQ 17456	Devillers et al. 1985	C
<i>Oryzias latipes</i>	<i>Medaka, high-eyes</i>	EC50	ITX; IMBL	TS: 98%	24	105000	AQ 5180	Canton et al. 1980	C
<i>Oryzias latipes</i>	<i>Medaka, high-eyes</i>	EC50	ITX; IMBL	TS: 98%	96	108000	AQ 5180	Canton et al. 1980	C
<i>Oryzias latipes</i>	<i>Medaka, high-eyes</i>	EC50	ITX; IMBL	TS: 98%	72	118000	AQ 5180	Canton et al. 1980	C
<i>Poecilia reticulata</i>	<i>Guppy</i>	EC50	BEH	TS: 98%	96	120000	AQ 5180	Canton et al. 1980	C
<i>Oryzias latipes</i>	<i>Medaka, high-eyes</i>	EC50	ITX; IMBL	TS: 98%	48	128000	AQ 5180	Canton et al. 1980	C
<i>Oncorhynchus mykiss</i>	<i>Rainbow trout, donaldson trout</i>	LC50	MOR	TS: 98%	24	133000	AQ 5180	Canton et al. 1980	C
<i>Poecilia reticulata</i>	<i>Guppy</i>	EC50	BEH	TS: 98%	48	135 000	AQ 5180	Canton et al. 1980	C
<i>Poecilia reticulata</i>	<i>Guppy</i>	EC50	BEH	TS: 98%	72	135 000	AQ 5180	Canton et al. 1980	C
<i>Poecilia reticulata</i>	<i>Guppy</i>	EC50	BEH	TS: 98%	24	187 000	AQ 5180	Canton et al. 1980	C

C = Complete

M = Moderate

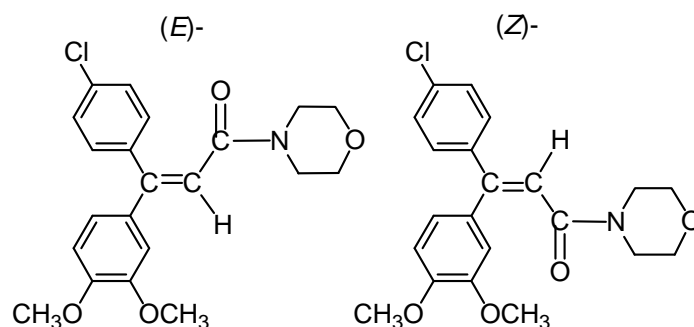
TS = Technical substance

AQ XXX = Acquire Ecotox database reference. The database is available in the Internet:

<http://www.epa.gov/ecotox/>

1. Dimethomorph

Dimethomorph is a systemic oomycete fungicide with preventive/curative and antisporulative effect. The mode of action is inhibition of fungal cell wall formation. Technical *dimethomorph* is a mixture of two optical isomers, E and Z. Only the Z-isomer is intrinsically active. *Dimethomorph* is used in potatoes and leak.



1.1 Physico-chemical properties

Physico-chemical properties of *dimethomorph* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *dimethomorph*.

		Reference
CAS-No.	110488-70-5	1
Empirical formula	C ₁₂ H ₂₂ Cl NO ₄	1
Molecular weight [g/mol]	388	1
Solubility in water [mg/kg]	E/Z = 48/52: 0.018 E-isomer: 0.012 Z-isomer: 0.006	1
Vapour pressure [Pa]	E-isomer: 9.7 · 10 ⁻⁷ Z-isomer: 1.0 · 10 ⁻⁶	1
Log P _{ow}	E-isomer: 2.63 Z-isomer: 2.73	1
Henry's law constant [Pa·m ³ /mol]	E-isomer: 3.1 · 10 ⁻⁵ Z-isomer: 6.7 · 10 ⁻⁵	1

1.2 Toxicity to aquatic organisms

The toxicity of *dimethomorph* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *dimethomorph*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	Growth rate	96 h	E _r C ₅₀ 84 NOE _r C 9.8	2
Crustaceans				

<i>Mysidopsis bahia</i>	Mortality	96 h	LC ₅₀ 33.0	3
<i>Daphnia magna</i>		48 h	EC ₅₀ 48.9	2
<i>Daphnia magna</i>	Mortality, reproduction	22 d	NOEC 0.1 ¹⁾	4
Fish				
<i>Salmo gairdneri</i>	Mortality	96 h	LC ₅₀ 6.2	1
<i>Cyprinodon veriegatus</i>	Mortality	96 h	LC ₅₀ 11.3	3
<i>Oncorhynchus mykiss</i>	Mortality	96 h	LC ₅₀ 6.2	3
<i>Oncorhynchus mykiss</i>	Mortality	96 h	LC ₅₀ 6.0	2
<i>Cyprinus carpio</i>	Mortality	96 h	LC ₅₀ 18.6	2
<i>Onchorhynchus mykiss</i>	Mortality, abnormal behaviour	21 d	NOEC 0.48	4

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.1 mg/L. Both short and long term studies are available, and three trophic levels have been tested. But according to the acute toxicity studies fish, and not crustaceans, seems to be the most sensitive group, therefore, an assessment factor of 50 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *dimethomorph* is calculated to 0.002 mg/L.

1.3 Bioaccumulation and persistence

Considering the relatively high log P_{ow} for *dimethomorph*, a slight potential for bioaccumulation can not be excluded, BCF is calculated to 48 and 57 for the E- and Z-isomers respectively (2), however, no bioaccumulation studies have been performed. *Dimethomorph* is hydrolytically stable, it is not readily biodegraded in water and there is no photochemical transformation of ecological relevance (1). No major metabolites in water have been detected. In sediment two unknown metabolites were found (16% after 51-105 d and 7.8% after 1 d) (2).

1.4 Proposed water quality objective

Since PNEC is 0.002 mg/L, the proposed water quality standard for *dimethomorph* is 0.002 mg/L.

1.5 Comments

Dimethomorph shows low mobility in soil and is therefore not expected to reach ground and surface waters via leaching through the soil profile.

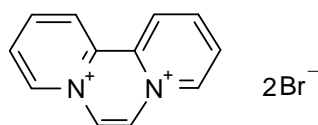
1.6 Literature

- (1) Dryselius, E., 1995. *Ecotoxicological evaluation of Dimethomorph*. National Chemicals Inspectorate. Sweden

- (2) Jansma, J.W. and Linders, J., 1993. *Dimethomorph*. Adviserapport: 93/679101/001. Holland.
- (3) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (4) Montforts, M.H.M.M. and Mensink, B.J.W.G., 1997. *Dimethomorph*. Adviserapport: 05216A00. Holland.

1. Diquat

Diquat is a non-selective contact herbicide, intended for use in legumes, potatoes and strawberries. *Diquat* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *diquat* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *diquat*.

		Reference
CAS-No.	2764-72-9 (ion) 85-00-7 (dibromide)	1
Empirical formula	C ₁₂ H ₁₂ N ₂ , C ₁₂ H ₁₂ Br ₂ N ₂ (dibromide)	1
Molecular weight [g/mol]	184.2, 344 (dibromide)	1
Solubility in water [mg/kg]	712000 at 20°C, pH 5.2 718000 at 20°C, pH 7.2 713000 at 20°C, pH 9.2	1
Vapour pressure [kPa]	<10 ⁻⁸ at 25°C	1
Log P _{ow}	-4.6 at 20°C	1
Henry's law constant [Pa×m ³ /mol]	< 5×10 ⁻¹²	1

1.2 Toxicity to aquatic organisms

The toxicity of *diquat* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *diquat*.

Species	End-point	Exposure duration	Result [mg/L]	Reference
Algae				
<i>Pseudokirchneriella Subcapitata</i>	biomass growth rate	96 h, static	EC ₅₀ 0.011 NOEC 0.0068 EC ₅₀ 0.019 ¹⁾ NOEC 0.0068	1, 2
Crustaceans				
<i>Daphnia magna</i>	mortality	48 h, static	EC ₅₀ 1.2	1, 2
<i>Daphnia magna</i>		21d	NOEC 0.125	1, 2
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 21.0	1, 2
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow through	LC ₅₀ 6.1	1, 2
<i>Pimephales promelas</i>	mortality	34 d	NOEC 0.12	1, 2
<i>Cyprinus carpio</i>	mortality	96 h, static	LC ₅₀ 67	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance *diquat* ion.

The most sensitive (acute effects) of the tested species was *Pseudokirchneriella subcapitata*, with an EC₅₀ of 0.019 mg/L and a NOEC of 0.0068 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.019 mg/L is divided by a factor of 100, which results in a PNEC of 0.00019 mg/L.

1.3 Bioaccumulation and persistence

Diquat is not expected to bioaccumulate. No hydrolysis occurs at environmental pH. Due to the strong adsorption to soil particles, *diquat* is very persistent in soil (1). The primary route of dissipation of *diquat* from natural water is through very rapid adsorption onto sediment or plant material. *Diquat* dissipates in water/sediment systems with a half-life of 12 to 24 hours, mainly due to partition into sediment.

1.4 Proposed water quality objective

Since PNEC is 1.9×10^{-4} mg/L, the proposed water quality objective for *diquat* is 0.0002 mg/L.

1.5 Comments

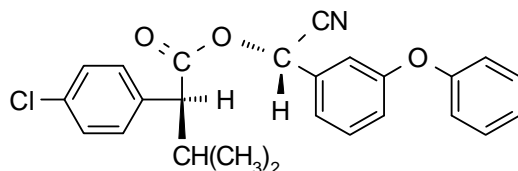
Even though *diquat* is very water-soluble it is unlikely to reach surface water, since *diquat* strongly adsorbs to soil particles (increase with clay content) and has little potential to leach through in the soil profile. Due to the strong adsorption, a water quality objective for the sediment compartment is relevant.

1.6 Literature

- (1) European Commission Peer Review Programme. *Diquat Monograph, 1996*. Rapporteur Member State: United Kingdom.
- (2) European Commission Peer Review Programme. *Diquat Review report. Appendix II - Endpoints and related information, 2000*. Rapporteur Member State: United Kingdom.

1. Esfenvalerate

Esfenvalerate is a pyrethroid insecticide, intended for use in legumes, fruit and cereals. *Esfenvalerate* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *esfenvalerate* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *esfenvalerate*.

		Reference
CAS-No.	66230-04-4	1
Empirical formula	C ₂₅ H ₂₂ ClNO ₃	1
Molecular weight [g/mol]	419.9	1
Solubility in water [mg/kg]	0.002 at 25°C	3
Vapour pressure [Pa]	1.17×10 ⁻⁹ at 20°C (estimated)	1
Log P _{ow}	6.24 at 25°C	1
Henry's law constant [Pa×m ³ /mol]	4.92×10 ⁻⁴	1

1.2 Toxicity to aquatic organisms

The toxicity of *esfenvalerate* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *esfenvalerate*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth rate	96 h, static	E _r C ₅₀ 0.010 NOEC 0.001	1, 2
Crustaceans				
<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 0.0009	1, 2
<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 0.0035	1
<i>Daphnia magna</i>	survival growth reproduction	21 d, semi-static	NOEC 0.000052	1, 2
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ 0.00021	1
<i>Pimephales promelas</i>	mortality	96 h, static	LC ₅₀ 0.00018	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.00026	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow-through	LC ₅₀ 0.0001	1, 2

<i>Oncorhynchus mykiss</i>		21 d, flow-through	NOEC 0.000001 ¹⁾	1
<i>Pimephales promelas</i>		260 d, flow-through	MATC 0.00009-0.00021 NOEC (0.00009/ $\sqrt{2}$) ≈ 0.0000636 ²⁾	1
Mesocosm				
			EAC 0.00008 NOEC 0.00001	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97%

²⁾ NOEC has been calculated from MATC (geometric mean of NOEC and LOEC). The equation is found in Technical guidance document.

The most sensitive of the tested species was *Oncorhynchus mykiss*, with a NOEC of 1×10^{-6} mg/L. Since both short and long term studies are available, and three trophic levels are tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *esfenvalerate* is calculated to 1×10^{-7} mg/L.

1.3 Bioaccumulation and persistence

Esfenvalerate has high potential for bioaccumulation. BCF for *esfenvalerate* was calculated to 2850-3650 based on fish. In natural water/sediment systems *esfenvalerate* was rapidly transferred from water to sediment and degraded with DT₅₀ values in the range of 54 to 80 days for the total system. Two metabolites were formed *CPIA* and *Pbacid*, exceeding 10%, but considered as much less toxic than parent compound (1).

1.4 Proposed water quality objective

Since PNEC is 1×10^{-7} , the proposed water quality objective for *esfenvalerate* is 1×10^{-7} mg/L.

1.5 Comments

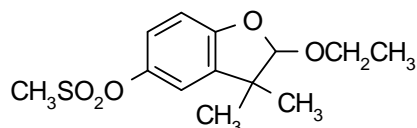
Esfenvalerate has low solubility in water and dissipates rapidly from the water-phase due to high adsorption to organic matter and sediment. Therefore, water quality objective for sediment compartment is relevant (1).

1.6 Literature

- (1) European Commission Peer Review Programme. *Esfenvalerate Monograph, 1996*. Rapporteur Member State: Portugal.
- (2) European Commission Peer Review Programme. *Esfenvalerate Review report. European Commission, 2000*. Rapporteur Member State: Portugal.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Ethofumesate

Ethofumesate is a systemic herbicide. *Ethofumesate* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *ethofumesate* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *ethofumesate*.

		Reference
CAS-No.	26225-79-6	1
Empirical formula	C ₁₃ H ₁₈ O ₅ S	1
Molecular weight [g/mol]	286.3	1
Solubility in water [mg/kg]	50 at 25 °C, pH 7.7	1
Vapour pressure [Pa]	6.5 × 10 ⁻⁴	1
Log P _{ow}	2.7 at 20 °C	1
Henry's law constant [Pa×m ³ /mol]	6.8 × 10 ⁻⁴ at 25 °C	1

1.2 Toxicity to aquatic organisms

The toxicity of *ethofumesate* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *ethofumesate*.

Species	End-point	Exposure duration	Result [mg ai/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>		120 h, static	EC ₅₀ >2.76 NOEC >2.7	2
<i>Scenedesmus subspicatus</i>	biomass growth rate	72 h, static 0-24 h	E _b C ₅₀ 3.9 E _r C ₅₀ 9.0 NOEC 1.25	1
<i>Nitzschia palea</i>	growth rate	96 h, static	E _r C ₅₀ 17 NOEC 2.2	1
Higher aquatic plants				
<i>Lemna minor</i>	biomass growth rate	14 d, semi-static	E _b C ₅₀ >50 E _r C ₅₀ >50 NOEC 4.3	1
Crustaceans				
<i>Mysidopsis bahia</i>	immobility	96 h, static	LC ₅₀ 5.3	2
<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 14	1
<i>Daphnia magna</i>	immobility	21 d, flow-through	NOEC 0.3	2
<i>Daphnia magna</i>	immobilisation reproduction	21 d, semi-static	NOEC 10 NOEC 0.32	1
<i>Daphnia magna</i>	reproduction	21 d, semi-static	NOEC 0.32	1

Molluscs				
<i>Crassostrea virginica</i>	shell deposition	96 h, flow-through	EC ₅₀ 2.6	2
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 17.5	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 20	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, semi-static	LC ₅₀ 12	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.75 ²⁾	2
<i>Lepomis macrochirus</i>	mortality	96 h, static-renewal	LC ₅₀ 21.8	2
<i>Lepomis macrochirus</i>	mortality	96 h, semi-static	LC ₅₀ 21	1
<i>Lepomis macrochirus</i>	mortality	96 h, semi-static	LC ₅₀ 12	1
<i>Cyprinodon variegatus</i>	mortality	96 h, static	LC ₅₀ 25	2
<i>Cyprinus carpio</i>		96 h, semi-static	LC ₅₀ 11	1
<i>Pimephales promelas</i>	mortality	28 d, flow-through	NOEC 2.56	2
<i>Pimephales promelas</i>		28 d, flow-through	NOEC <2.6	1
<i>Oncorhynchus mykiss</i>		21 d, flow-through	NOEC 3	1
<i>Oncorhynchus mykiss</i>		21 d, semi-static	NOEC 2.1	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96%

²⁾ This was the lowest short term LC₅₀ value. However, since three other studies with the same species gave significantly higher values, this is considered to be an outlier.

The most sensitive (acute effects) of the tested species was *Crassostrea virginica* with an EC₅₀ of 2.6 mg/L. In the long term studies, *Daphnia* was the most sensitive, with a NOEC of 0.3 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest LC₅₀ of 2.6 mg/L is divided by a factor of 100, which results in a PNEC of 0.026 mg/L.

1.3 Bioaccumulation and persistence

Ethofumesate is not expected to bioaccumulate. Hydrolytic and photolytic transformation has little importance for the dissipation of *ethofumesate* in natural aquatic environment. The substance is not readily biodegradable in the water phase. In water/sediment systems *ethofumesate* dissipates from the water phase and is slowly transformed in sediment (1).

1.4 Proposed water quality objective

Since PNEC is 0.026 mg/L, the proposed water quality standard for *ethofumesate* is 0.03 mg/L.

1.5 *Comments*

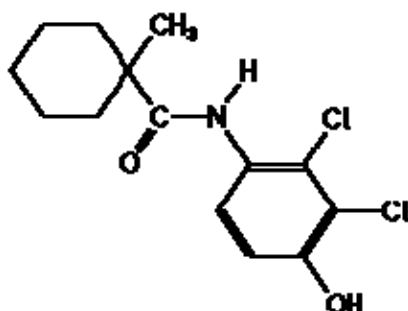
Ethofumesate is moderately mobile in soil and may reach ground and surface waters via transport through the soil profile. A quality objective is relevant for the sediment compartment.

1.6 *Literature*

- (1) European Commission Peer Review Programme. *Ethofumesate Monograph, 1998*. Rapporteur Member State: Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Fenhexamid

Fenhexamid is a fungicide, a member of the hydroxyanilids that inhibits spore germ tube development and hyphal growth. It is intended for use in cultivation of strawberries and fruit. *Fenhexamid* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *fenhexamid* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *fenhexamid*.

		Reference
CAS-No.	126833-17-8	1
Empirical formula	C ₁₄ H ₁₇ Cl ₂ NO ₂	1
Molecular weight [g/mol]	302.2	1
Solubility in water [mg/kg]	14 at pH 5 and 20° C 24 at pH 7 412 at pH 9	1
pKa	7.3	1
Vapour pressure [Pa]	9 × 10 ⁻⁷ at 25° C	1
Log P _{ow}	3.51	1
Henry's law constant [Pa×m ³ /mol]	5 × 10 ⁻⁶	1

1.2 Toxicity to aquatic organisms

The toxicity of *fenhexamid* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *fenhexamid*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth	72h, static	E _r C ₅₀ 26 NOEC >26	1
Aquatic toxicity				
<i>Lemna gibba</i>	growth	14d, static	EC ₅₀ >2.3	2
Crustaceans				
<i>Daphnia magna</i>	behaviour	48h, static	EC ₅₀ 105	2
<i>Daphnia magna</i>	not specified	48h, static	EC ₅₀ > 19	1
<i>Americamysis bahia</i>	mortality	96h, flow-through	LC ₅₀ 4.6	2
<i>Daphnia magna</i>	reproduction	21d, static	NOEC 1.0	1
Fish				
<i>Onchorhynchus</i>	mortality	96h	LC ₅₀ 1.2	2

<i>mykiss</i>				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.3	2
<i>Cyprinodon variegates</i>	mortality	96h, flow-through	LC ₅₀ 11	2
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.3	1
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 3.4	1
<i>Onchorhynchus mykiss</i>	early life stage test	35d, flow-through	NOEC 0.10 ¹⁾	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Onchorhynchus mykiss*, with a NOEC of 0.10 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *fenhexamid* is calculated to 0.010 mg/L.

1.3 **Bioaccumulation and persistence**

Fenhexamid is not expected to bioaccumulate. The major dissipation route for *fenhexamid* is microbial degradation and partitioning to sediment (DT₅₀ <7days). In sediment *fenhexamid* rose to account for maxima of ca 25-50% AR on day 3-7 then declined with first order DT₅₀ of 11-32 days. No major metabolites, exceeding 10%, were found.

1.4 **Proposed water quality objective**

Since PNEC is 0.010 mg/L, the proposed water quality standard for *fenhexamid* is 0.01mg/L.

1.5 **Comments**

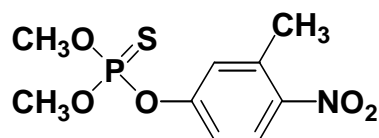
Fenhexamid is not mobile in soil, and it is therefore not expected to leach through the soil profile. A quality objective for sediment is recommended.

1.6 **Literature**

- (1) European Commission Peer Review Programme. *Fenhexamid Monograph*, 1998. Rapporteur Member State: United Kingdom.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Fenitrothion

Fenitrothion is an organophosphorus insecticide. It controls insects by contact and stomach action, intended for use against aphids in oleiferous plants. The insecticide has neither systemic nor vapour activity. *Fenitrothion* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *fenitrothion* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *fenitrothion*.

		Reference
CAS-No.	122-14-5	1
Empirical formula	C ₉ H ₁₂ NO ₅ PS	1
Molecular weight [g/mol]	277	1
Solubility in water [mg/kg]	19 at 20°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	6.8 x 10 ⁻⁴ at 20°C	1
Log P _{ow}	3.3 at 25°C	1
Henry's law constant [Pa×m ³ /mol]	9.9 x 10 ⁻³ at 20°C	1

1.2 Toxicity to aquatic organisms

The toxicity of *fenitrothion* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *fenitrothion*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	biomass	72h, static	EC ₅₀ 1.3 NOEC 0.61	1
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48h, static	EC ₅₀ 0.0086	1
<i>Daphnia magna</i>	immobilisation	21d, flow-through	NOEC 0.000087 ²⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.3	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ >2.1 ¹⁾	1
<i>Onchorhynchus mykiss</i>	mortality	96d, flow-through	NOEC 0.088	1

¹⁾ Test performed on preparation, IPM 400 (400g/l). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 94.5%

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.000087 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *fenitrothion* is calculated to 8.7×10^{-6} mg/L.

1.3 Bioaccumulation and persistence

Fenitrothion is not expected to bioaccumulate. Log P_{ow} indicates that *fenitrothion* and its metabolites may partition into fatty tissues. However BCF is low. *Fenitrothion* degrades rapidly in water/sediment systems, DT_{50} of 0.88-1.27 days. The formulation, IPM 400, is a suspension of micro-capsules (10 - 15 μ m) containing the active substance. The formulation differs in properties from active substance. If added as pure active substance *fenitrothion* mainly remains in water phase, 9-28% partitioning into the sediment. Added as capsule suspension (CS) the compound degrades within a DT_{50} of 84.3-96.6 days and the partition in sediment increases to 88.5-96.3%. Major metabolites in water are *NMC*, *AM-FNT* and *DM-AM-FNT*. *NMC* is also found in sediment. According to risk assessment the metabolites is expected to pose low risk to aquatic life. None of the metabolites is persistent.

1.4 Proposed water quality objective

Since PNEC is 8.7×10^{-6} mg/L, the proposed water quality standard for *fenitrothion* is 9×10^{-6} mg/L.

1.5 Comments

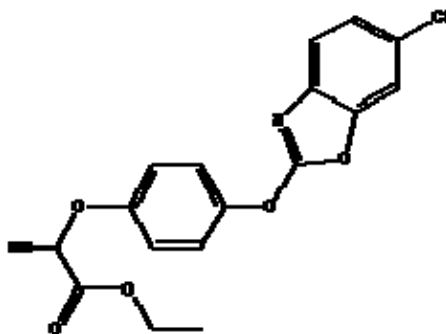
Added as preparation *fenitrothion* partitions into sediment. According to toxicity study the compound is toxicity to the sediment dwelling organisms, *Chironomus riparius*. Therefore a supplementary quality object for sediment is needed.

1.6 Literature

- (1) European Commission Peer Review Programme. *Fenitrothion Monograph*, 2003. Rapporteur Member State: United Kingdom.

1. Fenoxaprop-p-ethyl and propionic acid

Fenoxaprop-p-ethyl is a systemic herbicide, intended for use in cereals. *Fenoxaprop-p-ethyl* is under evaluation within the framework of EU Dir. 91/414. In plants the ester, *fenoxaprop-p-ethyl*, is rapidly transformed into *propionic acid*, which inhibits the synthesis of lipids.



1.1 Physico-chemical properties

Physico-chemical properties of *fenoxaprop-p-ethyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *fenoxaprop-p-ethyl*.

		Reference
CAS-No.	71238-80-2	2
Empirical formula	C ₁₈ H ₁₆ ClNO ₅	2
Molecular weight [g/mol]	361.8	2
Solubility in water [mg/kg]	0.7	2
pKa	Not relevant	
Vapour pressure [Pa]	0.53	2
Log P _{ow}	4.28	2

1.2 Toxicity to aquatic organisms

The toxicity of *fenoxaprop-p-ethyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *fenoxaprop-p-ethyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth inhibition	72h, static	EC ₅₀ 0.36	2
<i>Scenedesmus subspicatus</i>	growth inhibition	72h, static	EC ₅₀ 0.52 NOEC 0.36	1,2
Crustaceans				
<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ 4.6	1
<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ 1.9	2
<i>Daphnia magna</i>	mortality	21d, semi-static	NOEC 0.22	2
Fish				
<i>Onchohynchus mykiss</i>	mortality	96h	LC ₅₀ 0.62	1

<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.4	1,2
<i>Onchohynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.46	2
<i>Onchohynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.57	2

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.22 mg/L. Short term studies are available from three trophic levels. Chronic toxicity has only been tested for algae and daphnia. However fish is the most sensitive trophic level in acute tests. Due to the lack of long term study the assessment factor has to compensate for the uncertainty. An assessment factor of 100 is used for calculation of the predicted no effect concentration. *Fenoxaprop-p-ethyl* has shown to rapidly hydrolyse to *propionic acid*. Since the water quality objective is based on a semi-static long term test it will also account for the toxicity of the metabolite *propionic acid*. Hence, the PNEC for *fenoxaprop-p-ethyl* and *propionic acid* is calculated to 0.0022 mg/L.

1.3 Bioaccumulation and persistence

Fenoxaprop-p-ethyl is expected to bioaccumulate, log K_{ow} is 4.58. BCF in fish is 510 in whole fish. *Fenoxaprop-p-ethyl*, was in two water/sediment systems immediately hydrolysed to *propionic acid*. The parent compound and its main metabolite were both degraded with a DT₅₀ of 12-13 days, resulting in another metabolite, *Hoe 054014*. The substance was then adsorbed into the sediment or mineralised. No toxicity studies are available for *Hoe054014*.

1.4 Proposed water quality objective

Since PNEC is 0.0022 mg/L, the proposed water quality standard for *fenoxaprop-p-ethyl* and *propionic acid* is 0.002 mg/L.

1.5 Comments

Fenoxaprop-p-ethyl is strongly adsorbed to particles, K_{oc} 5600-16800 and is not expected to leach. However *propionic acid*, K_{oc} 110-190, may reach ground- and surface water due to leach through the soil profile. Toxicity studies are not sufficient regarding *Hoe054014*. Therefore the water quality object, complemented with a sediment quality objective, ought to be upgraded when additional studies are submitted.

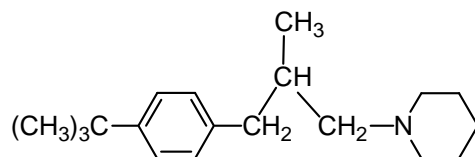
1.6 Literature

- (1) Silvo R., 1991. *Ekotoxikologisk utvärdering av fenoxaprop-p-ethyl*. Vatten- och miljöstyrelsen. Helsinki, Finland.

(2) *Sagens oplysninger og miljøstyrelsen vurdering*, 1996. Bekaempelsemiddelkontoret, miljøstyrelsen, Danmark.

1. Fenpropidin

Fenpropidin is a systemic fungicide. The compound is an ergosterol inhibitor with both curative and preventive effect. It is intended for use in cereals.



1.1 Physico-chemical properties

Physico-chemical properties of *fenpropidin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *fenpropidin*.

		Reference
CAS-No.	67306-008	1
Empirical formula	C ₁₉ H ₃₁ N	1
Molecular weight [g/mol]	273.9	1
Solubility in water [mg/kg]	3320 at pH 5 and 20°C 707 at pH 7 0.98 at pH 9	1
pKa	10.1	1
Vapour pressure [Pa]	1.7 × 10 ⁻²	1
Log P _{ow}	2.59	1
Henry's law constant [Pa×m ³ /mol]	8.8 × 10 ⁻³	1

1.2 Toxicity to aquatic organisms

The toxicity of *fenpropidin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *fenpropidin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Navicula pelliculosa</i>	biomass	96h, static	E _b C ₅₀ 0.0025 ²⁾ NOEC 0.0008	1
<i>Scendesmus subspicatus</i>	growth rate biomass	24h, static 96h, static	E _r C ₅₀ 0.0098 E _b C ₅₀ 0.0057 NOEC 0.001	1
<i>Scendesmus subspicatus</i>	growth rate biomass	24h, static 96h, static	E _r C ₅₀ 0.09 ¹⁾ E _b C ₅₀ 0.123 ¹⁾ NOEC 0.020 ¹⁾	1
Cyanobacteria				
<i>Microcystis aeruginosa</i>	biomass	96h, static	E _b C ₅₀ 4.4 NOEC 1.1	1
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.54	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.68 ¹⁾	1
<i>Daphnia magna</i>	reproduction immobility	21d, semi static	NOEC >1.0 <3.2 NOEC 0.32	1
<i>Daphnia magna</i>	reproduction immobility	21d, semi static	NOEC >1.0 <3.2 ¹⁾ NOEC 0.014 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ 2.57	1
<i>Lepomis macrochirus</i>	mortality	96h, static	EC ₅₀ 1.93	1
<i>Cyprinus carpio</i>	mortality	96h, static	EC ₅₀ 3.55	1
<i>Lepomis macrochirus</i>	mortality	96h, static	EC ₅₀ 2.09 ¹⁾	1
<i>Cyprinus carpio</i>	mortality	96h, static	EC ₅₀ 1.24 ¹⁾	
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ 2.93 ¹⁾	1
<i>Onchorhynchus mykiss</i>	Toxic symptoms and mortality	21d, flow-through	NOEC 0.32	1
<i>Onchorhynchus mykiss</i>	behaviour	21d, flow-through	NOEC 0.024 ¹⁾	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97%

The most sensitive (acute effects) of the tested species was *Navicula pelliculosa*, with an EC₅₀ of 0.0025 mg/L and. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.0025 mg/L is divided by a factor of 100, which results in a PNEC of 0.000025 mg/L.

1.3 Bioaccumulation and persistence

Fenpropidin may bioaccumulate with BCF 163 in fish. *Fenpropidin* is stable towards hydrolysis and photolysis. The dissipation half-life from water in sediment/water system is <14d. One major (exceeding 10%) transformation product was formed in the water phase, *Ro 15-6045*. The DT₅₀ in the whole systems is 21 and 65 days.

1.4 Proposed water quality objective

Since PNEC is 0.000025 mg/L, the proposed water quality standard for *Fenpropidin* is 0.00002 mg/L.

1.5 Comments

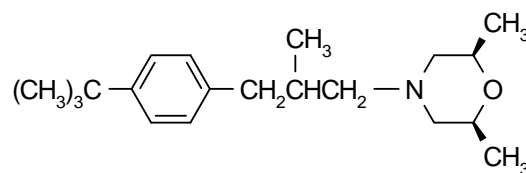
Fenpropidin is not expected to reach surface and ground waters through the soil profile. However some metabolites may leach. The toxicity of the metabolite *Ro 15-6045* is at the present not known, although this should be looked into when studies are available. Additional quality objectives for sediment and biota are recommended.

1.6 *Literature*

- (1) Lindbäck U., 1995. Ecotoxicological evaluation of Fenpropidin. National Chemical Inspectorate. Sweden.

1. Fenpropimorph

Fenpropimorph is a fungicide. The mode of action is by inhibiting the sterol biosynthesis. Intended for use in corn against mildew and rust.



1.1 Physico-chemical properties

Physico-chemical properties of *fenpropimorph* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *fenpropimorph*.

		Reference
CAS-No.	67564-91-4	2
Empirical formula	C ₂₀ H ₃₃ NO	2
Molecular weight [g/mol]	303.5	2
Solubility in water [mg/kg]	7 300 at pH 4.4 4.32 at pH 7 3.53 at pH 9-11	2
pK _b	7.02 at 20°C 7.19 at 25°C	2
Vapour pressure [Pa]	2.3 × 10 ⁻³ at 20°C 4.5 × 10 ⁻³ at 25°C	2
Log P _{ow}	2.6 at pH 5 4.1 at pH 7 4.4 at pH 9	2
Henry's law constant [Pa×m ³ /mol]	0.3	3

1.2 Toxicity to aquatic organisms

The toxicity of *fenpropimorph* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *fenpropimorph*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass	96 h	EC ₅₀ 0.17 NOEC 0.037	2
	growth rate	24 h	EC ₅₀ 0.18 NOEC 0.037	
Crustaceans				
<i>Daphnia magna</i>		48 h	EC ₅₀ 2.39	4
<i>Daphnia magna</i>	mortality	21 d, flow-through	EC ₅₀ 0.36 EC ₀ 0.071	4
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ 1.65 ¹⁾	5
<i>Oncorhynchus</i>	mortality	94 d, flow-through	NOEC 0.00016 ²⁾	1

<i>mykiss (Salmo gairdneri)</i>	toxic symptoms	94 d, flow-through	NOEC 0.0008	
<i>Oncorhynchus mykiss</i>	Modified Early life stage test	49 d, two applications with 28 d interval		6
	Body weight		NOEC 0.00195 ³⁾	

- 1) Test performed on preparation. Value expressed as active substance.
- 2) Effect concentration basis for calculation of former PNEC. Test substance purity 95.6 %.
- 3) Effect concentration basis for calculation of revised PNEC. Peak value corrected for analytical recovery.

Former water quality objective calculation

The lowest acute toxicity data is generated from *Scenedesmus subspicatus* with a growth rate EC₅₀ of 0.18 mg/L. The lowest NOEC, though, is generated from the fish *Oncorhynchus mykiss* with a mortality NOEC of 0.00016 mg/ml. In the same study there were indications of slight effects on growth at the same concentration level, but these effects are not expected to be of significance on population level. Both short-term and long-term results are available from two respectively three trophic levels. However for fish supportive data for acute toxicity has been presented therefore a factor of 10 is used to derive the PNEC for the substans. The PNEC is calculated to 1.6×10^{-5} mg/L.

Revised EQS calculation according to EU-harmonised methodology (7)

A new modified early life stage test with *Oncorhynchus mykiss* has been performed under, for the substance, more realistic exposure conditions (2 applications at 28 day interval). The NOEC_{growth} from this test is 1.95 µg/l and this result is preferred in the EU risk characterisation (5 & 6). There are chronic NOEC values representing three trophic levels (algae, crustacea and fish) available and therefore the use of an assessment factor of 10 is justified. The PNEC is calculated to 0.2 µg/L.

1.3 Bioaccumulation and persistence

Fenpropimorph is expected to bioaccumulate. BCF in fish has been determined to 1471-1842 in whole fish. *Fenpropimorph* is stable towards hydrolysis, but degraded by photolysis. However photolysis is expected to be a minor route of degradation due to rapid adsorption. Two water/sediment studies have been performed showing degradation to occur with a DT₅₀ of 5 days in water origin from Rhine and 13 days in pond water. One major metabolite is formed during degradation M1, *cis-4[3-[4-(1-methoxycarbonyl-1-methylethyl)phenyl]-2-methylpropyl]-2,6-dimethylmorpholine*.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.2 µg/L, the proposed EQS/water quality objective for *fenpropimorph* is 0.2 µg/L.

1.5 Comments

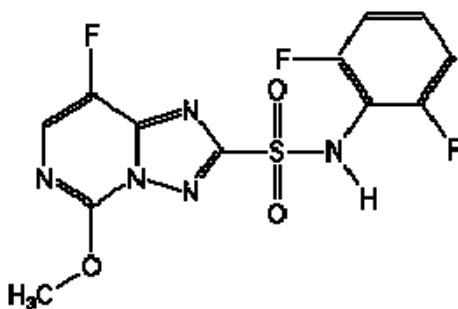
The potential mobility of *fenpropimorph* is low (K_{oc} 2772-5943). At low pH mobility may increase because of a positive charge. In water-sediment systems the main part of *fenpropimorph* is distributed to the sediment. A quality criterion for sediment is suggested as a complement to the water quality criterion. The metabolite is mainly distributed to the water-phase. The toxicity of the metabolite has not been investigated.

1.6 Literature

- (1) Hoffmann, H.D. & Munk, R., 1995, *Study Report: Early Life-Stage Toxicity Test on the Rainbow Trout (Oncorhynchus mykiss Walbaum 1972) with Fenpropimorph*, BASF, Germany.
- (2) Miljøstyrelsen, 1996, *Ecotoxicological Re-Evaluation of Fenpropimorph*, Carl Bro International a/s, Denmark.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (4) Wennell, T., 1991, *Ekotoxikologisk utvärdering av fungiciden Fenpropimorph*, Kemikalieinspektionen, Sverige
- (5) European Commission Peer Review Programme. *Fenpropimorph Draft Assessment Report vol 1*, 2005. Rapporteur Member State: Germany
- (6) European Commission Peer Review Programme. *Fenpropimorph Addendum vol 3*, 2007. Rapporteur Member State: Germany
- (7) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Florasulam

Florasulam is an herbicide, and a member of 1,5c triazolopyrimidine sulfonanilides. It inhibits the plant enzyme acetolactate synthase enzyme. The herbicide is intended for use in cereals and pasture. *Florasulam* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *florasulam* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *florasulam*.

		Reference
CAS-No.	145701-23-1	1
Empirical formula	C ₁₂ H ₈ O ₃ N ₅ F ₃ S	1
Molecular weight [g/mol]	359.3	1
Solubility in water [mg/kg]	84 at 20° and pH 5 6360 at pH 7 94200 at pH 9	1
pKa	4.54	1
Vapour pressure [Pa]	1 × 10 ⁻⁵ at 25°	1
Log P _{ow}	1.0 at pH 4 -1.22 at pH 7 -2.06 at pH 9	1
Henry's law constant [Pa×m ³ /mol]	4.35 × 10 ⁻⁷ at 20° and pH 7	1

1.2 Toxicity to aquatic organisms

The toxicity of *florasulam* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *florasulam*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth	72h, static	E _r C ₅₀ 0.0089 NOEC <7.9 × 10 ⁻⁴	1
Aquatic plants				
<i>Lemna gibba</i>	growth	96h, static	E _r C ₅₀ 0.0012 ¹⁾ NOEC 0.00062	1

Crustaceans				
<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ >292	1
<i>Palaemonetes pugio</i>	mortality	96h, static	LC ₅₀ >120	1
<i>Daphnia magna</i>	growth reproduction	21d, semi-static	NOEC 39 NOEC 65	1
Molluscs				
<i>Crassostrea virginica</i>	shell deposition	96h, static	EC ₅₀ >125	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >100	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ >100	1
<i>Menidia berylla</i>	mortality	96h, static	LC ₅₀ > 122	1
<i>Onchorhynchus mykiss</i>	growth	28d	NOEC 119	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 99.2%

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0012 mg/L and NOEC of 0.00062 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.0012 mg/L is divided by a factor of 100, which results in a PNEC of 0.000012 mg/L.

1.3 Bioaccumulation and persistence

Florasulam is not expected to bioaccumulate, the BCF in fish is 0.8-2.2. In water/sediment system the compound is primary degraded within a DT₅₀ of 8.7-18 days. It is transformed into a more persistent metabolite, 5-hydroxy, DT₅₀ of 68-243 days. *Florasulam* mainly remains in the water phase, while 5-hydroxy is distributed in water and sediment phases. The metabolite is less toxic to aquatic organisms than the parent compound. Therefore water quality for the metabolite is not needed.

1.4 Proposed water quality objective

Since PNEC is 1.2×10^{-5} mg/L, the proposed water quality standard for *florasulam* is 1×10^{-5} mg/L.

1.5 Comments

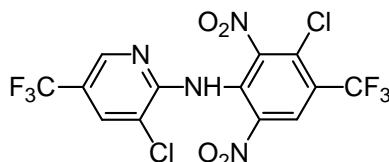
In soil *florasulam* is rapidly transformed (DT₅₀ 0.7-4.5 days) into metabolites; 5-hydroxy, DFP-ASTCA, ASTCA and TSA. The metabolites are more persistent, e.g. 5-hydroxy has a DT₅₀ of 31 days. The parent compound, as well as its metabolites, is considered as mobile in soil, and may reach surface- and groundwaters.

1.6 Literature

- (1) European Commission Peer Review Programme. *Florasulam Monograph, 1999*.
Rapporteur Member State: Belgium

1. Fluazinam

Fluazinam is a non selective fungicide and belongs to the group of chemicals aniline derivate. The compound is used on potatoes.



1.1 Physico-chemical properties

Physico-chemical properties of *fluazinam* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *fluazinam*.

		Reference
CAS-No.	79622-59-6	1
Empirical formula	C ₁₃ H ₄ Cl ₂ F ₆ N ₄ O ₄	1
Molecular weight [g/mol]	465.1	1
Solubility in water [mg/kg]	0.071 at pH 7 and 20°C	1
pKa	9.3	1
Vapour pressure [Pa]	1.1 × 10 ⁻³	1
Log P _{ow}	3.56	1
Henry's law constant [Pa×m ³ /mol]	7.2	1

1.2 Toxicity to aquatic organisms

The toxicity of *fluazinam* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *fluazinam*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	96h, static	EC ₅₀ >2.9 ¹⁾ NOEC 0.21 ¹⁾	1
<i>Selenastrum capricornutum</i>	growth rate	72h, static	EC ₅₀ 1.0 ¹⁾ NOEC 0.13 ¹⁾	5
<i>Selenastrum capricornutum</i>	growth rate	96h, static	EC ₅₀ 0.08 ¹⁾	3
<i>Selenastrum capricornutum</i>	growth rate	96h, static	EC ₅₀ >0.2 NOEC 0.048	4
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.06 ¹⁾	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.42 ¹⁾	5
<i>Daphnia magna</i>	immobility	48h, flow-through	EC ₅₀ 0.22	2
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.19	4
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.055	4
<i>Daphnia magna</i>	reproduction growth	21d, semi-static	NOEC 0.0125	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.08 ¹⁾	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.052 ¹⁾	5
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.036 ²⁾	2
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.11	2
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 0.053	2
<i>Cyprinus carpio</i>	mortality	96h, static	LC ₅₀ 0.15	4
<i>Onchorhynchus mykiss</i>	mortality	28d, flow-through	NOEC 0.012	1

¹⁾ Test performed on preparation; Epok (40g ai/l) and Shirilan (50g ai/l). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96.8%

The most sensitive (acute effects) of the tested species was *Onchorhynchus mykiss*, with a LC₅₀ of 0.036 mg/L and. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest LC₅₀ of 0.036 mg/L is divided by a factor of 100, which results in a PNEC of 0.00036 mg/L.

1.3 Bioaccumulation and persistence

Fluazinam is expected to bioaccumulate, log P_{ow} is 3.56 and BCF 465 in fish. The fungicide is hydrolysed with a DT₅₀ of 42 days at pH 7 and 6 day at pH 9. *Fluazinam* rapidly decreases from water in water/sediment systems, pH 7-7.6. However since no degradation products were found it is likely that the decrease is due to partition into the sediment. The time of dissipation is faster in water/sediment systems with higher organic content in the sediment, <1-7 days.

1.4 Proposed water quality objective

Since PNEC is 0.00036 mg/L, the proposed water quality standard for *fluazinam* is 0.0004 mg/L.

1.5 Comments

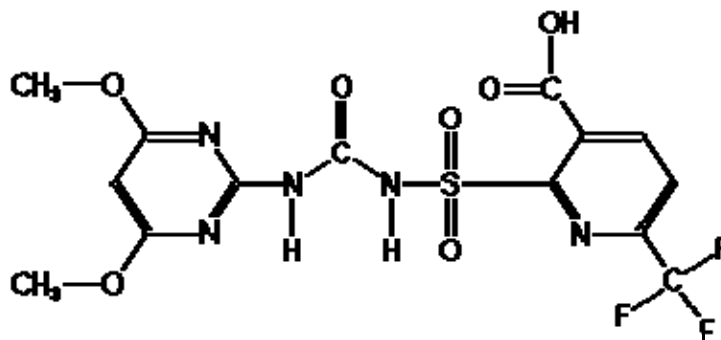
Fluazinam is not expected to reach surface and ground waters via leaching through the soil profile. The compound dissipates into the sediment and is expected to bioaccumulate, therefore additional quality objective are needed for sediment and biota.

1.6 Literature

- (1) Hanze K., 1993. Fluazinam. Scientific documentation and research. National Chemical Inspectorate. Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tuusa T., 1998. *Fluazinam, supplementary studies*. Finnish Environment Institute. Finland.
- (4) Adviescentrum toxicologie toxicology advisory center. 1993. RIVM, Netherland.
- (5) Spikkerud E., 1997. *Økotoksikologisk vurdering av Epok 600 EC (fluazinam + mefenoksam)*. Statens landbrukstilsyn, Seksjon plantevenmidler. Norge.

1. Flupyrulfuron-methyl

Flupyrulfuron-methyl is a selective herbicide against weed in cereals. *Flupyrulfuron-methyl* has been evaluated within the framework of EU Dir. 91/414



1.1 Physico-chemical properties

Physico-chemical properties of *flupyrulfuron-methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *flupyrulfuron-methyl*.

		Reference
CAS-No.	144740-54-5	2
Empirical formula	C ₁₅ H ₁₃ F ₃ N ₅ O ₇ SNa	2
Molecular weight [g/mol]	487.4	2
Solubility in water [mg/kg]	0.06 at pH 7 and 20° C	2
pKa	4.94	2
Vapour pressure [Pa]	<10 ⁻⁹	2
Log P _{ow}	9.17 at pH5 1.16 at pH6	2
Henry's law constant [Pa×m ³ /mol]	<10 ⁻⁸ at pH 5 <10 ⁻⁹ at pH 6	2

1.2 Toxicity to aquatic organisms

The toxicity of *flupyrulfuron-methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *flupyrulfuron-methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Anabeana flos-aquae</i>	biomass	72h, static	EC ₅₀ 0.099 NOEC 0.031	3
Higher aquatic plants				
<i>Lemna gibba</i>	biomass	14d, static	EC ₅₀ 0.0025 NOEC 0.00049 ¹⁾	1
Crustaceans				

<i>Daphnia magna</i>	immobilisation	48h, static	EC ₅₀ 720	1
<i>Daphnia magna</i>	growth	21 days	NOEC 16	1
Fish				
<i>Cyprinus carpio</i>	mortality	96h	LC ₅₀ 820	1
<i>Onchorhynchus mykiss</i>	mortality	96h	LC ₅₀ 470	1
<i>Onchorhynchus mykiss</i>	growth	28d, flow-through	NOEC 130	1
<i>Onchorhynchus mykiss</i>	sublethal effects	28d, flow-through	NOEC 9.2	1

¹⁴⁾ Effect concentration basis for calculation of PNEC. Test substance purity 92.8%

The most sensitive of the tested species was *Lemna gibba*, with a NOEC of 4.9×10^{-4} mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *flupyr sulfuron-methyl* is calculated to 4.9×10^{-5} mg/L.

1.3 Bioaccumulation and persistence

Flupyr sulfuron-methyl is not expected to bioaccumulate. Although the partition constant indicates bioaccumulation, due to rapid degradation and low use rate, the substance has little potential for accumulation. *Flupyr sulfuron-methyl* degrades rapidly in both soil and water. In water hydrolysis is a major degradation route. Hydrolysis is pH-dependent, in buffered water, the primary degradation occurs within a DT₅₀ of 44 days at pH 5, 12 days at pH 7 and 0.4 days at pH 9. The substance remains in the water phase. Half-life in water/sediment-studies (pH 6.3 and 7.3) is 3-6 days in water phase and the entire system. In the route of degradation two major metabolites are formed; *IN-JV460* and *IN-KV994*. Neither of the metabolites shows herbicidal or insecticidal activities.

1.4 Proposed water quality objective

Since PNEC is 0.000049 mg/L, the proposed water quality standard for *flupyr sulfuron-methyl* is 5×10^{-5} mg/L.

1.5 Comments

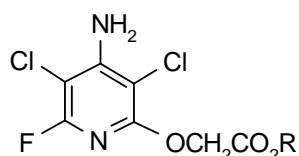
Flupyr sulfuron-methyl has potential to leach through the soil and reach both surface- and ground water.

1.6 **Literature**

- (1) European Commission Peer Review Programme. *Flupyr sulfuron-methyl Monograph, 1997*. Rapporteur Member State: France.
- (2) European Commission Peer Review Programme. *Flupyr sulfuron-methyl Review report, 2001*. Rapporteur Member State: France
- (3) European Commission Peer Review Programme. *Flupyr sulfuron-methyl Addendum, 2001*. Rapporteur Member State: France

1. Fluroxypyr

Fluroxypyr is an auxin type systemic herbicide, intended for use in cereals and pasture. The active moiety is the corresponding acid formed by hydrolysis of the ester. *Fluroxypyr* has been evaluated within the framework of EU Dir. 91/414.



Fluroxypyr ester

2-butoxy-1-methylethyl R = CH₃(CH₂)₃OCH₂CH(CH₃)-

meptyl (1-methylheptyl) R = CH₃(CH₂)₅CH(CH₃)-

1.1 Physico-chemical properties

Physico-chemical properties of *fluroxypyr acid* and *fluroxypyr-meptyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *fluroxypyr acid* and *fluroxypyr-meptyl*.

	Fluroxypyr acid	Reference	Fluroxypyr-meptyl	Reference
CAS-No.	69377-81-7	1	81406-37-3	1
Empirical formula	C₇H₅Cl₂FN₂O₃	1	C₁₅H₂₁Cl₂FN₂O₃	1
Molecular weight [g/mol]	255.0	1	367.3	1
Solubility in water [mg/kg]	125 at pH 3, 20 °C 5700 at pH 5.0, 20 °C 7300 at pH 9.2, 20 °C	1 1 1	0.0901 ± 0.01 at 20°C 0.0823 ± 0.01 at pH 5, 20°C 0.1096 ± 0.01 at pH 7, 20°C	1
pKa	2.94	1		1
Vapour pressure [Pa]	3.784 × 10⁻⁹	1	1.3 × 10⁻⁶	1
Log P_{ow}	1.7	1	4.5 ± 0.3	1
Henry's law constant [Pa×m³/mol]	1.06 × 10⁻⁸	1	5.5 × 10⁻³	1

1.2 Toxicity to aquatic organisms

The toxicity of *fluroxypyr acid* and *fluroxypyr-meptyl* to aquatic organisms are summarised in table 1.2.

Table 1.2:
Aquatic ecotoxicity data of *fluroxypyr-meptyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>		96 h, static	EC ₅₀ 1.4 NOEC 0.199 ¹⁾	2
<i>Scenedesmus subspicatus</i>	growth rate	96 h	EC ₅₀ >0.5	1
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ >2.31 NOEC 1.22	2
Crustaceans				

<i>Palaemonetes pugio</i>		96 h, flow-through	EC ₅₀ >0.135	2
<i>Daphnia magna</i>		48 h, semi-static	EC ₅₀ >0.2	1
<i>Daphnia magna</i>	mortality	21 d, flow through	NOEC 0.1	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, static-renewal	LC ₅₀ >0.63	2
<i>Cyprionodon variegatus</i>	mortality	96 h, flow-through	LC ₅₀ >0.087	2
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ >10	1
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ >0.2	1
<i>Pimephales promelas</i>	mortality	96 h	LC ₅₀ >0.9	1
<i>Leuciscus idus melanotus</i>	mortality	96 h	LC ₅₀ >0.7	1
<i>Oncorhynchus mykiss</i>	mortality	21 d, flow-through	NOEC 1.0	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Selenastrum capricornutum*, with a NOEC of 0.199 mg/L (*fluroxypyr-meptyl*). Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *fluroxypyr-meptyl* (ester) is calculated to 0.0199 mg/L.

The toxicity of *fluroxypyr-meptyl* to aquatic organisms are summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *fluroxypyr acid*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Chlorella vulgaris</i>		96 h	EC ₅₀ >100 NOEC 56	1
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ 12.3 NOEC <4.6	1
Crustaceans				
<i>Palaemonetes pugio</i>		96 h, flow-through	EC ₅₀ >120	2
<i>Daphnia magna</i>		48 h, static	EC ₅₀ >100	1, 2
<i>Daphnia magna</i>	mortality, reproduction	21 d, semi-static	NOEC 56	1
Molluscs				
<i>Crassostrea virginica</i>		96 h, flow-through	EC ₅₀ 51	2
Fish				
<i>Menidia beryllina</i>	mortality	96 h, flow-through	LC ₅₀ 40	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ >100	1
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ >100	2
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 14.3	1, 2
<i>Leuciscus idus melanotus</i>	mortality	96 h	LC ₅₀ >100	1
<i>Oncorhynchus</i>	mortality	21 d, semi-static	NOEC 100	1

mykiss				
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The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 12.3 mg/L and a NOEC of <4.6 mg/L. It is difficult to estimate the chronic toxicity from the long term test. Therefore the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 12.3 mg/L is divided by a factor of 100, which results in a PNEC of 0.123 mg/L.

1.3 Bioaccumulation and persistence

Fluroxypyr ester has a log P_{ow} of 4.5, indicating potential for bioaccumulation. However the hydrolysis to *fluroxypyr acid* (with a log P_{ow} of 1.7) is fast. Hence there is no reason to expect bioaccumulation (1). In water *fluroxypyr ester* adsorb to the sediment but hydrolysis releases *fluroxypyr acid* in the water. In water/sediment *fluroxypyr-meptyl* is degraded with a DT₅₀ of 2 days and *fluroxypyr-acid* with a DT₅₀ of 24 d in whole system. Major metabolites are *metabolite II* and *metabolite IV* (1).

1.4 Proposed water quality objective

Fluroxypyr-meptyl

Since PNEC is 0.0199 mg/L, the proposed water quality standard for *Fluroxypyr-meptyl* is 0.02 mg/L.

Fluroxypyr acid

Since PNEC is 0.123 mg/L, the proposed water quality standard for *fluroxypyr acid* is 0.1 mg/L.

1.5 Comments

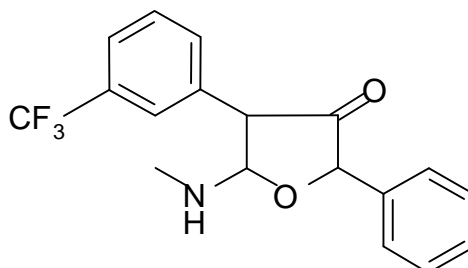
Fluroxypyr acid is mobile and may reach ground and surface waters via leaching through the soil profile. *Metabolite II (4-amino-3,5-dichloro-6-fluoro-2-pyridinol)* shows low toxicity toward algae, daphnia and fish.

1.6 Literature

- (1) European Commission Peer Review Programme. *Fluroxypyr Monograph*, 1996. Rapporteur Member State: Germany.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Flurtamone

Flurtamone is a contact and residual bleaching herbicide, intended for use in cereals. *Flurtamone* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *flurtamone* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *flurtamone*.

		Reference
CAS-No.	96525-23-4	1
Empirical formula	C ₁₈ H ₁₄ F ₃ NO ₂	1
Molecular weight [g/mol]	333.3	1
Solubility in water [mg/kg]	10.7 at pH 5 and 20°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	4.5 × 10 ⁻⁷	1
Log P _{ow}	3.1	1
Henry's law constant [Pa×m ³ /mol]	1.3 × 10 ⁻⁵	1

1.2 Toxicity to aquatic organisms

The toxicity of *flurtamone* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *flurtamone*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	biomass	72, static	E _b C ₅₀ 0.018 ¹⁾ NOEC 0.0057 ¹⁾	1
<i>Navilucula pelliculosa</i>	biomass	72, static	E _b C ₅₀ 0.011 NOEC 0.0013	1
Aquatic plants				
<i>Lemna gibba</i>	biomass	14d, semi-static	EC ₅₀ 0.0099 ²⁾ NOEC 0.0023	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 13	1
<i>Daphnia magna</i>	immobility	21d, flow-through	NOEC 0.071	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 7.0	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 11	1

<i>Onchorhynchus mykiss</i>	mortality	28d	NOEC 0.63	1
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¹⁾ Test performed on substance with purity <90%. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97.4%.

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0099 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.0099 mg/L is divided by a factor of 100, which results in a PNEC of 9.9×10^{-5} mg/L.

1.3 Bioaccumulation and persistence

Log P_{ow} indicated that *flurtamone* has potential to bioaccumulate. However bioaccumulation studies showed the risk for bioaccumulation to be low, BCF 27-28 in fish. *Flurtamone* is hydrolytically stable, but photolysis causes rapid degradation. However in Sweden photolysis is not a major degradation route. In water/sediment studies the substance has a DT₅₀ of 22-24 days, in the water phase, and 59-100 days, in the whole system. The substance is distributed 18-28% in the water phase and 22-57% in the sediment. No metabolites exceeded 10%.

1.4 Proposed water quality objective

Since PNEC is 0.000099 mg/L, the proposed water quality standard for *flurtamone* is 1×10^{-4} mg/L.

1.5 Comments

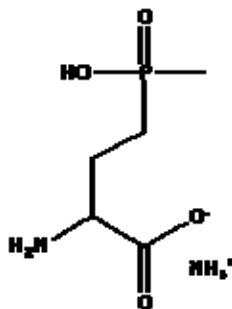
The insecticide is not mobile in soil and is therefore unlikely to leach through the soil profile.

1.6 Literature

- (1) European Commission Peer Review Programme. *Flurtamone Monograph, 1997*. Rapporteur Member State: France. Including addendum to monograph.

1. Glufosinate-ammonium and its metabolite MPP (3-methyl-phosphinico-propionic acid)

Glufosinate-ammonium is a broad spectrum herbicide for non-selective weed control in various crops. *Glufosinate-ammonium* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *glufosinate-ammonium* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *glufosinate-ammonium*.

		Reference
CAS-No.	77182-82-2	1
Empirical formula	C ₅ H ₁₂ O ₄ PH ₃ N	1
Molecular weight [g/mol]	198	1
Solubility in water [mg/kg]	>500 at 20°C	1
pKa	9.2	1
Vapour pressure [Pa]	<3.1×10 ⁻⁵ at 50°C	1
Log P _{ow}	-4.0 at pH 7	1
Henry's law constant [Pa×m ³ /mol]	4.5×10 ⁻⁹	1

1.2 Toxicity to aquatic organisms

The toxicity of *glufosinate-ammonium* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *glufosinate-ammonium*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	72h, static	E _r C ₅₀ >80 NOEC 2.5	1
<i>Scenedesmus subspicatus</i>	growth rate	72h, static	E _r C ₅₀ > 100 NOEC 100	1
<i>Selenastrum capricornutum</i>	growth rate	72h, static	E _r C ₅₀ 11-19 ¹⁾ NOEC 6.1 ¹⁾	1
Higher aquatic plants				
<i>Lemna gibba</i>	Growth inhibition	14d	I _b C ₅₀ 1.5 I _r C ₅₀ 2 - 3	1

			NOEC 0.8	
<i>Lemna gibba</i>	Growth inhibition	7d	E _b C ₅₀ 1.3 ¹⁾ E _r C ₅₀ 7.7 ¹⁾ NOEC 0.42 ¹⁾	1
<i>Lemna gibba</i>	Growth inhibition	7d	I _b C ₅₀ 1.8 ¹⁾ I _r C ₅₀ 2.3 ¹⁾ NOEC 0.57 ¹⁾	
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 670	1
<i>Mydopsis bahia</i>	immobility	96h, static	EC ₅₀ 7.5	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 2.5 ¹⁾	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 3.0 ¹⁾	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 2.7 ¹⁾	1
<i>Daphnia magna</i>	immobility	48, static	NOEC 18	1
<i>Daphnia magna</i>	reproduction	21 days, semi-static	NOEC 18	1
<i>Daphnia magna</i>	reproduction	21 days, semi-static	NOEC 0.59 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21 days, semi-static	NOEC 0.42 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 710	1
<i>Lepomis gibbosus</i>	mortality	96h, static	LC ₅₀ >320	1
<i>Cyprinidon variegatus</i>	mortality	96h, static	LC ₅₀ 1.9 ¹⁾	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 6.6 ¹⁾	1
<i>Onchorhynchus mykiss</i>	growth	21d, flow-through	NOEC 100	1
<i>Onchorhynchus mykiss</i>	growth	28d, flow-through	NOEC 0.11 ¹⁾	1
<i>Onchorhynchus mykiss</i>	growth	21d, flow-through	NOEC 0.09 ^{1, 2)}	1

¹⁾ Test performed on preparation; Basta SL14 (14%GA), Basta SL18 (19%GA). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC.

Most sensitive species for long term test was *Onchorhynchus mykiss*, NOEC 0.09 mg/L, in a test with the formulated product. Since short and long term studies are available from three trophic levels, the PNEC is calculated by dividing the lowest NOEC of 0.09 mg/L with a factor of 10, which results in a PNEC of 0.009 mg/L.

The toxicity of *MPP* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *MPP*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scendesmus subspicatus</i>	growth	72h, static	E _r C ₅₀ >1000 NOEC >1000	1
Higher aquatic plants				
<i>Lemna gibba</i>	growth	7 d	E _r C ₅₀ >78 NOEC >78	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ >100	1
<i>Daphnia magna</i>	reproduction	21 d	EC ₁₀ 2.1 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >100	1
<i>Onchorhynchus</i>	growth	28d, flow-through	NOEC 21	1

mykiss				
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¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with an EC₁₀ of 2.1 mg/L (regarded as a NOEC). Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for the metabolite *MPP* (*3-methylphosphinico-propionic acid*) is calculated to 0.21 mg/L.

1.3 **Bioaccumulation and persistence**

Glufosinate-ammonium is not expected to bioaccumulate. Glufosinate-ammonium is stable towards hydrolysis and photolysis. Hence, the degradation is mainly microbially mediated. In water/sediment-test DT₅₀ range from 1.4 to 13 days, water phase, and 2-11 days, whole system. The substance is mainly kept in water phase. Five metabolites are formed within the degradation pathways; *AE F061517 (MPP)*, *AE F 064619 (MPA)*, *AE F130947 (P-Y MPF)*, *AE 0015081 (P-X)* and the *N-acetylene derivative of the L-isomer of GA (NAG)*. Only *MPP*, *MPA* and *MPF* are considered to be relevant metabolites. The metabolites show low toxicity towards aquatic organisms. However the metabolite *MPP* is more persistent than the parent compound, DT₅₀ 150 days. Therefore a separate water quality objective is established for this metabolite.

1.4 **Proposed water quality objective**

Glufosinate-ammonium

Since PNEC is 0.009 mg/L, the proposed water quality standard for *glufosinate-ammonium* is 0.01 mg/L.

MPP

Since PNEC is 0.21 mg/L, the proposed water quality standard for the metabolite is 0.2 mg/L.

1.5 **Comments**

The parent compound and its metabolites may leach through the soil profile and reach both surface- and ground water in vulnerable areas.

1.6 **Literature**

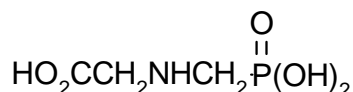
- (1) European Commission Peer Review Programme. *Glufosinate-ammonium Monograph*, 2002. Rapporteur Member State: Sweden.

(2) European Commission Peer Review Programme. *Glufosinate-ammonium List of endpoints, 2003*. Rapporteur Member State: Sweden.

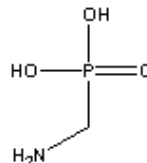
1. Glyphosate and its metabolite aminomethylphosphonic, AMPA

Glyphosate is a non-selective herbicide. Aminomethylphosphonic acid (AMPA) is a breakdown-product of the herbicide *glyphosate*. Other sources for AMPA are washing powders and other cleaning products in which phosphonates are used as stabilising and/or chelating agents (3). *Glyphosate* is under evaluation within the framework of EU Dir. 91/414.

Glyphosate:



AMPA:



1.1 Physico-chemical properties

Physico-chemical properties of *glyphosate* and AMPA are summarised in table 1.1 and table 1.1.2.

Table 1.1: Physico-chemical properties of *glyphosate*.

		Reference
CAS-No.	1071-83-6	1
Empirical formula	C ₃ H ₈ NO ₅ P	1
Molecular weight [g/mol]	169	1
Solubility in water [mg/kg]	10500±0.2 at 20°C, pH 2	1
pKa	2.34 (20°C), 5.73 (20°C) and 10.2 (25°C)	1
Vapour pressure [Pa]	1.31×10 ⁻⁵ at 25°C	1
Log P _{ow}	-3.2 at 25°C, pH 5-9	1
Henry's law constant [Pa × m ³ /mol]	2.1×10 ⁻⁷	1

Table 1.1.2: Physico-chemical properties of AMPA.

		Reference
CAS-No.	1066-51-9	3
Empirical formula	CH ₆ NO ₃ P	3
Molecular weight [g/mol]	111	-
Solubility in water [mg/kg]	1 × 10 ⁶ at 25°C	calculated ¹⁾
Vapour pressure [Pa]	7.68 × 10 ⁻³ at 25°C	calculated ²⁾
Log P _{ow}	-2.17	calculated ³⁾
Henry's law constant [Pa×m ³ /mol]	1.27 × 10 ⁻¹⁰	calculated ⁴⁾

¹⁾ EPIWIN software, estimated, log Pow used: -2.17, no-melting point equation used.

²⁾ EPIWIN software, estimated by Modified Grain Method.

³⁾ EPIWIN software, estimated.

⁴⁾ EPIWIN software, estimated by Bond SAR Method.

1.2 Toxicity to aquatic organisms

The toxicity of *glyphosate* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *glyphosate*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth rate	72 h	EC ₅₀ 60 NOEC 25	1
<i>Selenastrum capricornutum</i>	biomass	72 h	EC ₅₀ 48	1
	growth rate		EC ₅₀ 54	
<i>Skeletonema costatum</i>	chlorophyll	96 h	EC ₅₀ 1.3 ¹⁾	1
<i>Nitzschia palea</i>	growth	96 h	EC ₅₀ 4.5 NOEC 1 ²⁾	1
Aquatic plants				
<i>Lemna gibba</i>	frond counts	14 d, static	EC ₅₀ 25 NOEC 19	1
Crustaceans				
<i>Daphnia magna</i>		24 h	LC ₅₀ >100	1
		48 h	LC ₅₀ 40	
<i>Daphnia magna</i>		48 h	LC ₅₀ >100	1
<i>Daphnia magna</i>	mortality	21 d	NOEC 100	1
	reproduction	21 d	NOEC 100	
<i>Daphnia magna</i>	mortality	21 d	NOEC 95	1
	reproduction	21 d	NOEC 9	
<i>Daphnia magna</i>	mortality	21 d, flow-through	NOEC 397	1
	reproduction	21 d, flow-through	NOEC 50	
<i>Daphnia magna</i>	mortality	21 d	NOEC 56	1
	reproduction	21 d	NOEC 56	
Fish				
<i>Lepomis macrochirus</i>		24 h	LC ₅₀ 121	1
		48 h	LC ₅₀ 120	
		96 h	LC ₅₀ 120	
<i>Lepomis macrochirus</i>		96 h	LC ₅₀ 133-200 (NOEC 133)	1
<i>Lepomis macrochirus</i>		96 h	LC ₅₀ 78	1
<i>Oncorhynchus mykiss</i>		96 h	LC ₅₀ >100	1
<i>Oncorhynchus mykiss</i>		24 h	LC ₅₀ 170	1
		48 h	LC ₅₀ 120	
		72 h	LC ₅₀ 86	
		96 h	LC ₅₀ 50	
<i>Oncorhynchus mykiss</i>		96 h	LC ₅₀ 38	1
<i>Oncorhynchus</i>		96 h	LC ₅₀ 95-171	1

<i>mykiss</i>			(NOEC 95)	
<i>Cyprinus carpio</i>		96 h	LC ₅₀ 115	1
<i>Oncorhynchus mykiss</i>	behaviour	21 d	NOEC 50	1
	mortality	21 d	NOEC 50	
	growth	21d	NOEC 100	
<i>Oncorhynchus mykiss</i>	behaviour	21 d	NOEC 150	1
	mortality	21 d	NOEC150	
	growth	21d	NOEC 150	
<i>Pimephales promelas</i>		254 d, FLC-test	NOEC 25.7	1

- 1) Effect concentration basis for calculation of former PNEC. Test substance purity >94%.
- 2) Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Skeletonema costatum*, with an EC₅₀ of 1.3 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 1.3 mg/L is divided by a factor of 100, which results in a PNEC of 0.013 mg/L.

Revised EQS calculation according to EU-harmonised methodology (4)

Long term data is available for three trophic levels and thus an AF=10 is justified. When looking at biomass as an end-point the most sensitive of the tested species was *Skeletonema costatum*, with an E_bC₅₀ of 1.3 mg/L and a NOEC_{biomass} of 0.28 mg/L (value not included in table, see ref. 1). But since growth is the preferred end-point in algal tests the lowest NOEC is 1 mg/L, derived from the test with *Nitzschia palea*, which results in a PNEC of 0.1 mg/L.

The toxicity of AMPA to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of AMPA.

Species	End-point	Exposure duration	Result [mg/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth rate	72 h	EC ₅₀ 452 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>		48 h	EC ₅₀ >180	1
<i>Daphnia magna</i>		48 h	EC ₅₀ 690	1
Fish				
<i>Oncorhynchus mykiss</i>		96 h	EC ₅₀ 520	1
		96 h	EC ₅₀ >180	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity unknown.

The most sensitive of the tested species was *Scenedesmus subspicatus*, with a growth rate EC₅₀ of 452 mg/L. Since only short-term studies are available, and three trophic levels are tested, an assessment factor of 1000 is used for calculation of the predicted no effect concentration. Hence, the PNEC for AMPA is calculated to 0.452 mg/L.

1.3 Bioaccumulation and persistence

Neither *glyphosate* nor *AMPA* are expected to bioaccumulate. The substance is stable to hydrolytic and photolytic degradation. In water/sediment systems *glyphosate* disappears rapidly from water-phase with a half-life of 1-4 days. In the whole system half-life is between 27 and 146 days. In water/sediment degradation studies with *glyphosate*, *AMPA* is formed to a maximum of 16% of applied *glyphosate* after 14 days, followed by declination to 0.5% after 100 days (2). In field-studies half-life in soil has been determined to 35 days for *glyphosate* and to 697 days for the metabolite *AMPA*.

1.4 Proposed EQS/water quality objective

Glyphosate

Since PNEC is 0.1 mg/l, the proposed EQS/water quality objective for *glyphosate* is 0.1 mg/L.

1.5 Proposed water quality objective

AMPA

PNEC for *AMPA* is 0.452 mg/L, the proposed water quality objective is therefore 0.5 mg/L.

1.6 Comments

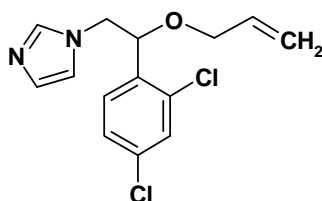
AMPA is less toxic than the parent compound. However, due to findings of *AMPA* in the surface waters, a quality objective for *AMPA* has been set. *AMPA* is more persistent.

1.7 Literature

- (1) European Commission Peer Review Programme. *Glyphosate* Monograph (draft), 1998. Rapporteur Member State: Germany.
- (2) European Commission Peer Review Programme. *Glyphosate* Review Report, 2002. Rapporteur Member State: Germany.
- (3) Ämnesregistret, 2001-12-20, Kemiska databaser [online], Solna, Kemikalieinspektionen, URL: <http://www.kemi.se/default.cfm?page=kemdatbas.htm>.
- (4) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Imazalil

Imazalil is a fungicide, intended for seedtreatment. The substance inhibits a cytochrome P-450 enzyme responsible for the demethylation of precursors of ergosteol. *Imazalil* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *imazalil* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *imazalil*.

		Reference
CAS-No.	73790-28-0	1
Empirical formula	C ₁₄ H ₁₄ Cl ₂ N ₂ O	1
Molecular weight [g/mol]	297.8	1
Solubility in water [mg/kg]	0.22 at pH 7	1
pKa	Does not dissociate	1
Vapour pressure [Pa]	1.58×10 ⁻⁴	1
Log P _{ow}	4.56	1
Henry's law constant [Pa×m ³ /mol]	1.09×10 ⁻⁹	1

1.2 Toxicity to aquatic organisms

The toxicity of *imazalil* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *imazalil*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth	72h	E _r C ₅₀ 1.2 NOEC 0.46 ¹⁾	1
<i>Selenastrum capricornutum</i>	growth	72h	E _r C ₅₀ 3.6 NOEC 1	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h	EC ₅₀ 3.5	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 3.2	2
<i>Daphnia magna</i>	immobility	48h	EC ₅₀ 3.5	2
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	EC ₅₀ 3.5	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.5	2
<i>Onchorhynchus mykiss</i>	mortality	96h	LC ₅₀ 2.0	2
<i>Lepomis</i>	mortality	96h	LC ₅₀ 4.0	2

<i>macrochirus</i>				
<i>Brachydanio rerio</i>	mortality	96h, semi-static	LC ₅₀ 2.8	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97%

The most sensitive of the tested species was *Selenastrum capricornutum*, with a NOEC of 0.46 mg/L. Short term studies are available tested on three trophic levels. However long term studies are only tested on algae, therefore an assessment factor of 100 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *imazalil* is calculated to 0.0046 mg/L.

1.3 **Bioaccumulation and persistence**

The octanol-water coefficient indicates a bioaccumulation of *imazalil*. However BCF range between 48-63, therefore the bioaccumulation is considered to be moderate. The half-life of *imazalil* is 53 days in water/sediment system. *Imazalil* is partitioned into the sediment. No metabolites exceed 10% of applied substance.

1.4 **Proposed water quality objective**

Since PNEC is 0.0046 mg/L, the proposed water quality standard for *imazalil* is 0.005 mg/L.

1.5 **Comments**

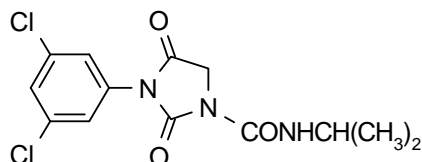
Because K_{oc} is high the substance is not expected to be mobile in soil. *Imazalil* is not volatile. The rapid partition into sediment motivates a quality objective for sediment and soil.

1.6 **Literature**

- (1) European Commission Peer Review Programme. *Imazalil Monograph, 1996*.
Rapporteur Member State: Luxemburg.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Iprodione and RP30228

Iprodione is a fungicide used as seed treatment in cultivation of among other crops, oleiferous plants, beets and potatoes. *RP 30228* is a structural isomer to *iprodion* and the major metabolite. *Iprodione* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *iprodione* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *iprodione*.

		Reference
CAS-No.	36734-19-7	1
Empirical formula	C ₁₃ H ₁₃ Cl ₂ N ₃ O ₃	1
Molecular weight [g/mol]	330.2	1
Solubility in water [mg/kg]	12.2 at 30 °C	1
Vapour pressure [Pa]	5×10 ⁻⁷	1
Log P _{ow}	3.0 at pH 5, 20 °C	1
Henry's law constant [Pa×m ³ /mol]	0.7×10 ⁻⁵ at 20 °C	1

1.2 Toxicity to aquatic organisms

The toxicity of *iprodione* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1:
Aquatic ecotoxicity data of *iprodione*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 7.2	2
<i>Daphnia magna</i>	immobility	48 h, static	EC ₅₀ 0.43	2
<i>Daphnia magna</i>	immobility	48 h, flow-through	EC ₅₀ 0.25	1
<i>Daphnia magna</i>		48h, static	EC ₅₀ 0.66	3
<i>Daphnia magna</i>	survival, reproduction, growth	21 d, flow-through	NOEC 0.17	1
Molluscs				
<i>Crassostrea virginica</i>		96 h, flow-through	EC ₅₀ 2.3	2
Fish				
<i>Ictalurus punctatus</i>	mortality	96 h, flow-through	LC ₅₀ 3.06	1, 2
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ 6.3	2

<i>Cyprinodon variegatus</i>	mortality	96 h, flow-through	LC ₅₀ 7.7	2
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ 3.7	1, 2
<i>Pimephales promelas</i>		34 d, flow-through	NOEC 0.26	1, 2
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow-through	LC ₅₀ 4.1	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Daphnia magna*, with an EC₅₀ of 0.25 mg/L and a NOEC of 0.17 mg/L. Since the acute/chronic ratio is low and a water quality object based on chronic effects does not guarantee appropriate protection against acute effects. Hence the PNEC is based on acute toxicity data. However the data set is not complete, the toxicity of *iprodione* towards algae is not completely studied. Supportive data suggests *iprodione* to be highly toxic towards algae, *Skeletonema costatum* EC₅₀ 0.23 mg/L. To compensate for missing data a higher assessment factor is needed. Hence, the lowest EC₅₀ of 0.25 mg/L is divided by a factor of 1000, which results in a PNEC of 0.00025 mg/L.

The toxicity of metabolite *RP30228* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2:

Aquatic ecotoxicity data of *RP 30228*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass	72 h, static	EC ₅₀ >0.5 NOEC 0.16	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48 h, flow-through	EC ₅₀ >50	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ 0.55 ¹⁾	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Lepomis macrochirus* LC₅₀ 0.55 mg/l (isomer *RP 30228*). Due to the rapid transformation of *iprodione* to *RP 30228* long term tests for *iprodione* can be presumed to include toxicity of *RP 30228*. *Scenedesmus subspicatus* was the most sensitive species towards chronic toxicity, NOEC 0.16 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest LC₅₀ of 0.55 mg/L is divided by a factor of 100, which results in a PNEC of 0.0055 mg/L.

1.3 Bioaccumulation and persistence

Iprodione may bioaccumulate. Log P_{ow} is 3 and BCF exceed 100 in fish, edible parts. The transformation route and rate of *iprodione*, strongly depends on pH. *Iprodione*, as well as *RP 30228*, is slowly degraded, DT₅₀ 149 days, in low pH. In neutral and higher pH the reaction proceeds to the major metabolite *RP 30228* with a DT₅₀ of 0.2 and 3 days, pH 8 and 7

respectively. In water/sediment systems *iprodione* is degraded with a DT₅₀ of less than 10 days. The metabolite *RP 30228* reaches 10% and adsorbs rapidly to the sediment.

1.4 Proposed water quality objective

Iprodione

Since PNEC is 0.00025 mg/L, the proposed water quality standard for *iprodione* is 0.0002 mg/L.

RP 30228

Since PNEC is 0.0055 mg/L, the proposed water quality standard for the isomer *RP 30228* is 0.005 mg/L.

1.5 Comments

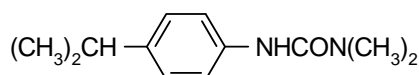
Neither *iprodione* nor *RP 30228* show potential for leach through the soil profile (1). *RP 30228* partitions into the sediment. Therefore a complementary quality objective is recommended.

1.6 Literature

- (1) European Commission Peer Review Programme. *Iprodione Monograph, 1996*. Rapporteur Member State: France.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *Iprodione Addendum, 2000*. Rapporteur Member State: France.

1. Isoproturon

Isoproturon is a selective herbicide belonging to the class phenyl ureas. The herbicide is intended for use in cereals. *Isoproturon* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *isoproturon* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *isoproturon*.

		Reference
CAS-No.	34123-59-6	1
Empirical formula	C ₁₂ H ₁₈ N ₂ O	1
Molecular weight [g/mol]	206.3	1
Solubility in water [mg/kg]	70.2, not pH dependent	1
Vapour pressure [Pa]	2.8-8.1 × 10 ⁻⁶ at 20°C	1
Log P _{ow}	2.5 at 25°C, not pH dependent	1
Henry's law constant [Pa×m ³ /mol]	1.46 × 10 ⁻⁵ at 22°C	1

1.2 Toxicity to aquatic organisms

The toxicity of *isoproturon* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *isoproturon*.

Species	End-point	Exposure duration	Result [mg/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>		72 h	EC ₅₀ 0.03 NOEC 0.0032 ¹⁾	1
<i>Scenedesmus subspicatus</i>	growth rate	72 h	EC ₅₀ 0.095	1
<i>Scenedesmus subspicatus</i>	biomass	96 h	EC ₅₀ 0.021	1
<i>Selenastrum capricornutum</i>		72 h	EC ₅₀ 0.072	1
<i>Selenastrum capricornutum</i>	growth rate	72 h	EC ₅₀ 0.148 NOEC 0.01	1
<i>Navicula pelliculosa</i>	growth rate	72 h	EC ₅₀ 0.046	1
Aquatic plants				
<i>Lemna minor</i>		10 d	EC ₅₀ 0.031	1
<i>Lemna gibba</i>	frond counts	14 d	EC ₅₀ 0.045	1
	biomass	14 d	EC ₅₀ 0.037	

Crustaceans				
<i>Daphnia magna</i>	immobility	48 h	EC ₅₀ >1000	1
<i>Daphnia magna</i>	immobility	48 h	EC ₅₀ 0.58	1
<i>Daphnia magna</i>	immobility	48 h	EC ₅₀ >56	1
<i>Daphnia magna</i>	mortality	21 d, semi-static	NOEC 8	1
	reproduction	21 d, semi-static	NOEC 0.064	
<i>Daphnia magna</i>	mortality	21 d, semi-static	NOEC 8.9	1
	reproduction	21 d, semi-static	NOEC >0.41	
<i>Daphnia magna</i>	mortality	21 d, semi-static	NOEC 0.03	1
	reproduction	21 d, semi-static	NOEC 0.01	
Insecta				
<i>Chironomus riparius</i>	emergence	28 d	NOEC 0.5	1
<i>Chironomus riparius</i>	emergence	28 d	NOEC 0.5	1
	development rate	28 d	NOEC 0.5	
Fish				
<i>Cyprinus carpio</i>	mortality	96 h	LC ₅₀ 54.4	1
<i>Leuciscus idus melanotus</i>	mortality	96 h	LOEC 25.5	1
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ >18	1
<i>Oncorhynchus mykiss</i>	mortality	96 h	LC ₅₀ 37.22	1
<i>Brachydanio rerio</i>	mortality	96 h	LC ₅₀ 40	1
<i>Poecilia reticulata</i>	mortality	96 h	LC ₅₀ 52	1
<i>Oncorhynchus mykiss</i>	mortality	21 d, semi-static	NOEC 10	1
	growth	21 d, semi-static	NOEC 1	
<i>Oncorhynchus mykiss</i>	mortality	21 d, semi-static	NOEC 8.9	1
	behaviour	21 d, semi-static	NOEC 3.2	
	growth	21 d, semi-static	NOEC 1.1	

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity as manufactured 97±2%.

The most sensitive of the tested species was *Scenedesmus subspicatus*, with a growth rate EC₅₀ of 0.095 mg/L and a NOEC of 0.0032 mg/L (different studies). Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *isoproturon* is calculated to 0.00032 mg/L.

1.3 Bioaccumulation and persistence

Isoproturon is not expected to bioaccumulate. *Isoproturon* is hydrolytically and photolytically stable. In water-sediment systems half-life is 20-61 days in the water phase and 44-276 days in the whole system.

1.4 Proposed water quality objective

Since PNEC is 0.00032 mg/L, the proposed water quality objective for *isoproturon* is 0.0003 mg/L.

1.5 *Comments*

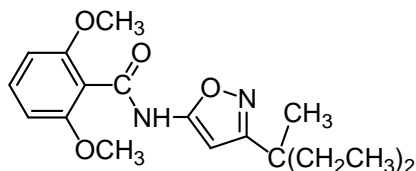
The only known relevant metabolite of *isoproturon* is *desmethylisoproturon*. Compared with *isoproturon*, *desmethylisoproturon* is less toxic; therefore a water quality objective for the metabolite is not necessary. *Isoproturon* is mobile in soil and can reach ground and surface waters via leaching through the soil profile.

1.6 *Literature*

- (1) European Commission Peer Review Programme. *Isoproturon Monograph (draft)*, 1999. Rapporteur Member State: Denmark.

1. Isoxaben

Isoxaben is a herbicide used in plantation of fruit trees and strawberries. The compound is an aniline derivate and its mode of action is by inhibiting plant cell division.



1.1 Physico-chemical properties

Physico-chemical properties of *isoxaben* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *isoxaben*.

		Reference
CAS-No.	82558-50-7	1
Empirical formula	C ₁₈ H ₂₄ N ₂ O ₄	1
Molecular weight [g/mol]	332.4	1
Solubility in water [mg/kg]	1.11 at 20°C	1
Vapour pressure [Pa]	5.8 × 10 ⁻⁹	1
Log P _{ow}	2.6-3.8 at 20°C	1
Henry's law constant [Pa×m ³ /mol]	1.29 × 10 ⁻⁴	2

1.2 Toxicity to aquatic organisms

The toxicity of *isoxaben* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *isoxaben*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ >1.3	1
<i>Daphnia magna</i>	reproduction growth	21d, semi-static	NOEC 0.69 ¹⁾	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	NOEC >1.1	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	NOEC >1.1	1
<i>Cyprinus carpio</i>	mortality	96h, static	NOEC >1.2	1
<i>Onchorhynchus mykiss/Pimephales promelas</i>	reproduction	33d/69d	NOEC >0.4	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.69 mg/L. Only two trophic levels have been tested. *Isoxaben* is an herbicide and is expected to be toxic towards algae. Supportive data indicates low toxicity, however the tests are not reliable. An

assessment factor of 1000 is used to compensate the lack of data. Hence, the PNEC for *isoxaben* is calculated to 0.00069 mg/L.

1.3 Bioaccumulation and persistence

Isoxaben may bioaccumulate, Log K_{ow} 2.6-3.8, however no bioaccumulation studies are available. *Isoxaben* is stable towards hydrolysis at environmental pH 5-9. *Isoxaben* is degraded photolytically with DT_{50} 14 days. The photolysis gives rise to several metabolites with unknown toxicity. Degradation in water/sediment system has not been studied.

1.4 Proposed water quality objective

Since PNEC is 0.00069 mg/L, the proposed water quality standard for *isoxaben* is 0.0007 mg/L.

1.5 Comments

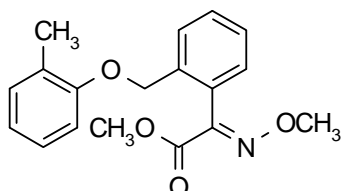
Isoxaben is not expected to reach ground and surface waters due to transport through the soil profile. When additional studies are available, the toxicity of the metabolites should be studied.

1.6 Literature

- (1) Stenström and Torstensson, 1995. *Ecotoxicological evaluation of Isoxaben*. Department of Microbiology, Swedish University of Agricultural Science.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Kresoxim-methyl

Kresoxim-methyl is a fungicide, intended for use in cultivation of fruit. *Kresoxim-methyl* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *kresoxim-methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *kresoxim-methyl*.

		Reference
CAS-No.	143390-89-0	1
Empirical formula	C ₈ H ₁₉ NO ₄	1
Molecular weight [g/mol]	313.4	1
Solubility in water [mg/kg]	2.0 at 20 °C	1
Vapour pressure [Pa]	2.3 × 10 ⁻⁶	1
Log P _{ow}	3.4 at pH 7, 25 °C	1
Henry's law constant [Pa×m ³ /mol]	3.6 × 10 ⁻⁴ at 20 °C	1

1.2 Toxicity to aquatic organisms

The toxicity of *kresoxim-methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *kresoxim-methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth	96 h, static	LC ₅₀ 0.055 NOEC 0.012	2
<i>Skeltonema costatum</i>	growth	96h, static	LC ₅₀ >0.293 NOEC 0.293	2
<i>Ankistrodesmus bibrianus</i>	growth	72 h, static	EC ₅₀ 0.063 (nominal)	1
Crustaceans				
<i>Mysidopsis bahia</i>	immobilisation	96 h, flow-through	LC ₅₀ 0.059	2
<i>Daphnia magna</i>	immobilisation	96 h, flow-through	LC ₅₀ 0.33	2
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.19 (nominal)	1
<i>Daphnia magna</i>	immobilisation	24 h, static	EC ₅₀ 1.51 (nominal)	1
<i>Daphnia magna</i>	reproduction	21 d, semi-static	NOEC 0.032 (nominal)	1
Molluscs				
<i>Crassostrea virginica</i>	shell deposition	96 h, flow-through	LC ₅₀ 0.015 ¹⁾	2
Fish				
<i>Cyprinodon</i>	mortality	96 h, flow-through	LC ₅₀ 1.17	2

<i>variegatus</i>				
<i>Pimephales promelas</i>	mortality	28 d, flow-through	NOEC 0.087	2
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ 0.5	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow-through	LC ₅₀ 0.19	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ >0.681<1.0 (nominal) LC ₅₀ >0.15<0.19 (measured)	1
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 3.2 (nominal) LC ₅₀ 0.5 (measured)	1
<i>Cyprinus carpio</i>	mortality	96 h, static	LC ₅₀ >1.0<2.2 (nominal) LC ₅₀ >0.25<0.33 (measured)	1
<i>Cyprinus carpio</i>	mortality	96 h, semi-static	LC ₅₀ 0.41 (nominal)	1
<i>Oncorhynchus mykiss</i>		28 d, flow-through	NOEC 0.02 (nominal) NOEC 0.013 (measured)	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 94.3%

The most sensitive of the tested species in short term studies was *Crassostrea virginica*, with a shell deposition EC₅₀ of 0.015 mg/L. For this species, no long term study was available. The most sensitive species in available long term studies was *Selenastrum capricornutum* with a NOEC of 0.012 mg/L. To account for the lack of long term data on the most sensitive species in short term tests, a factor of 50 is applied to the *Selenastrum capricornutum* NOEC, resulting in a long term PNEC of 0.0002 mg/L. However, since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.015 mg/L is divided by a factor of 100, which results in a PNEC of 0.00015 mg/L.

1.3 Bioaccumulation and persistence

Kresoxim-methyl may bioaccumulate, in fish BCF is more than 100 but is rapidly decreased during depuration. *Kresoxim-methyl* is not persistent; DT₅₀ is only a few days in both soil and water.

1.4 Proposed water quality objective

Since PNEC is 0.00015 mg/L, the proposed water quality standard for *kresoxim-methyl* is 0.0001 mg/L.

1.5 Comments

Kresoxim-methyl has a Koc of 219-372 and may leach through the soil profile. The main metabolite formed in soil is the corresponding acid, BF 490-1. The metabolite is very mobile

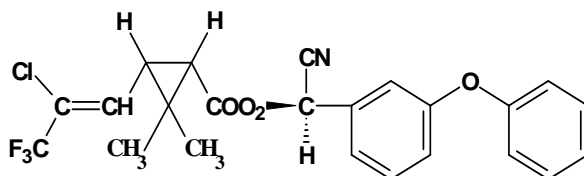
in soil (Koc 17-24) and tends to be persistent in water, but is not considered as toxic to aquatic organisms.

1.6 *Literature*

- (1) European Commission Peer Review Programme. *Kresoxim-methyl Monograph, 1997*. Rapporteur Member State: Belgium.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Lambda-cyhalothrin

Lambda-cyhalothrin is a synthetic pyrethroid. The insecticide exerts its effects on harmful organisms via contact and stomach action. The insecticide is intended for use in among other crops cereals, oleiferous plants and beets. *Lambda-cyhalothrin* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *lambda-cyhalothrin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *lambda-cyhalothrin*.

		Reference
CAS-No.	91465-08-6	1
Empirical formula	C ₂₃ H ₁₉ ClF ₃ NO ₃	1
Molecular weight [g/mol]	463	1
Solubility in water [mg/kg]	5×10 ⁻³ at pH 6.5 and 20°C	1
pKa	Not relevant	1
Vapour pressure [Pa]	2×10 ⁻⁷	1
Log P _{ow}	7.0	1
Henry's law constant [Pa×m ³ /mol]	0.02	1

1.2 Toxicity to aquatic organisms

The toxicity of *lambda-cyhalothrin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *lambda-cyhalothrin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth	96h	E _r C ₅₀ >0.3	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.00036	1
<i>Ceriodaphnia dubia</i>	mortality	48h, static	LC ₅₀ 0.0003	2
<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ 0.00104	2
<i>Gammarus pulex</i>	immobility	96h, semi-static	EC ₅₀ 0.000013	3
<i>Gammarus pulex</i>	immobility	96h	EC ₅₀ 0.000016 NOEC 0.000006 ¹⁾	3
Fish				
<i>Onchohynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.00024	1
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 0.00021	1
<i>Cyprinodon variegatus</i>	reproduction	28d, flow-through	NOEC 0.00025	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98%.

The most sensitive of the tested species was the aquatic invertebrate *Gammarus pulex*. In a study with neonates, the most sensitive life stage of gammarids, 96 hour EC₅₀ was 0.000013 mg/L and NOEC 0.000006 mg/L. Since the most sensitive life stage was included, this study is regarded as a long term study. Hence, sufficient long term data are available for three trophic levels.

Besides, two mesocosm studies are available, addressing long term effects and potential for recovery under more realistic exposure conditions. Although the results could not be directly compared with those from laboratory, it can be anticipated that the gammarid neonate NOEC would cover possible effects in the field. Therefore, an assessment factor of 1 is used, together with the NOEC, resulting in a PNEC of 6×10^{-6} mg/L.

1.3 Bioaccumulation and persistence

Lambda-cyhalothrin is expected to bioaccumulate; Log P_{ow} is 7 and BCF in fish 1660-2240, both indicate high bioaccumulation. *Lambda-cyhalothrin* will mainly be distributed to suspended organic matter and sediment. DT₅₀ in water/sediment system is 5-11h (water phase) and 7-15 days (whole system). Dissipation from the water phase is mainly due to partitioning into the sediment. Two relevant transformation products, cyclopropane acid and benzoic acid, are formed. In contrast to the parent compound the metabolites are mainly distributed to the water phase. Toxicity test show metabolites to be less toxic than the parent compound.

1.4 Proposed water quality objective

Since PNEC is 6×10^{-6} mg/L, the proposed water quality standard for *lambda-cyhalothrin* is 6×10^{-6} mg/L.

1.5 Comments

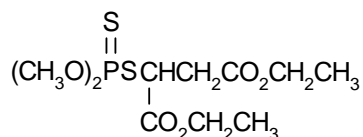
Lambda-cyhalothrin is degraded in soil with a DT₅₀ of 56days. High K_{oc}-value and low water solubility indicate low mobility. *Lambda-cyhalothrin* is not expected to volatilise. Due to the lipophilic properties of *lambda-cyhalothrin*, a quality objective for sediment is needed.

1.6 Literature

- (1) European Commission Peer Review Programme. *Lambda-cyhalothrin Monograph*, 1996. Rapporteur Member State: Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *Lambda-cyhalothrin Review Report*, 2001. Rapporteur Member State: Sweden.

1. Malathion

Malathion is an organophosphorous insecticide/acaricide. The herbicide is a non-systemic insecticide and acaricide with contact, stomach, and respiratory action. The substance has been forbidden in Sweden since 1995.



1.1 Physico-chemical properties

Physico-chemical properties of *malathion* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *malathion*.

		Reference
CAS-No.	121-75-5	3
Empirical formula	C ₁₀ H ₁₉ O ₆ PS ₂	3
Molecular weight [g/mol]	330.3	3
Solubility in water [mg/kg]	145-148 at 25 °C	1, 3
Vapour pressure [Pa]	4.5 × 10 ⁻⁴ at 25 °C	3
Log P _{ow}	2.75	3
Henry's law constant [Pa×m ³ /mol]	1.21 × 10 ⁻²	3

1.2 Toxicity to aquatic organisms

The toxicity of *malathion* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *malathion*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Daphnia pulex</i>	immobilisation	48 h, static	EC ₅₀ 0.0018	2
<i>Gammarus lacustris</i>		48 h, static	LC ₅₀ 0.0018	2
<i>Simocephalus serrulatus</i>	immobilisation	48 h, static	EC ₅₀ 0.00059	2
<i>Gammarus fasciatus</i>		96 h, flow-through	LC ₅₀ 0.0005 ¹⁾	2
<i>Mysidopsis bahia</i>		96 h, flow-through	LC ₅₀ 0.0022	2
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.001	2
<i>Mysidopsis bahia</i>		96 h, flow-through	LC ₅₀ 0.0022	2
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.0022	2
<i>Daphnia magna</i>		21 d, flow-through	NOEC 0.00006	2
Molluscs				
<i>Crassostrea virginica</i>		96 h, flow-through	EC50 >1	2
<i>Crassostrea</i>	shell deposition	96 h, flow-through	EC50 2.9	2

<i>virginica</i>				
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 0.02	2
<i>Lepomis microlophus</i>	mortality	96 h, static	LC ₅₀ 0.062	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.004	2
<i>Perca flavescens</i>	mortality	96 h, static	LC ₅₀ 0.26	2
<i>Micropterus salmonides</i>	mortality	96 h, static	LC ₅₀ 0.25	2
<i>Pimephales promelas</i>	mortality	96 h, static	LC ₅₀ 8.7	2
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ 7.6	2
<i>Cyprinodon variegatus</i>	mortality	96 h, static	LC ₅₀ 0.033	2
<i>Oncorhynchus kisutch</i>	mortality	96 h, static	LC ₅₀ 0.17	2
<i>Oncorhynchus clarki</i>	mortality	96 h, static	LC ₅₀ 1.7	2
<i>Salmo trutta</i>	mortality	96 h, static	LC ₅₀ 0.10	2
<i>Salvelinus namaycush</i>	mortality	96 h, static	LC ₅₀ 0.076	2
<i>Ictalurus melas</i>	mortality	96 h, static	LC ₅₀ 12	2
<i>Lepomis cyanellus</i>	mortality	96 h, static	LC ₅₀ 1.5	2
<i>Cyprinodon variegatus</i>	mortality	96 h, flow-through	LC ₅₀ 1.5	2
<i>Oncorhynchus mykiss</i>	mortality	97 d, flow-through	NOEC 0.002	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 95%

Toxicity data for primary consumers are missing. However *malathion* is an insecticide. The insecticide operates by contact, stomach, and respiratory action, specific for insects. Thus primary producers are expected to be less toxic than daphnia and/or fish. This is confirmed by supportive data. The most sensitive (acute effects) of the tested species was *Gammarus fasciatus*, with an EC₅₀ of 0.0005 mg/L. Since the acute/chronic ratio is low a PNEC based on long term studies does not guarantee appropriate protection against acute effects. Hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.0005 mg/L is divided by a factor of 100, which results in a PNEC of 0.000005 mg/L.

1.3 **Bioaccumulation and persistence**

Malathion is not expected to bioaccumulate (log P_{ow} 2.75), but no bioaccumulation studies are available. In water *malathion* is hydrolysed and half-lives depend on pH (pH 5: 107 d, pH 7: 6,2 d, pH 9: 12 h) (1).

1.4 **Proposed water quality objective**

Since PNEC is 0.000005 mg/L, the proposed water quality standard for *malathion* is 5×10^{-6} mg/L.

1.5 *Comments*

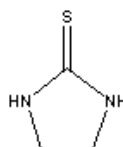
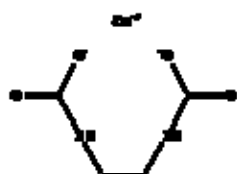
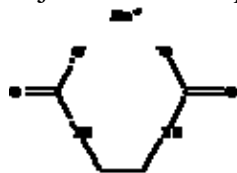
Malathion has a medium mobility in soil, leach through the soil is therefore not very likely (1).

1.6 *Literature*

- (1) National Chemicals Inspectorate, 1991. *PM-Etotal puder*. Solna, Stockholm.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, US EPA, Washington, D.C.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Mancozeb

Mancozeb is a fungicide of ethylenebisdithiocarbamate type, intended for use in potatoes and leak. *Mancozeb* is under evaluation within the framework of EU Dir. 91/414. *ETU* is the major breakdown product.



Mancozeb

ETU

1.1 Physico-chemical properties

Physico-chemical properties of *mancozeb* are summarised in table 1.1.1. and 1.1.2.

Table 1.1.1: Physico-chemical properties of *mancozeb*.

		Reference
CAS-No.	8018-01-07	1
Empirical formula	$(C_4H_6MnN_2S_4)_x(Zn)_y$	1
Molecular weight [g/mol]	271.3 (tentative; not defined for the polymeric complex)	1
Solubility in water [mg/kg]	9.92 at pH 4.2 6.2 at pH 7.5, 25°C	1 2
Log P_{ow}	Insoluble in most organic solvents	2
Vapour pressure	Negligible at 20°C	1,2
Henry's law constant	Not determined	1

Table 1.1.2: Physico-chemical properties of *ETU*.

		Reference
CAS-No.	96-45-7	4
Empirical formula	$C_3H_6N_2S$	4
Molecular weight [g/mol]	102.15	4
Solubility in water [mg/kg]	20 000 at 30°C	3
Vapour pressure [Pa]	0.02 (recalc. from mmHg)	5
Log P_{ow}	-0.66	4
Henry's law constant [$Pa \times m^3/mol$]	4.1×10^{-8} (recalc. from mmHg)	5

1.2 Toxicity to aquatic organisms

The toxicity of *mancozeb* to aquatic organisms is summarised in table 1.2.1. Most values are uncertain due to rapid hydrolysis.

Table 1.2.1: Aquatic ecotoxicity data of *mancozeb*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	72h, static	EC ₅₀ 1.25 NOEC 0.25	6
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48h	EC ₅₀ 0.073	6
<i>Daphnia magna</i>	reproduction	21 d, flow-through	NOEC 0.0073 ¹⁾	1
Fish				
<i>Salmo gairdneri</i>	mortality	96h	EC ₅₀ 0.074	1
<i>Pimephales promelas</i>		34 d, early life stage test, flow-through	NOEC 0.0022 ²⁾	1
Mesocosm				
Zooplankton, macroinvertebrates, phytoplanktion		12 weeks	EAC 0.032	6

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance of technical quality with 88.1% purity.

The most sensitive species tested was *Pimephales promelas*; with a NOEC of 0.0022 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *mancozeb* is calculated to 0.00022 mg/L.

The toxicity of *ETU* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *ETU*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Daphnia magna</i>		48 h	LC ₅₀ 49	3
<i>Daphnia magna</i>	reproduction and growth	21 d	NOEC 2.0 ¹⁾	3
Fish				
<i>Oncorhynchus mykiss</i>		96 h	LC ₅₀ >490 NOEC 490	3

¹⁾ Effect concentration basis for calculation of PNEC. Test substance of technical quality with unknown purity.

Supporting data on algae are available, but results not listed because the tests exceed optimal exposure duration time. The most sensitive species tested was *Daphnia magna*; with a reproduction NOEC of 2.0 mg/L. Fish seems to be more tolerant to *ETU* than *Daphnia*. Supportive studies suggest that *Daphnia* is more sensitive to *ETU* than fish and algae. One long-term NOEC from *Daphnia*, the most sensitive trophic level, is available and also supportive chronic data from fish; therefore an assessment factor of 50 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *ETU* is calculated to 0.04 mg/L

1.3 **Bioaccumulation and persistence**

Neither *mancozeb* nor the metabolite *ETU* is expected to bioaccumulate. *Mancozeb* degrades rapidly in water. *Mancozeb* is degraded mainly due to hydrolysis. Reported degradation time of hydrolysis is pH dependent, however the information is contradictory and varies from 4h-20 days in different studies. The most important metabolite, *ethylenethiourea (ETU)*, is hydrolytically stable. Both *mancozeb* and *ETU* are photochemically stable, but *ETU* has been reported to rapidly photodegrade in water with natural photosensitizers (3). In river and pond water, half-lives between 4 and 11 days has been reported (2). *ETU* can be more relevant than *mancozeb* in monitoring studies. However, *mancozeb* is more toxic towards aquatic organisms and should be paid attention to.

1.4 **Proposed water quality objective**

Mancozeb

PNEC is 0.000044 mg/L, the proposed water quality objective for *mancozeb* is 2×10^{-4} mg/L.

ETU

PNEC is 0.04 mg/L, the proposed water quality objective for *ETU* is 0.04 mg/L.

1.5 **Comments**

The main metabolites of *mancozeb* are ethylenebisisothiocyanate sulfide (*EBIS*), ethyleneurea (*EU*) and ethylenethiourea (*ETU*). The proposed metabolic route is: [*Mancozeb* → *EBIS* → *ETU* → *EU* → CO_2]. Potentially toxic metabolites are *EBIS* and *ETU*. However *EBIS* degrades very quickly. *ETU* is the ecotoxicologically most relevant metabolite.

Because *mancozeb* binds strongly to soil and degrades rapidly, leakage to groundwater is not expected. The metabolite *ETU* on the contrary is very mobile and leaching through the soil can be expected to both surface water and ground water. In monitoring program *mancozeb* is measured for as *ETU* in the aquatic environment.

Mancozeb and *ETU* are suspected to cause endocrine disrupting effects. Thyroidea may be affected. One study reports effects on frog (*Xenopus*). However the information is uncertain.

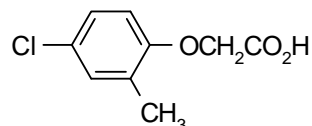
1.6 **Literature**

- (1) European Commission Peer Review Programme. *Mancozeb* Monograph (draft), 1998. Rapporteur Member State: Italy.
- (2) European Commission Peer Review Programme. *Mankozebe* Monograph (draft), 2000. Rapporteur Member State: Italy.
- (3) Environmental Fate Database (EFDB), 2001, Syracuse Research Corporation (SRC), State of New York, U.S.

- (4) Stenström, J. and Torstensson, L., 1992, *Ecotoxicological evaluation of ETU*, Sveriges Lantbruksuniversitet, inst. för mikrobiologi, Uppsala, Sweden.
- (5) Verschueren, K., 1996, *Handbook of Environmental Data on Organic Chemicals*, 3rd ed., John Wiley & Sons, Inc., New York, U.S.
- (6) European Commission Peer Review Programme. *Mancozeb* list of endpoint, 2003.
Rapporteur Member State: Italy.
- (7) European Commission Peer Review Programme. *Mancozeb* addendum, 2002.
Rapporteur Member State: Italy.

1. MCPA

MCPA [(4-chloro-2-methylphenoxy) acetic acid] is a selective, systemic herbicide with auxinic mode of action. Intended use for the substance is in cereals, potatoes and pasture. *MCPA* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *MCPA* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *MCPA*.

		Reference
CAS-No.	94-74-6	1
Empirical formula	C ₉ H ₉ ClO ₃	1
Molecular weight [g/mol]	200.6	1
Solubility in water [mg/kg]	26.2 g/l at pH 5 25°C 294 g/l at pH 7 25°C 320 g/l at pH 5 25°C	1
pKa	3.73	1
Log P _{ow}	2.70 (0.001 m/l) at pH 1 2.80 (0.0001 m/l) at pH 1 0.28 (0.01 m/l) at pH 5 0.59 (0.001 m/l) at pH 5 -0.81 (0.01 m/l) at pH 7 -0.71 (0.001 m/l) at pH 7 -1.07 (0.01 m/l) at pH 9 -0.88 (0.001 m/l) at pH 9	1
Vapour pressure	4×10 ⁻⁴ Pa at 32°C 4×10 ⁻³ Pa at 45°C	1
Henry's law constant	5.5×10 ⁻⁵ Pa × m ³ /mol at 25°C	1

1.2 Toxicity to aquatic organisms

The toxicity of *MCPA* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *MCPA*.

Species	End-point	Exposure duration	Result [mg ai/L]	Reference
Algae				
Selenastrum capricornutum	Growth inhibition	96 h	EC50 414 ¹⁾	3
Pseudokirchneriella	Biomass	72 h	EC50 57 ¹⁾	3
Aquatic plants				

<i>Lemna gibba</i>	Growth	14 d, static	EC ₅₀ 0.105 NOEC 0.011 ²⁾⁵⁾	2
<i>Lemna minor</i>	Fronnd numbers	7 d	E _r C ₅₀ >2.5 NOEC 0.13 ⁴⁾	3
<i>Lemna gibba</i>		7 d	E _b C ₅₀ 2.6 NOEC 0.32	3
Mollusca				
<i>Crassostrea virginica</i>		48 h, embryo-larval test, static	EC ₅₀ 147	2
<i>Crassostrea virginica</i>	shell deposition	96 h, flow-through	EC ₅₀ 18 ²⁾	2
Crustaceans				
<i>Daphnia magna</i>		48 h, flow-through	EC ₅₀ >155 ²⁾	2
<i>Mysidopsis bahia</i>		96 h, flow-through	LC ₅₀ 120 ²⁾	2
<i>Daphnia magna</i>	reproduction	21 d, semi-static	NOEC 41 ²⁾	1
Fish				
<i>Oncorhynchus mykiss</i>		96, static	LC ₅₀ 95 ^{2,3)}	1
<i>Oncorhynchus mykiss</i>		96 h, flow-through	LC ₅₀ 41 ^{1,2)}	1
<i>Oncorhynchus mykiss</i>		96 h, flow-through	LC ₅₀ 457 ²⁾	1
<i>Oncorhynchus mykiss</i>		96 h, static	LC ₅₀ 86	2
<i>Lepomis macrochirus</i>		96 h, static	LC ₅₀ 250 ^{2,3)}	1
<i>Lepomis macrochirus</i>		96 h	LC ₅₀ 250 ^{2,3)}	1
<i>Lepomis macrochirus</i>		96, static	LC ₅₀ 91	2
<i>Menidia beryllina</i>		96 h	LC ₅₀ 180 ^{2,3)}	1
<i>Menidia menidia</i>		96 h, static	LC ₅₀ 169	2
<i>Oncorhynchus mykiss</i>		28 d, flow-through	NOEC 40 ^{1,2)}	1

¹⁾ Test performed on preparation (Herbicide Marks M, 495g/l and U 46-M Fluid, 610g/l). Value expressed as active substance.

²⁾ Test performed on salt compound. Value expressed as active substance.

³⁾ Test performed on substance with purity <90%. Value expressed as active substance.

⁴⁾ Effect concentration basis for calculation of former PNEC.

⁵⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive of the tested species was *Lemna minor*, with a NOEC of 0.13 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for MCPA is calculated to 0.013 mg/L.

Revised EQS calculation according to EU-harmonised methodology (4)

The most sensitive of the tested species is *Lemna gibba* with a NOEC på 16.2 µg/l (14 d, growth). As this test was performed on salt compound (80 %) the NOEC expressed as active substance is 11 µg/l. This test was previously assigned the wrong unit (NOEC = 11 mg/l instead of µg/L), and was therefore not considered to be the lowest test result in the former PNEC calculation. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for MCPA is calculated to 0.0011 mg/L.

1.3 Bioaccumulation and persistence

MCPA is not expected to bioaccumulate. Photolysis is a potential route of degradation of *MCPA* in aquatic systems. The substance is stable to hydrolysis at pH between 5 and 9. In a study using ditch water/sediment the time of degradation was 1-2 weeks. *MCPA* remains mainly in the water phase.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.0011 mg/L, the proposed EQS/water quality objective for the substance is 0.001 mg/L.

1.5 Comments

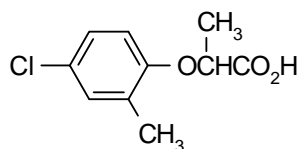
MCPA is mobile in soil and may leach through the soil profile. The metabolite *4-chloro-2-methylphenol* is expected to be more toxic to aquatic organisms than the parent substance. This metabolite may be a significant residue of *MCPA* degradation. A quality objective for the metabolite cannot be established at the moment due to lack of data.

1.6 Literature

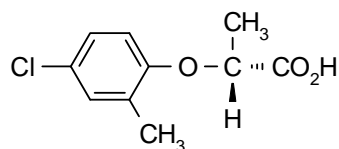
- (1) European Commission Peer Review Programme. *MCPA* Monograph (draft), 2001. Rapporteur Member State: Italy.
- (2) Pesticide Ecotoxicity Database, 2001, Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *MCPA* Addendum vol 3, 2003. Rapporteur Member State: Italy
- (4) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Mecoprop, mecoprop-p

Mecoprop is an auxin type systemic herbicide, intended for weed control in cereals and pastures. *Mecoprop* and *mecoprop-p* are under evaluation within the framework of EU Dir. 91/414.



Mecoprop



Mecoprop-p

1.1 Physico-chemical properties

Physico-chemical properties of *mecoprop* and *mecoprop-p* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *mecoprop* and *mecoprop-p*.

	<i>Mecoprop</i>	<i>Mecoprop-p</i>	Reference
CAS-No.	7085-19-0	16484-77-8	1, 2
Empirical formula	C ₁₀ H ₁₁ ClO ₃	C ₁₀ H ₁₁ ClO ₃	1, 2
Molecular weight [g/mol]	214.65	214.65	1, 2
Solubility in water [mg/kg]	734 at 25°C	860 at 20°C	1, 2
pKa	3.78	3.68 at 20°C	4
Vapour pressure [Pa]	0.12 at 22.5°C	4.0×10 ⁻⁴ at 20°C	1, 2
Log P _{ow}	1.18 at 23°C	1.43 at pH 5, 20°C 0.02 at pH 5, 20°C -0.18 at pH 5, 20°C	1, 2
Henry's law constant [Pa×m ³ /mol]	3.51×10 ⁻² at 25°C	9.98×10 ⁻⁵ at 20°C	1, 2

1.2 Toxicity to aquatic organisms

The toxicity of *mecoprop* and *mecoprop-p* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *mecoprop* and *mecoprop-p*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudokirchneriella Subcapitata</i>		70 h, static MCP-P	EC ₅₀ 270 NOEC 27	2
<i>Anabaena flos-aquae</i>	growth rate	72 h	E _r C ₅₀ 23.9 NOEC 6.0	5
Higher aquatic plant				
<i>Lemna minor</i>	frond numbers	14 d	EC ₅₀ 1.6 ³⁾ LOEC 0.44 ⁴⁾	5
Crustaceans				

<i>Daphnia magna</i>		48 h, static MCP	EC ₅₀ >100	3
<i>Daphnia magna</i>		48 h, static MCP	EC ₅₀ >100	1
<i>Daphnia magna</i>		48 h, static MCP	EC ₅₀ >91	1
<i>Daphnia magna</i>	reproduction	21 d, semi-static MCP-P	NOEC 50	2
<i>Daphnia magna</i>	reproduction	28 d, semi-static MCP	NOEC 22.2 ¹⁾	1
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static MCP	LC ₅₀ 124.8	3
<i>Lepomis macrochirus</i>	mortality	96 h, static MCP	LC ₅₀ >69 ^{1,2)}	3
<i>Oncorhynchus mykiss</i>	mortality	96 h, static MCP	LC ₅₀ 69 ^{1,2)}	3
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow through MCP	LC ₅₀ 198 ¹⁾	1
<i>Cyprinus carpio</i>	mortality	96 h, static MCP	LC ₅₀ 264-469 ¹⁾	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static MCP	LC ₅₀ 147-215	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static MCP-P	LC ₅₀ 147-215	2
<i>Lepomis macrochirus</i>	mortality	96 h, static MCP	LC ₅₀ ≥100	1
<i>Oncorhynchus mykiss</i>		21 d, flow through MCP	NOEC >89 ¹⁾	1
<i>Oncorhynchus mykiss</i>	sub lethal	28 d, flow through MCP-P	NOEC 50	2

¹⁾ Test performed on salt compound. Value expressed as active substance.

²⁾ Test performed on substance with purity <90%. Value expressed as active substance.

³⁾ Effect concentration basis for calculation of PNEC. Test substance purity 68.4%

⁴⁾ Effect concentration basis for calculation of revised PNEC. Test substance purity 68.4%

Former water quality objective calculation

The most sensitive (acute effects) group of species was *Lemna minor*, with an EC₅₀ of 1.6 mg/L and LOEC of 0.4 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 1.6 mg/L is divided by a factor of 100, which results in a PNEC of 0.016 mg/L.

Revised EQS calculation according to EU-harmonised methodology (6)

There is chronic data available from three trophic levels. The lowest NOEC is < 0.44 mg/l (LOEC =0.44 mg/l) for *Lemna minor*. A NOEC can according to the TGD be derived from the LOEC with the equation LOEC/2 if the effect is below >10% and <20% (as it is in this case). The estimated NOEC is thus 0.22 mg/l, dividing this value with an assessment factor of 10, gives a PNEC of 0.02 mg/l.

1.3 Bioaccumulation and persistence

Mecoprop and *mecoprop-p* are expected to have a low bioaccumulation potential. The degradation time is approximately 20 days in water (laboratory conditions, 20°C). In

water/sediment systems the main portion of *mecoprop* and *mecoprop-p* is located in the water phase (1,2).

1.4 Proposed EQS/water quality objective

Since PNEC is 0.02 mg/L, the proposed EQS/water quality objective for *mecoprop* and *mecoprop-p* is 0.02 mg/L.

1.5 Comments

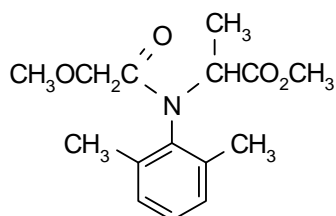
Mecoprop-p does not show more or higher ecotoxicological effects than racemic *mecoprop*. Degradation route and major metabolites are unknown. *Mecoprop* and *mecoprop-p* may reach surface- and ground waters through the soil profile (1,2).

1.6 Literature

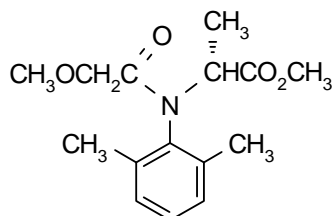
- (1) European Commission Peer Review Programme. *Mecoprop Monograph, 1999*. Rapporteur Member State: Denmark.
- (2) European Commission Peer Review Programme. *Mecoprop-P Monograph, 1998*. Rapporteur Member State: Denmark.
- (3) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide Programs, U.S. EPA. Washington DC.
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (5) European Commission Peer Review Programme. *Mecoprop-p Review report, 2003*, Rapporteur Member State: Denmark.
- (6) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Metalaxyl and metalaxyl-M

Metalaxyl and *metalaxyl-M* (*metalaxyl-M* is the R-enantiomer of *metalaxyl* which is a R/S racemic mixture) are systemic fungicides. The substance is intended for use in potatoes. *Metalaxyl* and *metalaxyl-M* is under evaluation within the framework of EU Dir. 91/414.



Metalaxyl



Metalaxyl-M

1.1 Physico-chemical properties

Physico-chemical properties of *metalaxyl* and *metalaxyl-M* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *metalaxyl* and *metalaxyl-M*.

	Metalaxyl	Reference	Metalaxyl-M	Reference
CAS-No.	57837-19-1	1	70630-17-0	2
Empirical formula	C ₁₅ H ₂₁ NO ₄	1	C ₁₅ H ₂₁ NO ₄	2
Molecular weight [g/mol]	279.3	1	279.3	2
Solubility in water [mg/kg]	8.4 at 22°C	1	26 at 25°C	2
pKa	Not relevant	1	Not relevant	2
Vapour pressure [Pa]	7.5×10 ⁻⁴ at 25°C	1	3.3×10 ⁻³ at 25°C	2
Log P _{ow}	1.75 at 25°C	1	1.71 at 25°C	2
Henry's law constant [Pa×m ³ /mol]	1.6×10 ⁻⁵	1	3.5×10 ⁻⁵	2

1.2 Toxicity to aquatic organisms

The toxicity of *metalaxyl* and *metalaxyl-M* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *metalaxyl* and *metalaxyl-M*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass	72 h, static	E _b C ₅₀ 46 NOE _b C <5.8	2
<i>Scenedesmus subspicatus</i>	biomass	72 h, static	E _b C ₅₀ 36 ²⁾ NOE _b C 9.6 ²⁾	2
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ 77.01 ²⁾ NOEC < 3.0 ²⁾	3
<i>Lemna gibba</i>		14 d, static	EC ₅₀ 85 ¹⁾ NOEC 56 ¹⁾	3
Crustaceans				

<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 28 ¹⁾	1,3
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 121 ¹⁾	3
<i>Daphnia magna</i>	mortality, reproduction	42 d, flow-through	NOEC 1.2 ¹⁾	1,3
<i>Mysidopsis bahia</i>	immobilisation	96 h, flow-through	LC ₅₀ 25 ¹⁾	1,3
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ >100 ²⁾	2
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ >113 ²⁾	3
Molluscs				
<i>Crassostrea virginica</i>	reproduction of shell deposition	96 h, flow-through	EC ₅₀ 5.6 ^{1,3)}	1
<i>Crassostrea virginica</i>	reproduction of shell deposition	96 h, flow-through	EC ₅₀ 9.7 ²⁾	2,3
Fish				
<i>Pimephales promelas</i>	hatchability of eggs, survival, growth of fry	30 d, flow-through	NOEC >9.1 ¹⁾	1,3
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 150 ¹⁾	1,3
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 139 ¹⁾	3
<i>Onchorynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 132 ¹⁾	3
<i>Onchorynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 130 ¹⁾	3
<i>Onchorynchus mykiss</i>	mortality	96 h, static	LC ₅₀ >100 ²⁾	2
<i>Onchorynchus mykiss</i>	mortality	96 h, static	LC ₅₀ >121 ²⁾	2,3

¹⁾ *Metalaxyl* used as test compound.

²⁾ *Metalaxyl-M* used as test compound.

³⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96.1%

The most sensitive (acute effects) of the tested species was *Crassostrea virginica*, with an EC₅₀ of 5.6 mg/L. Since the acute/chronic ratio is low, a PNEC based on long term studies does not guarantee appropriate protection against acute effects. Hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 5.6 mg/L is divided by a factor of 100, which results in a PNEC of 0.056 mg/L.

1.3 Bioaccumulation and persistence

Metalaxyl and *metalaxyl-M* are not expected to bioaccumulate. In water *metalaxyl* and *metalaxyl-M* are stable to hydrolysis and photolysis at environmental pH, and are not readily biodegradable. In natural water/sediment systems *metalaxyl* and *metalaxyl-M* distribute evenly between both water and sediment phases (1, 2).

1.4 Proposed water quality objective

Since PNEC is 0.056, the proposed water quality standard for *metalaxyl* and *metalaxyl-M* is 0.06 mg/L.

1.5 *Comments*

Metalaxyl and *metalaxyl-M* may leach through the soil profile.

Metalaxyl acid (CGA 62826) is the major metabolite. Also CGA 67868, formed by degradation of the acid, can be of interest as a major metabolite. Both of them are less toxic than *metalaxyl* and *metalaxyl-M* according to toxicity studies, but more persistent (1, 2).

1.6 *Literature*

- (1) European Commission Peer Review Programme. *Metalaxyl Monograph, 2000*.
Rapporteur Member State: Portugal.
- (2) European Commission Peer Review Programme. *Metalaxyl-M Monograph, 1999*.
Rapporteur Member State: Belgium.
- (3) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of
Office of Pesticide programs, U.S. EPA, Washington, D.C.

1. Metamitron

Metamitron is a systemic herbicide of the triazinone group. The mode of action is by inhibition of photosynthesis and thereby plant growth is inhibited. Intended use against grass and broad-leaved weeds in beets and strawberries (3).



1.1 Physico-chemical properties

Physico-chemical properties of *metamitron* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *metamitron*.

		Reference
CAS-No.	41394-08-2	1
Empirical formula	C ₁₀ H ₁₀ N ₄ O	1
Molecular weight [g/mol]	202.2	1
Solubility in water [mg/kg]	1700 at 20°C	1
pKa	Not relevant	
Vapour pressure [Pa]	8.6 × 10 ⁻⁹ at 20°C	1
Log P _{ow}	0.83	1
Henry's law constant [Pa×m ³ /mol]	1 × 10 ⁻⁷	2

1.2 Toxicity to aquatic organisms

The toxicity of *metamitron* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *metamitron*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	72h, static	E _r C ₅₀ 1.8 NOE _r C 0.12	1
<i>Selenastrum capricornutum</i>	growth rate	96h, static	E _r C ₅₀ 0.14 ²⁾ NOE _r C 0.1 ³⁾	4
<i>Selenastrum capricornutum</i>	growth rate	72h, static	E _r C ₅₀ 3.2 ¹⁾ NOE _r C 0.36 ¹⁾	3
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 101.7	3
<i>Daphnia magna</i>	immobility	48h	EC ₅₀ 145 ¹⁾	3
<i>Daphnia magna</i>	reproduction	21d	NOEC 32	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 10	1
Fish				
<i>Onchorhynchus mykiss</i>	sublethal effects	21d, semi-static	NOEC 9.9	3
<i>Onchorhynchus mykiss</i>	sublethal effects	21d, semi-static	NOEC 3.2 ¹⁾	3

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of former PNEC.

³⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 0.14 mg/L and NOEC of 0.1 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.14 mg/L is divided by a factor of 100, which results in a PNEC of 0.0014 mg/L.

Revised EQS calculation according to harmonised methodology (5)

There is chronic data available for three trophic levels. The most sensitive of the tested species was *Selenastrum capricornutum*, with a NOEC of 0.1 mg/L. Dividing this NOEC with an AF=10 results in a PNEC of 0.01 mg/l.

1.3 Bioaccumulation and persistence

Metamitron is not expected to bioaccumulate. Log P_{ow} is low hence no bioaccumulation studies have been performed. *Metamitron* is slowly partitioned into the sediment, and is evenly distributed between aqueous and the sediment phase after 50 days (3). The substance is degraded with a DT₅₀ of 7-9 days. One major metabolite is formed, *desamino-metamitron*. The metabolite is not persistent, and shows lower toxicity towards aquatic organisms than the parent compound (1). Therefore, no separate water quality standard is proposed for that compound.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.01 mg/L, the proposed EQS/water quality objective for *metamitron* is 0.01 mg/L.

1.5 Comments

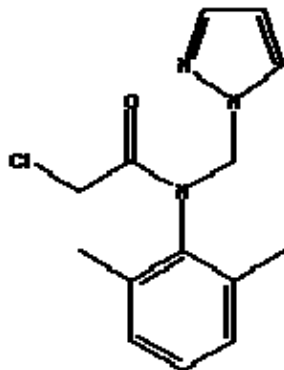
The metabolite is mobile in soil and may reach ground and surface water due to leach through the soil profile (1).

1.6 Literature

- (1) Miljøstyrelsen, 2000. *Miljømaessig grundvurdering. Metamitron*, Bilaga 1.a. Pesticidkontoret, Denmark.
- (2) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (3) Hanze K., 1993. *Ecotoxicological evaluation of the herbicide Metamitron*. National Chemicals inspectorate.
- (4) Vaittinen S-L., 1987. *Metamitron: Upptredande och verkan i naturen*. KUIPIO, Finland.
- (5) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Metazachlor

Metazachlor is a systemic herbicide, adsorbed by the hypocotyls and roots and inhibitions germination. The substance is intended for use in cabbage, potatoes and olieferous plants.



1.1 Physico-chemical properties

Physico-chemical properties of *metazachlor* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *metazachlor*.

		Reference
CAS-No.	67129-08-2	1
Empirical formula	C ₁₄ H ₁₆ ClN ₃ O	1
Molecular weight [g/mol]	277.8	1
Solubility in water [mg/kg]	4.3	1
pKa	Not relevant	
Vapour pressure [Pa]	9.3 × 10 ⁻⁵	3
Log P _{ow}	2.13	1
Henry's law constant [Pa×m ³ /mol]	5.7 × 10 ⁻⁵	3

1.2 Toxicity to aquatic organisms

The toxicity of *metazachlor* to aquatic organisms is summarised in table 1.2.1.

Table 1.21.: Aquatic ecotoxicity data of *metazachlor*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Clorella fusca</i>	biomass	96h, static	EC ₅₀ 0.34 NOEC 1.6	1
<i>Ankistodesmus bibrianus</i>	growth rate	72h, static	E _r C ₅₀ 0.02 ¹⁾	2
<i>Pseudokirchneriella subxapitata</i>	growth rate	72h, static	E _r C ₅₀ 0.027	2
Crustaceans				

<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ 22	1
<i>Daphnia magna</i>	mortality	48h	LC ₅₀ >100	2
<i>Daphnia magna</i>		21d	NOEC 50	2
Fish				
<i>Cyprinus carpio</i>	mortality	96h, static	LC ₅₀ 15	1
<i>Salmo gairdneri rich</i>	mortality	96h, static	LC ₅₀ 4.4	1
<i>Salmo gairdneri rich</i>	mortality	96h, static	LC ₅₀ 10	1
<i>Onchorhynchus mykiss</i>		28d	NOEC 3.2	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity not reported.

The most sensitive (acute effects) of the tested species was *Ankistodemus bibraianus*, with an EC₅₀ of 0.02 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.02 mg/L is divided by a factor of 100, which results in a PNEC of 0.0002 mg/L.

The toxicity of *BH-479-4* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *BH-479-4*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Clorella fusca</i>	biomass	72h, static	EC ₅₀ 79 NOEC 9	1
<i>Ankistodesmus bibraianus</i>	biomass	72h, static	EC ₅₀ 9.6 NOEC 1.5 ¹⁾	
Crustaceans				
<i>Daphnia magna</i>	mortality	48h, static	LC ₅₀ >100	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >100	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity not reported.

The most sensitive of the tested species was *Ankistodesmus bibraianus*, with a NOEC of 1.5 mg/L. Short term studies are available from three trophic levels. Only one trophic level has been tested for long term effects. Therefore an assessment factor of 100 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *BH-479-4* is calculated to 0.015 mg/L.

1.3 Bioaccumulation and persistence

Metazachlor is not expected to bioaccumulate, log K_{ow} is lower than 3. *Metazachlor* is stable towards hydrolysis and photolysis in water. The degradation has been studied in river- and pond waters. The DT₅₀ was 28 and 33 days respectively, the degradation is mainly due to microbial activity. Two metabolites have been found and identified as *BH 479-1* and *BH 479-4*. *BH 479-4* is considered to be major, exceeding 10%. A separate quality objective for the metabolite has been established.

1.4 Proposed water quality objective

Metazachlor

Since PNEC is 0.0002 mg/L, the proposed water quality standard for *metazachlor* is 0.0002 mg/L.

BH-479-4

Since PNEC is 0.015 mg/L, the proposed water quality standard for *BH-479-4* is 0.01 mg/L.

1.5 Comments

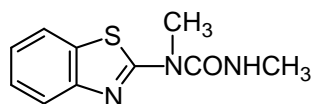
Metazachlor and *BH 479-4* are mobile in soil. They stay in the water phase and may be transported by water through soil profile. Therefore both substances may reach surface- and ground water.

1.6 Literature

- (1) Wrangstadh M., 1994. *Metazaklor, ekotoxikologisk utvärdering*. BIOTA handelsbolag. Möndal.
- (2) Lindqvist L., Concha G., 2002. *Butisan S*. PM inför beslut. Kemikalieinspektionen. Sverige.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Methabenzthiazuron

Methabenzthiazuron is a selective herbicide and belongs to the group arylurea, which inhibits the formations of ATP and NADPH₂. The herbicide is used for weed control in culturing of grass seeds.



1.1 Physico-chemical properties

Physico-chemical properties of *methabenzthiazuron* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *methabenzthiazuron*.

		Reference
CAS-No.	18691-97-9	1
Empirical formula	C ₁₀ H ₁₁ N ₃ OS	1
Molecular weight [g/mol]	221.3	1
Solubility in water [mg/kg]	59	1
Vapour pressure [Pa]	5.9 × 10 ⁻³	2
Log P _{ow}	2.64	2
Henry's law constant	2.2 × 10 ⁻⁷	3

1.2 Toxicity to aquatic organisms

The toxicity of *methabenzthiazuron* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *methabenzthiazuron*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate biomass	96h, static	E _r C ₅₀ 0.12 ²⁾ NOE _b C 0.018	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 30.6	1
<i>Daphnia magna</i>	immobility	21d	NOEC 1.4 ¹⁾	3
Fish				
<i>Leuciscus idus mela</i>	mortality	96h, static	EC ₅₀ 29	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ 15.9	1
<i>Cyprinus carpio</i>	mortality	96h, static	EC ₅₀ 8.4	1
<i>Cyprinus carpio</i>	mortality	96h, static	EC ₅₀ 8.5	1
<i>Cyprinus carpio</i>	mortality	96h, static	EC ₅₀ 20 ¹⁾	1
<i>Leuciscus idus mela</i>	mortality	96h, static	EC ₅₀ 48.7 ¹⁾	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ 20 ¹⁾	1

¹⁾ Test performed on preparation, Tribunil (70% ai). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97.1%

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 0.12 mg/L and a NOEC of 0.018 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.12 mg/L is divided by a factor of 100, which results in a PNEC of 0.0012 mg/L.

1.3 Bioaccumulation and persistence

Methabenzthiazuron may bioaccumulate, log P_{ow} 2.64. Studies for bioaccumulation are missing. *Methabenzthiazuron* is stable towards hydrolysis. In water/sediment systems the time of degradation is 90-182 days.

1.4 Proposed water quality objective

Since PNEC is 0.0012 mg/L, the proposed water quality standard for *methabenzthiazuron* is 0.001 mg/L.

1.5 Comments

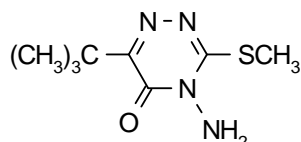
Methabenzthiazuron is not expected to reach ground- and surface waters through the soil profile.

1.6 Literature

- (1) Wenell T., 1992. *Ecotoxicological evaluation of Methabenzthiazuron*. Division of scientific documentation and research. National Chemical Inspectorate, Sweden.
- (2) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (3) Eriksson, Rudin och Steckó, 1992. Tribunil, reg nr 2439. PM. Kemikalieinspektionen. Sverige.

1. Metribuzin

Metribuzin is a systemic herbicide, used in cultivation of potatoes and carrots.



1.1 Physico-chemical properties

Physico-chemical properties of *metribuzin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *metribuzin*.

		Reference
CAS-No.	21087-64-9	3
Empirical formula	C ₈ H ₁₄ N ₄ OS	3
Molecular weight [g/mol]	214.3	3
Solubility in water [mg/kg]	1050 at 20 °C	3
Vapour pressure [Pa]	5.8 × 10 ⁻⁵	3
Log P _{ow}	1.6 at pH 5.6, 20 °C	3
Henry's law constant [Pa×m ³ /mol]	1 × 10 ⁻⁵ at 20 °C	3

1.2 Toxicity to aquatic organisms

The toxicity of *metribuzin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *metribuzin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass growth rate	96 h, static	E _b C ₅₀ 0.007 E _r C ₅₀ 0.02 ¹⁾	1
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ 0.16 NOEC 0.04	1 ³⁾
<i>Lemna gibba</i>	fronds	14 d, semi-static	EC ₅₀ 0.0079 ²⁾	4
Crustaceans				
<i>Daphnia magna</i>		48 h, static	EC ₅₀ 4.2	2
<i>Daphnia magna</i>		48 h, static	EC ₅₀ 4	2
<i>Daphnia magna</i>		48 h, static	EC ₅₀ 35	1
<i>Penaeus duorarum</i>		96 h, static	LC ₅₀ 48	2
<i>Penaeus duorarum</i>		96 h, semi-static	LC ₅₀ 44	1
<i>Daphnia magna</i>		21 d, flow-through	NOEC 1.3	2
<i>Daphnia magna</i>		21 d, static-renewal	NOEC 3.3	2
<i>Daphnia magna</i>	immobilisation reproduction	21 d, semi-static	NOEC 1.5 NOEC 1.5	1

Molluscs				
<i>Crassostrea virginica</i>	shell deposition	96 h, static	EC ₅₀ 50	2
			EC ₅₀ 52	1
<i>Crassostrea virginica</i>	shell deposition	96 h, static-renewal	EC ₅₀ 42	1
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 42	2
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 92	2
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ >100	2
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 76	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 77	2
<i>Cyprinodon variegatus</i>	mortality	96 h, static	LC ₅₀ 85	1, 2
<i>Leuciscus idus melanotus</i>	mortality	96 h, static	LC ₅₀ 142	1
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 80	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 76	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 64	1
<i>Oncorhynchus mykiss</i>		21 d, semi-static	NOEC 5.6	1

- 1) Effect concentration basis for calculation of former PNEC. Test substance purity 99%
- 2) Effect concentration basis for calculation of revised PNEC. Test substance purity 99%
- 3) This test could not be found in the reference (2007-10-03)

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Scenedesmus subspicatus*, with an E_rC₅₀ of 0.02 mg/L and. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.02 mg/L is divided by a factor of 100, which results in a PNEC of 0.0002 mg/L.

Revised EQS calculation according to EU-harmonised methodology (5)

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0079 mg/L and. Since this value is lower than all NOECs derived from long term studies the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.0079 mg/L is divided by a factor of 100, which results in a PNEC of 0.000079 mg/L.

1.3 Bioaccumulation and persistence

Metribuzin is not expected to bioaccumulate. The compound is hydrolytically stable, and slowly degraded in soil (1).

1.4 Proposed EQS/water quality objective

Since PNEC is 0.000079 mg/L, the proposed EQS/water quality objective for metribuzin is 0.00008 mg/L.

1.5 Comments

Due to potential for leach through the soil profile *Metribuzin* may reach surface- and ground waters. *Metribuzin* have three metabolites of interest, *desaminometribuzin* (DA),

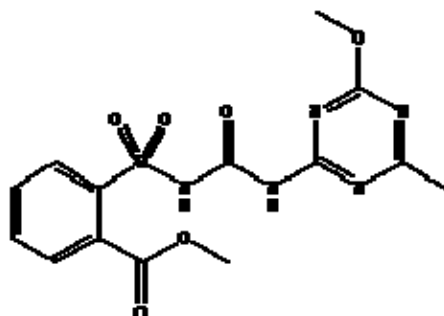
diketometribuzin (DK) and *desaminodiketometribuzin (DADK)* (1).

1.6 Literature

- (1) Dryselius, E., (1994). *Ecotoxicological evaluation of metribuzin*. National Chemicals Inspectorate, Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (4) European Commission Peer Review Programme. *Metribuzin* Draft Assessment Report vol 1, 2004. Rapporteur Member State: Germany
- (5) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Metsulfuron methyl

Metsulfuron methyl is a selective herbicide, acting primarily through foliar and root uptakes. It affects sensitive weeds through inhibition of the enzyme acetolactate synthase (ALS). The herbicide is intended for use in potatoes and carrots. *Metsulfuron methyl* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *metsulfuron methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *metsulfuron methyl*.

		Reference
CAS-No.	74223-64-6	1
Empirical formula	C ₁₄ H ₁₅ N ₅ O ₆ S	1
Molecular weight [g/mol]	381.4	1
Solubility in water [mg/kg]	548 at 25° pH 5 2790 at pH 7 213000 at pH 9	1
pKa	3.8	1
Vapour pressure [Pa]	1.1×10 ⁻¹⁰	1
Log P _{ow}	-1.7	1
Henry's law constant [Pa×m ³ /mol]	2.3×10 ⁻¹⁰ at pH 5 4.5×10 ⁻¹¹ at pH 7	1

1.2 Toxicity to aquatic organisms

The toxicity of *metsulfuron methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *metsulfuron methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	biomass growth	72h 48h	E _b C ₅₀ 3.9 E _r C ₅₀ 2.9 NOEC 0.5	1
<i>Selenastrum capricornutum</i>	biomass	72h	E _b C ₅₀ 0.045	1
<i>Selenastrum capricornutum</i>	biomass	96h, static	E _b C ₅₀ 0.19	2

Aquatic plants				
<i>Lemna minor</i>	frond number	14d	EC ₅₀ 0.00036 NOEC 0.00016 ²⁾	1
<i>Lemna minor</i>		7d	EC ₅₀ 0.0003 ¹⁾	2
Crustaceans				
<i>Daphnia magna</i>	immobility	48h	EC ₅₀ >150	1
<i>Daphnia magna</i>	reproduction and mortality	21d	NOEC 150	1
Fish				
<i>Bluegill sunfish</i>	mortality	96h	LC ₅₀ >150	1
<i>Onchorhynchus mykiss</i>	mortality	96h	LC ₅₀ >150	2
<i>Onchorhynchus mykiss</i>	mortality	96h	LC ₅₀ >150	2
<i>Claris batrachus</i>	mortality	96	LC ₅₀ 100	2
<i>Onchorhynchus mykiss</i>	growth	21d	NOEC 68	1

¹⁾ Effect concentration basis for calculation of former PNEC.

²⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Lemna minor*, with an EC₅₀ of 0.0003 mg/L. The lowest chronic toxicity showed *Lemna gibba*, with a NOEC of 0.00016 mg/L. Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.0003 mg/L is divided by a factor of 100, which results in a PNEC of 0.000003 mg/L.

Revised EQS calculation according to EU-harmonised methodology (3)

There is chronic data available from three trophic levels. The most sensitive (acute effects) of the tested species was *Lemna minor*, with an EC₅₀ of 0.0003 mg/L. The lowest chronic toxicity showed *Lemna minor*, with a NOEC of 0.00016 mg/L. Dividing the lowest NOEC with an AF=10 results in a PNEC of 0.000016 mg/L.

1.3 Bioaccumulation and persistence

Metsulfuron methyl is not expected to bioaccumulate. *Metsulfuron methyl* is stable in water at pH 7 and 9, but hydrolysed at pH 5. In water the substance is transformed into *sulfonamide (IN-D5803)*, *saccharin (IN-00581)* and *triazine amine (IN-A4098)*. The primary degradation occurs with DT₅₀ 81-148 days. *Metsulfuron methyl* is slowly degraded in water/sediment systems, DT₅₀ 15-25 weeks for the entire systems. Major metabolite in water/sediment system is *bis-O-demthyl metsulfuron methyl (IN-JX909)*. The metabolite occurs in both water and sediment. Toxicity tests have been performed of metabolite *IN-JX909*. In toxicity studies the metabolite show low toxicity towards aquatic organisms.

1.1 Proposed EQS/water quality objective

Since PNEC is 0.000016 mg/L, the proposed EQS/water quality objective for *metsulfuron methyl* is 0.00002 mg/L.

1.2 **Comments**

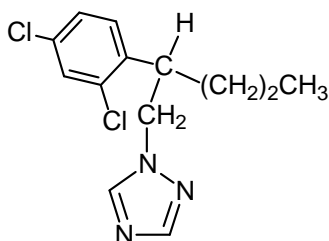
Metsulfuron methyl is weakly adsorbed to soils, K_{oc} 3-18. It is highly mobile in soil columns, but shows no significant leaching in lysimeter studies or MACRO simulations. *Metsulfuron methyl* degrades with DT_{50} 23 days, and degradation tends to be faster in acidic soils. Vapour pressure and Henry's law constant are low; therefore no significant concentration of *metsulfuron methyl* is expected in air.

1.3 **Literature**

- (1) European Commission Peer Review Programme. *Metsulfuron methyl Monograph*, 1997. Rapporteur Member State: France.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Penconazol

Penconazole is a fungicide belonging to a group of systemic triazoles. The fungicide acts by inhibition of the ergosterol biosynthesis (3). *Penconazole* is used in cultivation of fruit and strawberries.



1.1 Physico-chemical properties

Physico-chemical properties of *penconazole* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *penconazole*.

		Reference
CAS-No.	66 246-88-6	2
Empirical formula	C ₁₃ H ₁₅ Cl ₂ N ₂	2
Molecular weight [g/mol]	284.2	2
Solubility in water [mg/kg]	70 at 20°C	2
pKa	1.51 at 20°C	3
Vapour pressure [Pa]	3.6 × 10 ⁻⁴ at 25°C	3
Log P _{ow}	3.7 at pH 5.6 and 25°C	3
Henry's law constant [Pa×m ³ /mol]	6.6 × 10 ⁻⁴ at 20°C	4

1.2 Toxicity to aquatic organisms

The toxicity of *penconazole* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *penconazole*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Higher aquatic plants				
<i>Lemna gibba</i>	frond number	14d, static	EC ₅₀ 0.22	2
Crustaceans				
<i>Daphnia magna</i> Straus	immobility	24h, static	IC ₅₀ 8.4	1
<i>Daphnia magna</i> Straus	immobility	24h, static	IC ₅₀ 9.1	3
<i>Daphnia magna</i>	reproduction	21d, flow-through	NOEC 0.069 ¹⁾	2,3
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 1.3	3
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 4.3	3
<i>Pimephales</i>	larval growth	30d, flow-through	NOEC 0.36	3

<i>promelas (early life stage test)</i>				
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¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 87.3%

The most sensitive of the tested species was *Daphnia magna*, with a NOEC 0.069 of mg/L. Short term studies are available from three trophic levels and long term studies from two. According to available studies *Onchorhynchus mykiss* is the most sensitive species for acute toxicity. However long term toxicity has not been tested for *Onchorhynchus mykiss*. Hence a higher assessment factor (100) is chosen to compensate the uncertainty. The PNEC for *penconazole* is calculated to 0.00069 mg/L.

1.3 **Bioaccumulation and persistence**

Penconazole is expected to bioaccumulate. The log P_{ow} of 3.7 indicates a potential for bioaccumulation, which is confirmed by studies with the result BCF 320. *Penconazole* is stable for hydrolysis (1). The degradation has been studied in two water/sediment systems; Rhine water system and pond water system. The degradation proceeded very slowly with an approximate DT_{50} of 11 weeks. However *penconazole* is readily adsorbed onto the sediments. After 7 days in the tests 35-54% of the added amount of *penconazole* is partitioned into sediment. (3)

1.4 **Proposed water quality objective**

Since PNEC is 0.00069 mg/L, the proposed water quality standard for *penconazole* is 0.0007 mg/L.

1.5 **Comments**

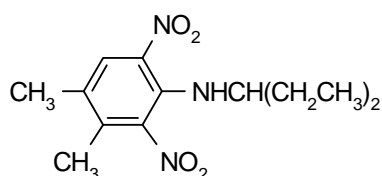
Penconazole is not expected to reach surface and ground waters through the soil profile (1). Due to rapid adsorption onto the sediment, an additional quality objective is recommended for sediment.

1.6 **Literature**

- (1) Gustafsson K., 1988. *Ekotoxicologisk utvärdering av Penkonazol, verksam beståndsdel I Topas EC*. Vetenskaplig utredning och dokumentation. Kemikalieinspektionen. Sverige.
- (2) Björk M., 1993. *Amendment to ecotoxicological evaluation of penconazole*. Scientific documentation and research. National Chemical Inspectorate. Sweden.
- (3) Mattsoff L., 1995. *Penconazole, ecotoxicological evaluation*. Helsinki.
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Pendimethalin

Pendimethalin is an herbicide, intended for use in potatoes and carrots. *Pendimethalin* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *pendimethalin* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *pendimethalin*.

		Reference
CAS-No.	40487-42-1	1
Empirical formula	C ₁₃ H ₁₉ N ₃ O ₄	1
Molecular weight [g/mol]	281.3	1
Solubility in water [mg/kg]	0.54 at pH 4, 20 °C 0.33 at pH 7, 20 °C 0.44 at pH 10, 20 °C	1
pKa	2.8	1
Vapour pressure [Pa]	1.94 × 10 ⁻³ at 25 °C	1
Log P _{ow}	5.2	1
Henry's law constant [Pa×m ³ /mol]	2.73	1

1.2 Toxicity to aquatic organisms

The toxicity of *pendimethalin* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *pendimethalin*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>		72 h, static	E _b C ₅₀ 0.0081 NOEC 0.0076	1
<i>Selenastrum capricornutum</i>	growth rate	72 h, static	E _r C ₅₀ 0.024 NOEC 0.0044	1
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ 0.0125 ¹⁾ NOEC 0.0056	2
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.28	1, 2
<i>Penaeus duoratum</i>	immobilisation	96 h, static	EC ₅₀ 1.6	1, 2
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.40	1
<i>Daphnia magna</i>	reproduction	21 d, flow-through	NOEC 0.015	1

Molluscs				
<i>Crassostrea virginica</i> (embryo larvae)		48 h, static	EC ₅₀ 0.21	1, 2
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, static	EC ₅₀ 0.2	1, 2
<i>Cyprinodon variegatus</i>	mortality	96 h, static	EC ₅₀ 0.71	1, 2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	EC ₅₀ 0.14	1
<i>Ictalurus punctatus</i>	mortality	96 h, static	EC ₅₀ 0.42	1
<i>Pimephales promelas</i>	survival of fry	30 d, flow-through	NOEC 0.022	1
Mesocosm				
<i>Macrophytes, periphyton etc.</i>	chlorophyll a, cryptophyceaea and chlorophyceaea	128 d, outdoor mesocosm, ponds	NOAEC 0.15 LOEC 0.0011 NOEC 0.00023	3

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Lemna gibba*, with an EC₅₀ of 0.013 mg/L and NOEC of 0.0056 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.013 mg/L is divided by a factor of 100, which results in a PNEC of 1.3×10^{-4} mg/L.

1.3 Bioaccumulation and persistence

Pendimethalin is expected to bioaccumulate, BCF 5100. *Pendimethalin* is also persistent in the environment; mineralisation is low. In water *pendimethalin* rapidly binds to sediment.

1.4 Proposed water quality objective

Since PNEC is 1.3×10^{-4} mg/L, the proposed water quality standard for *pendimethalin* is 1×10^{-4} mg/L.

1.5 Comments

Pendimethalin dissipates in the environment by binding to soil and by volatilisation. The substance does not have any metabolites of concern. Water quality objectives recommended to be set for both sediment and biota.

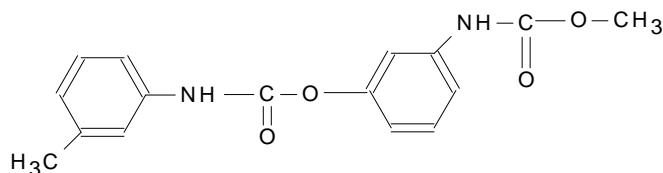
1.6 Literature

- (1) European Commission Peer Review Programme. *Pendimethalin Monograph*, 1998. Rapporteur Member State: Spain.

- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *Pendimethalin Addendum*, 2002. Rapporteur Member State: Spain.

1. Phenmedipham

Phenmedipham is a non-systemic contact herbicide used against weeds in sugar beets and strawberries. *Phenmedipham* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *phenmedipham* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *phenmedipham*.

		Reference
CAS-No.	13684-63-4	1
Empirical formula	C ₁₆ H ₁₆ N ₂ O ₄	1
Molecular weight [g/mol]	300.3	1
Solubility in water [mg/kg]	6 at 20°C, and pH 4	1
pKa	Not relevant	1
Vapour pressure [Pa]	7×10 ⁻¹⁰	1
Log P _{ow}	3.6 at 22°C and pH 4	1
Henry's law constant [Pa×m ³ /mol]	5×10 ⁻⁸	1

1.2 Toxicity to aquatic organisms

The toxicity of *phenmedipham* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *phenmedipham*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Nitzshia palea</i>	growth rate	72h, static	E _r C ₅₀ 0.62 NOEC 0.29	1
<i>Chlorella vulgaris</i>	growth rate	72h, static	E _r C ₅₀ 3.5 ¹⁾ NOEC <0.048 ¹⁾	1
<i>Selenastrum capricornutum</i>	growth rate	72h, static	E _r C ₅₀ 0.19 ^{1,2)} NOEC 0.025 ¹⁾	1
Higher aquatic plants				
<i>Lemna minor</i>	frond numbers	14d, semi-static	EC ₅₀ 0.23 NOEC 0.028	1
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, flow-through	EC ₅₀ 0.5	1
<i>Daphnia magna</i>	immobility	48h, semi-static	EC ₅₀ 0.9 ¹⁾	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 1.25 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.065	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.025 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, semi-static	LC ₅₀ 2.7	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 3	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.3 ¹⁾	1
<i>Onchorhynchus mykiss</i>	clinical signs	21d, flow-through	NOEC 0.4	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 0.19 mg/L and NOEC 0.025 mg/L separate studies. Since the acute/chronic ratio for algae is low, a PNEC based on chronic toxicity does not guarantee appropriate protection against acute effects. Hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.19 mg/L is divided by a factor of 100, which results in a PNEC of 0.0019 mg/L.

The toxicity of the metabolite *MHPC* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *MHPC*

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudokrichneriella subcapitata</i>	growth rate	96h, static	E _r C ₅₀ 79 NOEC 6.2	2
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 14 ¹⁾	2
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, semi-static	LC ₅₀ 75	2

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with an EC₅₀ 14 mg/L. Since only short-term studies are available from three trophic levels, an assessment factor of 1000 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *MHPC* is calculated to 0.014 mg/L.

1.3 Bioaccumulation and persistence

Phenmedipham is expected to bioaccumulate. BCF is 165, in whole fish. Hydrolysis of *phenmedipham* is pH-dependent; DT₅₀ is 0.16h in alkaline waters and 14.5-119.5 hours at pH 7 and 5, respectively. In water/sediment systems the substance is primarily degraded within a DT₅₀ of 0.1-0.3 days in the water phase and 0.11-0.18 days in the sediment. *Phenmedipham* is mainly partitioned into the sediment. In water/sediment systems the substance is hydrolysed under neutral/alkaline conditions and *MHPC* is the main metabolite. The half-life of *MHPC* is ca 20 days. Because the metabolite is more persistent than the parent compound, although not more toxic, a separate water quality standard has been established.

1.4 Proposed water quality objective

Phenmedipham

Since PNEC is 0.0019 mg/L, the proposed water quality standard for *phenmedipham* is 0.002 mg/L.

MHPC

Since PNEC is 0.014 mg/L, the proposed water quality standard for *MHPC* is 0.01 mg/L.

1.5 Comments

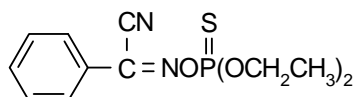
Phenmedipham is partitioned to sediment; hence a quality standard for sediment is recommended.

1.6 Literature

- (1) European Commission Peer Review Programme. *Phenmedipham Monograph, 1999*. Rapporteur Member State: Finland.
- (2) European Commission Peer Review Programme. *Phenmedipham Addendum, 2001*. Rapporteur Member State: Finland.
- (3) European Commission Peer Review Programme. *Phenmedipham List of endpoints, 2001*. Rapporteur Member State: Finland.

1. Phoxim

Phoxim is an organophosphorus insecticide intended for use against insects in soil and indoor to control housing and storage room pests.



1.1 Physico-chemical properties

Physico-chemical properties of *phoxim* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *phoxim*.

		Reference
CAS-No.	14186-18-3	1, 3
Empirical formula	C ₁₂ H ₁₆ N ₂ O ₃ PS	1, 3
Molecular weight [g/mol]	298.3	1, 3
Solubility in water [mg/kg]	1.5 at 20°C	1, 3
Vapour pressure [Pa]	0.0021 at 20 °C	3
Log P _{ow}	4.39 at 20 °C	1, 3
Henry's law constant [Pa×m ³ /mol]	0.42	1, 3

1.2 Toxicity to aquatic organisms

The toxicity of *phoxim* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *phoxim*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	growth inhibition	96 h, static	EC ₅₀ 0.65 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 6.7×10 ⁻⁴ ¹⁾	1
<i>Daphnia magna</i>	reproduction and body lengths of parent animals	21 d, flow-trough	NOEC 4.2×10 ⁻⁵ ^{1,2)}	2

Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.68 ¹⁾	1
<i>Leuciscus idus</i>	mortality	96 h, static	LC ₅₀ 1.8 ¹⁾	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.53 ¹⁾	1
<i>Lepomis macrochirus</i>			LC ₅₀ 0.22 ¹⁾	

¹⁾ Test performed on preparation (Volaton, 84.5%, Volaton VL 83,6% and Volaton technical, 89%).

Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 83.6%

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 4.2×10^{-5} mg/L. Since short-term studies from three trophic levels, but only one long-term study are available, an assessment factor of 100 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *phoxim* is calculated to 4.2×10^{-7} mg/L.

1.3 Bioaccumulation and persistence

Phoxim may bioaccumulate, the octanol/water partition coefficient is higher than three, but no experimental data exist on the bioconcentration factor, BCF. Degradation in sediment/water systems has not been investigated (1).

1.4 Proposed water quality objective

Since PNEC is 4.2×10^{-7} mg/L, the proposed water quality objective for *phoxim* is 4×10^{-7} mg/L.

1.5 Comments

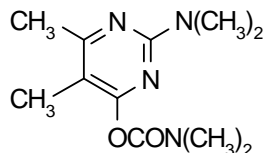
Phoxim is strongly adsorbed in soil and is not expected to reach surface and ground waters through the soil profile.

1.6 Literature

- (1) Lundberg, I. (1990). *Ekotoxikologisk utvärdering av insekticiden foxim*. National Chemicals inspectorate.
- (2) Lundberg, I. (1993). *Kompletterade ekotoxikologisk utvärdering av insekticiden foxim*. National chemicals inspectorate.
- (3) Tomlin, C. (2000). *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Pirimicarb

Pirimicarb is a systemic carbamate insecticide with contact, stomach or respiratory action. *Primicarb* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *pirimicarb* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *pirimicarb*.

		Reference
CAS-No.	23103-98-2	1
Empirical formula	C ₁₁ H ₁₈ O ₂ N ₄	1
Molecular weight [g/mol]	238	1
Solubility in water [mg/kg]	3 060 at pH 7.4	1
Vapour pressure [Pa]	4.4 × 10 ⁻⁴ at 20°C 21 × 10 ⁻⁴ at 30°C	1
Log P _{ow}	1.7 at 20°C	1
Henry's law constant [Pa×m ³ /mol]	3.6 × 10 ⁻⁵	5

1.2 Toxicity to aquatic organisms

The toxicity of *pirimicarb* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *pirimicarb*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudokirschneriella subcapitatus</i>	growth rate	96 h, static	EC ₅₀ 180 NOEC 50	1
Crustaceans				
<i>Daphnia magna</i>		48 h, static	LC ₅₀ 0.014 ¹⁾	3
<i>Daphnia magna</i>		48 h, static	LC ₅₀ 0.019	3
<i>Daphnia magna</i>		48 h, flow-through	EC ₅₀ 0.0065 ²⁾	1
<i>Daphnia magna</i>	mortality	21 d, semi-static	NOEC 0.0017	1
	growth	21 d, semi-static	NOEC 0.0009 ³⁾	
	reproduction	21 d, semi-static	NOEC 0.0017	
Fish				
<i>Oncorhynchus mykiss</i>		96 h, semi-static	LC ₅₀ 32	1

<i>Oncorhynchus mykiss</i>		96 h, semi-static	LC ₅₀ 62 ¹⁾	1
<i>Oncorhynchus mykiss</i>		96 h, flow-through	LC ₅₀ 29	3
<i>Cyprinus carpio</i>		96 h, semi static	LC ₅₀ 36	3
<i>Cyprinus carpio</i>		96 h, semi static	LC ₅₀ 158 ¹⁾	3
<i>Lepomis macrochirus</i>		96 h, flow-through	LC ₅₀ 55	3
<i>Oncorhynchus mykiss</i>		28 d, semi-static	NOEC >18	4
<i>Pimephales promelas</i>	survival	36 d, flow-through	NOEC 24	5
	hatchability	36 d, flow-through	NOEC 24	
	growth	36 d, flow-through	NOEC 10	

¹⁾ Test performed on preparation (Primor 50 DP). Value expressed as active substance.

²⁾ Effect concentration basis for calculation of former PNEC. Test substance purity 99.13%

³⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive of the tested species was *Daphnia magna*, with an EC₅₀ of 0.0065 mg/L and a NOEC of 0.0009 mg/L. Since the acute/chronic ratio is low, a PNEC based on long term data does not guarantee appropriate protection against acute effects. Hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.0065 mg/L is divided by a factor of 100, which results in a PNEC of 6.5×10^{-5} mg/L.

Revised EQS calculation according to EU-harmonised methodology (5)

There is chronic data available for three trophic levels. The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.0009 mg/L. Dividing this NOEC with an assessment factor of 10 gives a PNEC of 0.00009 mg/l.

1.3 Bioaccumulation and persistence

Pirimicarb is not expected to bioaccumulate, Log P_{ow} is low. In water, photolysis is pH-dependent and increases with pH (half-lives between 3 and >20 days including metabolites). Hydrolysis is slow with a half-life of >>23 days. The substance degrades biologically within a pH-dependent half-life varying from 7-56 days at alkaline conditions to 105-300 days at acidic conditions at 30°C. In water-sediment systems *pirimicarb* is mainly remained in the water-phase.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.00009 mg/L, the proposed EQS/water quality objective for *pirimicarb* is 0.00009 mg/L.

1.5 Comments

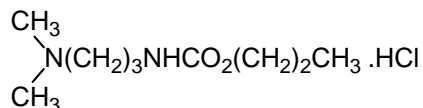
Primicarb may reach the surface- and ground water through the soil profile. *Pirimicarb* gives rise to several active photolytic metabolites. None of the metabolites is more toxic than the parent compound. The metabolite *R34885*, is, however, due to the active carbamate structure, is very toxic to *Daphnia magna* EC₅₀ 0.018 mg/L.

1.6 Literature

- (1) Fischer, S., 1990, *Ekotoxikologisk utvärdering av pirimikarb*, Enheten för vetenskaplig utredning och dokumentation, Kemikalieinspektionen, Solna.
- (2) Pesticide Ecotoxicity Database, 2001, Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Tapp, J. F. et al., 1989, *PIRIMICARB: Determination of the 28 day LC₅₀ to rainbow trout (Salmo gairdneri)*, Imperial Chemical Industries PLC, Brixham Devon, UK
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (5) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Propamocarb hydrochloride

Propamocarb hydrochloride is a systemic fungicide. It is used in cultivation of potatoes, leak, cucumber, tomatoes and salad.



1.1 Physico-chemical properties

Physico-chemical properties of *propamocarb hydrochloride* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *propamocarb hydrochloride*.

		Reference
CAS-No.	25606-41-1	2
Empirical formula	C ₉ H ₂₁ ClN ₂ O ₂	2
Molecular weight [g/mol]	224.7	2
Solubility in water [mg/kg]	>7000 at 20°C	1
pKa	9.3	2
Vapour pressure [Pa]	3.85 × 10 ⁻² at 20°C	2
Log P _{ow}	-2.6	1
Henry's law constant [Pa×m ³ /mol]	1.7 × 10 ⁻⁸	2

1.2 Toxicity to aquatic organisms

The toxicity of *propamocarb hydrochloride* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *propamocarb hydrochloride*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	Growth rate	93h, static	E _r C ₅₀ 595 ¹⁾ NOEC 126 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	LC ₅₀ 422	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 8.9 ²⁾	1
Fish				
<i>Cyprinus carpio</i>	mortality	72h, static	LC ₅₀ 646	1
<i>Cyprinus carpio</i>	mortality	96h, static	LC ₅₀ 235	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 410	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 415	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 616	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 8.9 mg/L. Short term studies are available from three trophic levels and long term studies from two. According to available studies fish is the most sensitive species regarding acute toxicity. However long term toxicity has not been tested on fish. Hence a higher assessment factor (100) is chosen to compensate the uncertainty. The PNEC for *propamocarb hydrochloride* is calculated to 0.089 mg/L.

1.3 Bioaccumulation and persistence

Propamocarb hydrochloride is not expected to bioaccumulate. BCF is 39-43. *Propamocarb hydrochloride* is stable towards hydrolysis at environmental pH, and photolysis. Microbial degradation seems to be the major route of degradation in water. Time of degradation in water was DT₅₀ 21days, if an extra carbon source was added, otherwise DT₅₀ >35 days.

1.4 Proposed water quality objective

Since PNEC is 0.089 mg/L, the proposed water quality standard for *propamocarb hydrochloride* is 0.09 mg/L.

1.5 Comments

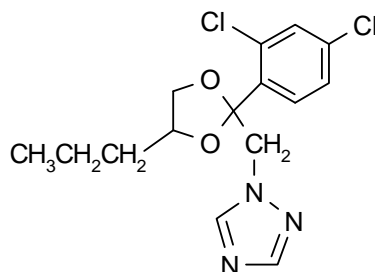
Propamocarb hydrochloride is mobile in soil may reach surface and ground waters via transport through the soil profile.

1.6 Literature

- (1) Elzvik, 1991. *Ekotoxikologisk utvärdering av fungiciden propamocarb-hydroklorid*. Vetenskaplig utredning och dokumentation. Kemikalieinspektionen. Sverige.
- (2) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Propiconazole

Propiconazole is a fungicide consisting of four isomers, all biologically active.



1.1 Physico-chemical properties

Physico-chemical properties of *propiconazole* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *propiconazole*.

		Reference
CAS-No.	60207-90-1	1
Empirical formula	C ₁₅ H ₁₇ Cl ₂ N ₃ O ₂	1
Molecular weight [g/mol]	342.2	1
Solubility in water [mg/kg]	100-150 mg/l at 20°C	1
Vapour pressure [Pa]	2.1 × 10 ⁻⁴ at 20°C	1
Log P _{ow}	3.51 at 20°C and pH 4.7 3.72 at 20°C and pH 6.6	1
Henry's law constant [Pa×m ³ /mol]	9.2 × 10 ⁻⁵ (calc.) 4.78 × 10 ⁻⁴ (calc.)	1

1.2 Toxicity to aquatic organisms

The toxicity of *propiconazole* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *propiconazole*.

Species	End-point	Exposure duration	Result [mg/L]	Reference
Aquatic plants				
<i>Lemna gibba</i>	frond production	14 d	EC ₅₀ 9.02 EC ₁₀ 2.94	1
Crustaceans				

<i>Daphnia magna</i>		48 h, static	EC ₅₀ 4.8	2
<i>Daphnia magna</i>		48 h, static	EC ₅₀ 11.3	2
<i>Mysidopsis bahia</i>		96 h, flow-through	LC ₅₀ 0.51	1,2
<i>Procambrus sp.</i>		96 h, static	LC ₅₀ 42	1
<i>Daphnia magna</i>		21 h, flow-through	NOEC 0.31	1,2
<i>Mysidopsis bahia</i>		28 h, intermittent flow	NOEC 0.114	1
Mollusca				
<i>Crassostrea virginica</i>	shell deposition	96 h, static	EC ₅₀ 1.7	1,2
<i>Crassostrea virginica</i>		96 h, static	EC ₅₀ 3.4	2
Fish				
<i>Oncorhynchus mykiss</i>		96 h, static	LC ₅₀ 0.83	2
<i>Lepomis macrochirus</i>		96 h, static	LC ₅₀ 5.5	2
<i>Lepomis macrochirus</i>		96 h, static	LC ₅₀ 1.3	2
<i>Leistomus xanthurus</i>		96 h, static	LC ₅₀ 2.6	1
<i>Ictalurus punctatus</i>		96 h, static	LC ₅₀ 4.87	2
<i>Pimephales promelas</i>	toxicological symptoms	31 d, early life stage	NOEC 0.43	1
<i>Cyprinodon variegates</i>	reproduction	100 d, FLC-test	NOEC 0.068	1
<i>Cyprinodon variegates</i>		100 d, flow-through	NOEC 0.15	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance of technical quality with unknown purity.

PNEC is based on the toxicity to *Cyprinodon variegates* with a NOEC of 0.068 mg/L. The species with the lowest toxicity values was *Skeletonema costatum*, with an EC₅₀ of 0.021 mg/L and a NOEC of 0.018 mg/L. However the test is considered to be supportive only, due to longer duration time than normally accepted. Tests on algae with shorter duration are not expected to lower the toxicity values. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *propiconazole* is calculated to 0.0068 mg/L.

1.3 Bioaccumulation and persistence

Bioaccumulation of *propiconazole* may be of concern. In *Lepomis macrochirus* BCF was established to 116 in the whole fish. However steady state was never reached, therefore the concentration fluctuated with in a range of 68-203. *Propiconazole* is slowly degraded in soil and breakdown is mainly due to biodegradation. Breakdown is influenced by pH, and decreases with increasing pH. The metabolite 1,2,4-triazole has a half-life in soil between 1 and 84 days. Hydrolysis and photolysis does not represent important pathways for - degradation of *propiconazole* and its metabolite 1,2,4-triazole from water-sediment systems. Dissipation from the water-phase is rapid due to adsorption.

1.4 Proposed water quality objective

Since PNEC is 0.0068 mg/L, the proposed water quality objective for *propiconazole* is 0.007 mg/L.

1.5 Comments

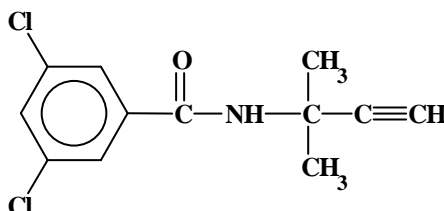
The most stable metabolite of *propiconazole* is *1,2,4-triazole*, which is a metabolite of several triazole fungicides. The metabolite is toxic to algae, but less toxic than the parent substance. *Propiconazole* is adsorbed to particles. However *1,2,4-triazole* may reach ground- and surface water due to leach through the soil profile. The substance dissipates to the sediment; therefore an additional quality objective for sediment ought to be established.

1.6 Literature

- (1) European Commission Peer Review Programme. *Propiconazole* Monograph, 1998. Rapporteur Member State: Finland.
- (2) Pesticide Ecotoxicity Database, 2001, Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Propyzamide

Propyzamide is a selective herbicide. The uptake occurs through roots and acts by inhibition of the cell division in plants and roots. *Propyzamide* has been is under evaluation within the framework of EU Dir. 91/414/EEC.



1.1 Physico-chemical properties

Physico-chemical properties of *propyzamide* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *propyzamide*.

		Reference
CAS-No.	23950-58-5	1
Empirical formula	C ₁₂ H ₁₁ Cl ₂ NO	1
Molecular weight [g/mol]	256.13	1
Solubility in water [mg/kg]	9.0 at pH 7	1
pKa	Not relevant	1
Vapour pressure [Pa]	2.67 x 10 ⁻⁵	1
Log P _{ow}	3.0	1
Henry's law constant [Pa×m ³ /mol]	7.6 x 10 ⁻⁴ (calculated)	1

1.2 Toxicity to aquatic organisms

The toxicity of *propyzamide* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *propyzamide*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth biomass	72h 120h	EC ₅₀ 0.98 NOEC 0.49	1
Higher plants				
<i>Lemna gibba</i>	fronds numbers	14d, static	EC ₅₀ 1.4 NOEC 0.56	1
<i>Lemna gibba</i>	growth	14d, static	EC ₅₀ 1.18	2
Crustaceans				

<i>Daphnia magna</i>	immobility	48h	NOEC>5.6	1
<i>Daphnia magna</i>	reproduction	21d	NOEC 0.60	1
<i>Americamysis bahia</i>	mortality	96h, flow-through	LC ₅₀ > 3.9	2
Molluscs				
<i>Crassostea virginica</i>	intoxication	96h, flow-through	EC ₅₀ 3.5	2
Fish				
<i>Cyprinus carip</i>	mortality	96h, flow-through	LC ₅₀ >5.1	1
<i>Onchorhyncus mykiss</i>	mortality	96h, flow-through	LC ₅₀ >4.7	1
<i>Onchorhyncus mykiss</i>	growth	21d	NOEC 0.94	1
<i>Onchorhyncus mykiss</i>	mortality	96h, static	LC ₅₀ 72	2
<i>Poecilia reticulata</i>	mortality	96h, static	LC ₅₀ 150	2
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ >100	2
<i>Ictalurus punctatus</i>	mortality	96h, static	LC ₅₀ >500	2
<i>Carassius auratus</i>	mortality	96h, static	LC ₅₀ 350	2
<i>Bufo bufo japonicus</i>	mortality	24h, static	LC ₅₀ >40	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97%

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 0.98 mg/L and a NOEC of 0.49mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.98 mg/L is divided by a factor of 100, which results in a PNEC of 0.0098 mg/L.

1.3 Bioaccumulation and persistence

Although log P_{ow} is 3.0, which indicates a possibility for bioaccumulation, *propryzamide* is not expected to bioaccumulate in the aquatic environment. Measured BCF in fish is 49 and CT₉₀, clearance time, is approx. 3 days. Water/sediment studies show a moderate rate of transformation in the water phase of 18 - 24 days. Half-life in the whole water/sediment system is about 118 - 69 days. *Propryzamide* is the main residue in the water phase.

1.4 Proposed water quality objective

Since PNEC is 0.0098 mg/l, the proposed water quality standard for *propryzamide* is 0.01 mg/L.

1.5 Comments

Propryzamide is expected to partition into organic material in soil, sediment and to biota. This indicates that the substance is not mobile in soil. K_{oc} ranges from 548 to 1340, depending on type of soil. Due to low vapour pressure the substance is not expected to dissipate from water to atmosphere. Hence the substance is most likely to be found in soil, and in some extent also in sediment and biota. In soil the degradation results in two metabolites; *RH-24580* and *RH-24644*.

1.6 Literature

- (1) European Commission Peer Review Programme. *Propyzamide Monograph, 1998*.
Rapporteur Member State: Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the
Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Prosulfocarb

Prosulfocarb is a selective herbicide and belongs to the chemical group of thiolcarbamates. It is used for weed control in winter cereals and potatoes.



1.1 Physico-chemical properties

Physico-chemical properties of *prosulfocarb* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *prosulfocarb*.

		Reference
CAS-No.	52888-80-9	1
Empirical formula	$\text{C}_{14}\text{H}_{21}\text{NOS}$	1
Molecular weight [g/mol]	251.4	1
Solubility in water [mg/kg]	13.2 at 20°C	1
pKa	Not relevant	
Vapour pressure [Pa]	6.9×10^{-3} at 25°C	1
Log P_{ow}	4.7 at 25°C	2
Henry's law constant [$\text{Pa} \times \text{m}^3/\text{mol}$]	0.1	2

1.2 Toxicity to aquatic organisms

The toxicity of *prosulfocarb* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *prosulfocarb*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	96h, static	EC_{50} 0.16 ¹⁾ NOEC 0.048	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC_{50} 1.3	1
<i>Daphnia magna</i>	reproduction growth	21d, semi-static	$\text{NOEC}_{\text{repro}}$ 0.2 $\text{NOEC}_{\text{growth}}$ 0.047 ²⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, semi-static	LC_{50} 4.2	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC_{50} 4.7	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.047 mg/L. Short term studies have been tested at three trophic levels, however long term studies have only been tested for two trophic levels. Therefore an assessment factor of 50 is used for

calculation of the predicted no effect concentration. Hence, the PNEC for *prosulfocarb* is calculated to 0.00094 mg/L.

1.3 Bioaccumulation and persistence

Prosulfocarb is expected to bioaccumulate. Log P_{ow} 4.65, indicates bioaccumulation and this is confirmed by studies resulting in BCF 700-800. *Prosulfocarb* is stable toward hydrolysis in water. The herbicide is photochemically unstable in water. Degradation in water/sediment has not been studied. In soil the substance is degraded with in DT_{50} of 49-60 days.

1.4 Proposed water quality objective

Since PNEC is 0.00094 mg/L, the proposed water quality standard for *prosulfocarb* is 0.0009 mg/L.

1.5 Comments

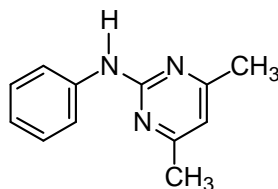
The degradation of *prosulfocarb* in water has not been studied. Thus, no metabolites have been reported. The compound is not expected to reach surface and ground waters through the soil profile, due to low mobility in soil. Additional quality objectives for biota and sediment are recommended.

1.6 Literature

- (1) Hedenberg M., 1992. Ekotoxikologisk utvärdering av herbiciden Prosulfokarb. Examensarbete, Stockholms Universitet.
- (2) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (3) Debourg, Steckó, Wistrand, 1992. PM BOXER, Kemikalieinspektionen, Sverige.

1. Pyrimethanil

Pyrimethanil is an aniline-pyrimidine fungicide with both protective and curative actions. It is used in cultivation of fruit and strawberries.



1.1 Physico-chemical properties

Physico-chemical properties of *pyrimethanil* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *pyrimethanil*.

		Reference
CAS-No.	53112-28-0	1
Empirical formula	C ₁₂ H ₁₃ N ₃	1
Molecular weight [g/mol]	199.3	1
Solubility in water [mg/kg]	0.21 at 25°C and pH 6.1	1
pKa	3.5	1
Vapour pressure [Pa]	1.1 × 10 ⁻³ at 20°C	1
Log P _{ow}	2.8 at 25°C	1
Henry's law constant [Pa×m ³ /mol]	3.6 × 10 ⁻³	1

1.2 Toxicity to aquatic organisms

The toxicity of *pyrimethanil* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *pyrimethanil*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	96h, static	EC ₅₀ 5.8 NOEC 1.0	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	LC ₅₀ 2.9 ¹⁾	1
<i>Daphnia magna</i>	immobility	21d, semi-static	NOEC 0.97	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 10.6	1
<i>Cyprinus carpio</i>	mortality	96h, static	LC ₅₀ 19.8	1
<i>Onchorhynchus mykiss</i>	Fry weight	21d, flow-through	NOEC 1.6	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Daphnia magna*, with an EC₅₀ of 2.9 mg/L and NOEC of 0.97 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 2.9 mg/L is divided by a factor of 100, which results in a PNEC of 0.029 mg/L.

1.3 Bioaccumulation and persistence

Pyrimethanil is not expected to be highly bioaccumulative. Log P_{ow} is 2.79, however no bioaccumulation studies are available. *Pyrimethanil* is stable towards hydrolysis at environmental pH (7-9). Photochemical transformation in water may be rapid. Two water/sediment studies have been carried out. *Pyrimethanil* decreased with in a DT₅₀ of 40-121 days resulting in one major (>10%) metabolite; ZK 512723. However the dissipation was partly due to the formation of unextractable residues in the sediment.

1.4 Proposed water quality objective

Since PNEC is 0.029 mg/L, the proposed water quality standard for *pyrimethanil* is 0.03 mg/L.

1.5 Comments

Pyrimethanil is not expected to reach surface and ground waters due to transport through the soil profile. Toxicity of the metabolite should be examined when data are available.

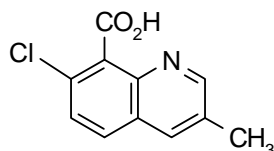
Pyrimethanil is rapidly partitioned into the sediment; therefore a complementary quality objective for sediment is recommended.

1.6 Literature

- (1) *Evaluation on: Pyrimethanil*. Food and environment protection act, 1985, PART III. Issue no 85. Ministry of Agriculture, Fisheries and Food, Pesticides Safety Directorate. York, Great Brittan.

1. Quinmerac

Quinmerac is a systemic herbicide, intended for weed control in beets.



1.1 Physico-chemical properties

Physico-chemical properties of *quinmerac* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *quinmerac*.

		Reference
CAS-No.	90717-03-6	2
Empirical formula	C ₁₁ H ₈ ClNO ₂	2
Molecular weight [g/mol]	221.6	2
Solubility in water [mg/kg]	223	2
pKa	4.31	2
Vapour pressure [Pa]	< 1 × 10 ⁻⁵	2
Log P _{ow}	-0.38 at pH 5, 20 °C -1.1 at pH 7, 20 °C -1.15 at pH 9, 20 °C	2
Henry's law constant [Pa×m ³ /mol]	< 9.9 × 10 ⁻⁶	2

1.2 Toxicity to aquatic organisms

The toxicity of *quinmerac* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *quinmerac*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Chlorella fusca</i>	biomass	96 h, static	E _b C ₅₀ 48.5 NOEC 20	1, 2
<i>Selenastrum capricornutum</i>		72 h, static	EC ₅₀ 255 EC ₁₀ 82	2
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 148.7	2, 3
<i>Daphnia magna</i>	reproduction	21 d, semi-static	NOEC < 1.95 NOEC 1 ¹⁾	2 1
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 87	2, 3
<i>Cyprinus carpio</i>	mortality	96 h, static	LC ₅₀ >100	2, 3
<i>Oncorhynchus mykiss</i>	sublethal effects	28 d, flow-through	NOEC 3.16	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 95-99%

The most sensitive of the tested species was *Daphnia magna*, with a reproduction NOEC of 1 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *quinmerac* is calculated to 0.1 mg/L.

1.3 Bioaccumulation and persistence

Quinmerac is not expected to bioaccumulate since $\log P_{ow}$ is very low. *Quinmerac* is hydrolytically stable and seems to persist to biotic degradation in water (2).

1.4 Proposed water quality objective

Since PNEC is 0.1 mg/L, the proposed water quality standard for *quinmerac* is 0.1 mg/L.

1.5 Comments

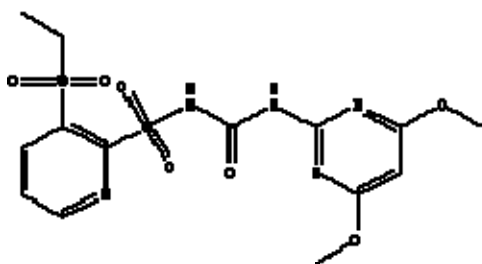
Quinmerac has a high potential to leach through the soil profile and reach surface- and groundwater (2).

1.6 Literature

- (1) Cardinaals, J.H., Geuijen, W.H.C., Gubbels, I., Pluilmens, M.H.M., & Willems, H., 1998. *Quinmerac -summary of environmental fate, parts G and H*. National Institute of Public Health and Environmental Protection (RIVM). Holland.
- (2) Lindbäck, U., (1994). *Ecotoxicological evaluation of quinmerac*. National Chemicals Inspectorate, Sweden.
- (3) Otermann, K., & Linders, J., 1991. *Quinmerac*. Toxicology advisory center, National Institute of Public Health and Environmental Protection (RIVM). Holland.

1. Rimsulfuron

Rimsulfuron is a selective herbicidal belonging to the class of sulfonylureas. The uptake occurs through leaves and inhibits the enzyme acetolactate synthase (ALS). The herbicide is intended for use in potatoes and corn. *Rimsulfuron* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *rimsulfuron* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *rimsulfuron*.

		Reference
CAS-No.	122931-48-0	1
Empirical formula	C ₁₄ H ₁₇ N ₅ O ₇ S ₂	1
Molecular weight [g/mol]	431.45	1
Solubility in water [mg/kg]	0.135 at pH 5 7.3 at pH 7 5.56 at pH 9	1
pKa	4.0	1
Vapour pressure [Pa]	8.9 × 10 ⁻⁹	1
Log P _{ow}	0.288 at pH 5	1
Henry's law constant [Pa×m ³ /mol]	4.6 × 10 ⁻⁶	1

1.2 Toxicity to aquatic organisms

The toxicity of *rimsulfuron* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *rimsulfuron*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Anabaena flos-aqua</i>	growth	96h, static	EC ₅₀ 5.2 NOEC 0.45	1
<i>Selenastrum capricornutum</i>	biomass	72h, static	EC ₅₀ 1.2 NOEC 0.63	1
Aquatic plants				
<i>Lemna gibba</i>	fronds	14d, static	EC ₅₀ 0.027 NOEC 0.00012 ¹⁾	1
	biomass	14d	EC ₅₀ 0.02	

			NOEC 0.00093	
<i>Lemna minor</i>	fronds	14d, semistatic	EC ₅₀ 0.0046 NOEC 0.001	1
<i>Lemna gibba</i>	biomass	14d, static	EC ₅₀ 0.012	2
Crustaceans				
<i>Daphnia magna</i>	growth reproduction	21d, semistatic	NOEC 1 NOEC 1	1
<i>Daphnia magna</i>	immobility	48h, static	LC ₅₀ 1000	2
<i>America mysis bahia</i>	mortality	96h, flow-through	LC ₅₀ >110	2
Mollusc				
<i>Crassostrea virginica</i>	immobility	96h, flow-through	EC ₅₀ >120	2
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ >390	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >390	1
<i>Onchorhynchus mykiss</i>	growth behaviour	21d, flow-through	NOEC 125 NOEC 1000	1
<i>Onchorhynchus mykiss</i> (Early life stage)	hatch rate growth behaviour	90d	NOEC 250 NOEC 125 NOEC 250	1
<i>Cyprinodon variegatus</i>	mortality	96h, flow-through	LC ₅₀ >110	2
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >180	2
<i>Onchorhynchus mykiss</i>	mortality	96h, static-renewal	LC ₅₀ >110	2
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >180	2

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98.8%

The most sensitive of the tested species in short-term was *Lemna minor* with an EC₅₀-value of 0.0046 mg/L. The lowest toxicity value generated from the target organism group is a NOEC of *Lemna gibba*, of 0.00012 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *rimsulfuron* is calculated to 1.2×10^{-5} mg/L.

1.3 Bioaccumulation and persistence

Rimsulfuron is not expected to bioaccumulate in the aquatic environment, log P_{ow} is 0.288 at pH 5 and -1.46 at pH 7. The substance dissociated in water (pK_a 4.0). Hydrolysis is an important degradation pathway and contributes to a rapid transformation of the parent compound in water. Contraction of the sulfonylurea bridge leads to the formation of IN-70941 and further to IN-70942 as the major metabolites in water. In water/sediment studies *rimsulfuron* degrades rapidly in water and sediment, DT₅₀ 1-7 days in water phase and 7-12 days in sediment. *Rimsulfuron* is not expected to participate to the sediment.

1.4 Proposed water quality objective

Since PNEC is 1.2×10^{-5} mg/L, the proposed water quality standard for *rimsulfuron* is 1.0×10^{-5} mg/L.

1.5 Comments

Volatilisation is not expected. In soil the DT₅₀-values for *rimsulfuron* are with in a range of 21-40 days at 20°. The temperature shows big influence on the degradation rates. In lower temperatures the time of degradation increases. However in European field studies *rimsulfuron* was primary degraded with DT₅₀ ranging from 6-14 days. Metabolites, exceeding 10%, in soil are *IN-70941*, *IN-70942* and *IN-E9620*. *Rimsulfuron* and two of its metabolites show mobility in soil.

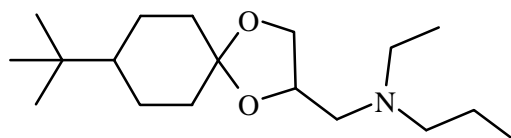
Results of the submitted studies indicate that compared to *rimsulfuron* the acute toxicity of both metabolites is not increasing.

1.6 Literature

- (1) European Commission Peer Review Programme. *Rimsulfuron Monograph*, 2003. Rapporteur Member State: Germany.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Spiroxamine

Spiroxamine is a systemic fungicide with apoplastic translocation in plants. It inhibits the biosynthesis of fungal sterols. The fungicide consists of two diastereomers. *Spiroxamine* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *spiroxamine* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *spiroxamine*.

	Diastereomer A	Diastereomer B	Reference
CAS-No.	1181134-30-8	1181134-30-8	1
Empirical formula	C ₁₈ H ₃₅ NO ₂	C ₁₈ H ₃₅ NO ₂	1
Molecular weight [g/mol]	297.5	297.5	1
Solubility in water [mg/kg]	470 at pH 7, 20°C 14 at pH 9, 20°C	340 at pH 7, 20°C 10 at pH 9, 20°C	1
pK _b	6.9	6.9	1
Vapour pressure [Pa]	3.0×10 ⁻³ -4.0×10 ⁻³ Pa	5.5 × 10 ⁻³ - 5.7×10 ⁻³ Pa	1
Log P _{ow}	1.28 at pH 5, 20°C 2.79 at pH 7 4.88 at pH 9	1.41 at pH 5, 20°C 2.98 at pH 7 5.08 at pH 9	1
Henry's law constant [Pa×m ³ /mol]	2.5×10 ⁻³	5.0×10 ⁻³	1

1.2 Toxicity to aquatic organisms

The toxicity of *spiroxamine* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *spiroxamine*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass	72h	EC ₅₀ 0.003 NOEC 0.0012	1
<i>Selenastrum capricornutum</i>	biomass	72h	EC ₅₀ 0.005 NOEC 0.0003 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>		48h	EC ₅₀ 6.1	1
<i>Daphnia magna</i>	reproduction	21d	NOEC 0.1	1
Fish				
<i>Lepomis macrochirus</i>		96h	LC ₅₀ 7.13	1

<i>Onchorhynchus mykiss</i>		96h	LC ₅₀ 18.5	1
<i>Onchorhynchus mykiss</i>	growth flow through	93d	NOEC 0.014	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity unknown.

The most sensitive of the tested species was *Selenastrum capricornutum*, with a NOEC of 0.0003 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *spiroxamine* is calculated to 0.00003 mg/L.

1.3 **Bioaccumulation and persistence**

Spiroxamine is not expected to bioaccumulate. Although a quick uptake, after conversion to non-contaminated water *spiroxamine* is almost completely excreted after 14 days.

Spiroxamine does not transform in water. In water/sediment studies the fungicide rapidly bind to sediment. Hence the concentration in water decreases, whilst it increases in sediment.

1.4 **Proposed water quality objective**

Since PNEC is 0.00003 mg/L, the proposed water quality standard for *spiroxamine* is 3×10^{-5} mg/L.

1.5 **Comments**

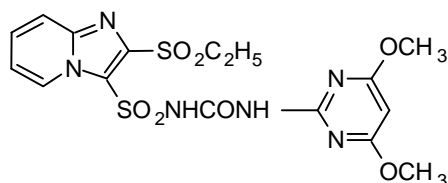
The substance is not mobile in soil, K_{oc} 659-6417. The rate of primary degradation varies in soil within DT₅₀ 35-64 days. The substance show tendency to volatilise. In water-sediment systems the active substance is strongly bound to the sediment; therefore a quality objective for sediment may be relevant.

1.6 **Litterature**

- (1) European Commission Peer Review Programme. *Spiroxamine Monograph*, 1997
Rapporteur Member State: Germany.

1. Sulfosulfuron

Sulfosulfuron is a member of the sulphonyl urea family of herbicides. It acts by inhibition of acetolactate synthase in aliphatic amino acid pathway. The herbicide is intended for use in cereals. *Sulfosulfuron* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *sulfosulfuron* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *sulfosulfuron*.

		Reference
CAS-No.	141776-32-1	1
Empirical formula	C ₁₆ H ₁₈ N ₆ O ₇ S ₂	1
Molecular weight [g/mol]	470.49	1
Solubility in water [mg/kg]	17.6 at 20°, pH 5 1627 at pH 7 482 at pH 9	1
pKa	3.51	1
Vapour pressure [Pa]	3.05×10 ⁻⁸	1
Log P _{ow}	0.73 at pH 5 -0.77 at pH 7 -1.44 at pH 9	1
Henry's law constant [Pa×m ³ /mol]	8.15×10 ⁻⁷ at pH 5 8.83×10 ⁻⁹ at pH 7 2.97×10 ⁻⁸ at pH 9	1

1.2 Toxicity to aquatic organisms

The toxicity of *sulfosulfuron* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *sulfosulfuron*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth	72h	EC ₅₀ 0.67 NOEC 0.094	1
<i>Scenedesmus subspicatus</i>	biomass	72h	EC ₅₀ 3.1 NOEC 0.31	1
Aquatic plants				
<i>Lemna gibba</i>	frond number	14d, static	EC ₅₀ >0.001 NOEC 0.0005 ¹⁾	1

Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ >96	1
<i>Daphnia magna</i>	immobility reproduction	21d, static-renewal	EC ₅₀ > 102 NOEC 102	1
<i>Americamykiss bahia</i>	mortality	96h, static	LC ₅₀ >106	2
Molluscs				
<i>Crassostrea virginica</i>	mortality	96h, static	LC ₅₀ >116	2
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >95	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ >96	1
<i>Cyprinus carpio</i>	mortality	96h, static	LC ₅₀ >91	1
<i>Cyprinodon variegates</i>	mortality	96h, static	LC ₅₀ >101	2
<i>Onchorhynchus mykiss</i>	hatching growth	86d, flow-through	NOEC 100 NOEC 100	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98.5%

Former water quality objective calculation

The most sensitive of the tested species was *Lemna gibba*, with a NOEC of 0.0005 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *sulfosulfuron* is calculated to 0.00005 mg/L.

Revised EQS calculation according to EU-harmonised methodology (3)

The PNEC of 0.00005 mg/L is still valid. In a new study in which other monocotyledonous and dicotyledonous species were exposed to *sulfosulfuron* under more realistic conditions (4) nominal NOECs were in the same order of magnitude as the laboratory test with *Lemna gibba*, the exposure concentrations, however, decreased during the study (27-36 % of initial concentrations at 14 d and 19-21 % at day 21) and a new PNEC cannot be calculated based on the given information.

1.3 Bioaccumulation and persistence

Sulfosulfuron is not expected to bioaccumulate. In water the substance degrades mainly by photolysis or hydrolysis depending on pH. Aqueous photolysis occurs with DT₅₀ values for *sulfosulfuron* of 2.4 and 21.7 days at the water surface, for summer and winter respectively. The hydrolytic half-life varies from 7-159 days depending on pH. Hydrolysis of *sulfosulfuron* is most rapid at acidic pH values. In sediment/water systems, *sulfosulfuron* dissipates from the water with a DT₅₀ of 16 - 20 days and from the whole system with DT₅₀ of 20 - 32 days. *Sulfosulfuron* is transformed into the metabolite *desmethyl sulfosulfuron*.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.00005 mg/L, the proposed EQS/water quality objective for *sulfosulfuron* is 5 × 10⁻⁵ mg/L.

1.5 **Comments**

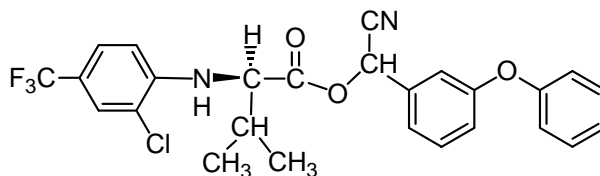
Sulfosulfuron is moderately persistent in soil with DT₅₀ values ranging from 33-176 days. Both *sulphonamide* and *aminopyrimidine* are persistent metabolites. Although toxicity was not studied specifically for these metabolites, they are both formed by cleavage and therefore likely to be less toxic than the parent chemical. The metabolite *desmethyl sulfuron* is also formed in soil. *Sulfosulfuron* may leach to groundwater. It is essentially non-volatile.

1.6 **Literature**

- (1) European Commission Peer Review Programme. *Sulfosulfuron Monograph, 1998*. Rapporteur Member State: Ireland.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.
- (4) Davies, J., Honegger, J., Tencalla, F., Meregalli, G., Brain, P., Newman, J. and Pitchford, H. (2003). *Herbicide risk assessment for non-target aquatic plants: sulfusulfuron – a case study*. *Pest Manag Sci* 59:231-237.

1. Tau-fluvalinate

Tau-fluvalinate belongs to the group of pyrethroids. It is a foliar applied insecticide used in cultivation of cereals, legumes and oiliferous crops.



1.1 Physico-chemical properties

Physico-chemical properties of *tau-fluvalinate* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *tau-fluvalinate*.

		Reference
CAS-No.	102851-06-9	4
Empirical formula	C ₂₆ H ₂₂ ClF ₃ N ₂ O ₃	4
Molecular weight [g/mol]	502.9	4
Solubility in water [mg/kg]	0.001 at pH 7 and 20°C	4
Vapour pressure [Pa]	9 × 10 ⁻¹¹ at 20°C	4
Log P _{ow}	4.26	4
Henry's law constant [Pa×m ³ /mol]	4.04 × 10 ⁻⁵	4

1.2 Toxicity to aquatic organisms

The toxicity of *tau-fluvalinate* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *tau-fluvalinate*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass		E _b C ₅₀ 180-320 NOEC 180	5
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.001	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.074	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.077 ¹⁾	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.00085	2
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.001	2
<i>Mysidopsis bahia</i>	mortality	48h, static	LC ₅₀ 0.000018 ²⁾	2
<i>Daphnia magna</i>	reproduction	21d, flow-through	NOEC 0.000037	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.0026	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.00089	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.0029	1

<i>Cyprinus carpio</i>	mortality	96h, static	LC ₅₀ 0.004	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.000504 ¹⁾	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.0088	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.0027	2
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.0062	2
<i>Pimephales promelas</i>	length	30d, flow-through	NOEC 0.000064	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 93.1%

The most sensitive (acute effects) of the tested species was *Mysidopsis bahia*, with a LC₅₀ of 0.000018 mg/L and. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest LC₅₀ 0.000018 mg/L of *tau-fluvalinate* mg/L is divided by a factor of 100, which results in a PNEC of 0.00000018 mg/L.

1.3 Bioaccumulation and persistence

Tau-fluvalinate has potential for bioaccumulation. Log P_{ow} 4.26 indicates risk for bioaccumulation, which is confirmed by studies, BCF is 240 in whole fish, *Lepomis macrochirus*. *Tau-fluvalinate* is rapidly hydrolysed in water with high pH; DT₅₀ 1-2 days at pH 9 and >30 days in pH 3-6. Studied in mesocosms, pH not specified, the substance rapidly dissipates from the water phase into the sediment. DT₅₀ in water phase is estimated to 0.5 days. Although the substance is partitioned into the sediment it is rapidly degraded, DT₅₀ 3-14 days. Therefore *tau-fluvalinate* is not considered to be persistent in aquatic systems (3).

1.4 Proposed water quality objective

Since PNEC is 1.8×10^{-7} mg/L, the proposed water quality standard for *tau-fluvalinate* is 2×10^{-7} mg/L.

1.5 Comments

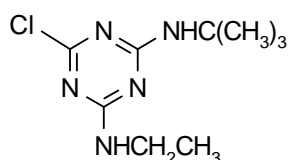
Tau-fluvalinate has low potential for transport through the soil profile and is therefore not expected to leach to ground and surface water.

1.6 Literature

- (1) Otermann K., Linders J., 1991. *Tau-fluvalinate*, Adviesrapport 90/670104/001, RIVM. The Netherlands.
- (2) COWIconsult, 1991. *Økotoksikologisk vurdering af fluvalinat*. Miljøstyrelsen. Norge.
- (3) Lefebvre, 1999. *Tau-fluvalinate (SAN 527) Formulated as MAVRIK 2F (A-10085A). Environmental safety risk assessment for the aquatic environment from higher tier studies*. Risk assessment. CP 6.43, version 2.
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (5) Lindkvist L., 1999. *PM MARVIK 2F*. Kemikalieinspektionen. Sverige.

1. Terbutylazine

Terbutylazine is an herbicide mainly taken up by the roots. The substance is no longer in use in Sweden. The intended use was weed control in cereals.



1.1 Physico-chemical properties

Physico-chemical properties of *terbutylazine* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *terbutylazine*.

		Reference
CAS-No.	227-637-9	4
Empirical formula	C ₉ H ₁₆ ClN ₅	4
Molecular weight [g/mol]	229.7	4
Solubility in water [mg/kg]	8.5 at pH 7 and 20 °C	4
pKa	2.0	4
Vapour pressure [Pa]	1.5 × 10 ⁻⁴	4
Log P _{ow}	3.2	4
Henry's law constant [Pa×m ³ /mol]	4.1 × 10 ⁻³	4

1.2 Toxicity to aquatic organisms

The toxicity of *terbutylazine* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *terbutylazine*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scenedesmus subspicatus</i>	biomass	72 h, static	E _b C ₅₀ 0.016 NOE _b C 0.0033	2
<i>Microcystis aeruginosa</i>	biomass	96 h, static	E _b C ₅₀ 0.019 NOE _b C 0.011	2
<i>Chlorella pyrenoidosa</i>	growth inhibition	24 h, static	EC ₅₀ 0.02	1
<i>Chlorococcum sp.</i>	photosynthesis inhib.	24 h, static	EC ₅₀ 0.09	
<i>Anabaena variabilis</i>	growth inhibition	24 h, static	EC ₅₀ 0.67	
<i>Lyngbya sp.</i>	photosynthesis inhib.	24 h, static	EC ₅₀ 0.09	
<i>Anabaena variabilis</i>	growth inhibition	48 h, static	EC ₅₀ 1	
<i>Lyngbya sp.</i>	photosynthesis inhib.	24 h, static	EC ₅₀ 0.08	
<i>Lyngbya sp.</i>	growth inhibition	24 h, static	EC ₅₀ <0.02	
<i>Lyngbya sp.</i>	photosynthesis inhib.	24 h, static	EC ₅₀ <0.02	
Higher aquatic plants				

<i>Lemna gibba</i>		14 d, static	EC ₅₀ 0.016 NOEC 0.002 ¹⁾	3
<i>Lemna gibba</i>	frond germination	14 d, static	EC ₅₀ 0.019 EC ₁₀ 0.0027	2
Crustaceans				
<i>Daphnia magna</i>	immobilisation	96 h, static	EC ₅₀ 50.9	3
<i>Mysidopsis bahia</i>		96 h, static	EC ₅₀ 0.109	3
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 21	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 7.5	3
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 3.4	3
<i>Oncorhynchus mykiss</i> <i>Cyprinus carpio</i> <i>Ictalurus punctatus</i> <i>Lepomis macrochirus</i> <i>Poecilia reticulata</i>	mortality	96 h, static	LC ₅₀ 4.6 LC ₅₀ 66 LC ₅₀ ≈ 7 LC ₅₀ 52 LC ₅₀ 1.6	1
<i>Lepomis macrochirus</i> <i>Pimephales promelas</i> <i>Ictalurus punctatus</i> <i>Salvelinus fontinalis</i> <i>Notemigonus crysoleucas</i>	mortality	96 h, flow-through	LC ₅₀ 1.8 LC ₅₀ 0.8 LC ₅₀ 1.2 LC ₅₀ 1.2 LC ₅₀ 3.5	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97.1%.

The most sensitive of the tested species is *Lemna gibba*, with an EC₅₀ of 0.016 mg/L and a NOEC of 0.0021 mg/L. Chronic toxicity data origin from the trophic levels primary consumers, algae and higher aquatic plants. In the absence of chronic toxicity data for crustacean and fish, PNEC is based on NOEC 0.0021 mg/L and divided by a factor of 100, which results in a chronic PNEC of 0.000021 mg/L.

1.3 Bioaccumulation and persistence

Terbuthylazine is not expected to bioaccumulate. BCF is 34 in *Lepomis macrochirus*, whole fish. Hydrolysis and photolysis occurs slowly. Time for degradation is very long.

1.4 Proposed water quality objective

Since PNEC is 0.000021 mg/L, the proposed water quality standard for *terbuthylazine* is 2×10^{-5} mg/L.

1.5 Comments

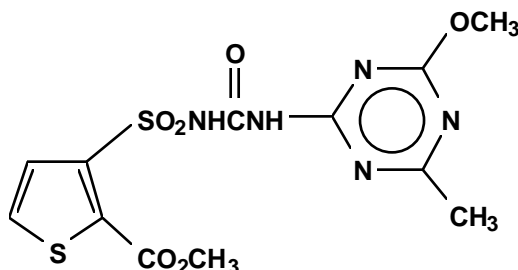
Mobility through soil is expected to be high (K_{oc} 60-200). *Terbuthylazine* has several metabolites but none of them are more toxic than *terbuthylazine*.

1.6 Literature

- (1) Fischer, S., (1988). *Ekotoxikologisk utvärdering av terbutylazin*. National Chemicals Inspectorate, Sweden.
- (2) Hanze, K., (1995). *Ecotoxicological evaluation of the herbicide Terbuthylazine – Supplement to Ecotoxicological Evaluation in 1988*. National Chemicals Inspectorate, Sweden.
- (3) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Thifensulfuron methyl

Thifensulfuron methyl is a sulfonylurea selective herbicide intended for use in cereals. The herbicide primarily acts through foliar uptake, inhibiting the acetolactate synthetase (ALS). *Thifensulfuron methyl* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *thifensulfuron methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *thifensulfuron methyl*.

		Reference
CAS-No.	79277-27-3 Methylester	1
Empirical formula	C ₁₁ H ₁₁ N ₅ O ₆ S ₂ (C ₁₂ H ₁₃ N ₅ O ₆ S ₂)	1
Molecular weight [g/mol]	387.4	1
Solubility in water [mg/kg]	223 at pH 5, 25 °C 2240 at pH 7 8830 at pH 9	1
pKa	4.0	1
Vapour pressure [Pa]	7.5×10 ⁻⁹ at 20 °C 1.7×10 ⁻⁸ at 25 °C	1
Log P _{ow}	1.06 at pH 5, 25 C 1.7 at pH 7 2.1 at pH 9	1
Henry's law constant [Pa×m ³ /mol]	1.3×10 ⁻¹²	1

1.2 Toxicity to aquatic organisms

The toxicity of *thifensulfuron methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *thifensulfuron methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	24-48 h	E _r C ₅₀ 0.017	1
<i>Navicula pelliculosa</i>	growth rate	48h	E _r C ₅₀ 0.0159	1
<i>Anabaena Flos-aquae</i>		72h	EC ₅₀ 0.84	1

Aquatic plants				
<i>Lemna gibba</i>		14d	EC ₅₀ 0.0013 ¹⁾ NOEC 0.0005 ²⁾	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h	EC ₅₀ 470	1
<i>Daphnia magna</i>	growth	21d	NOEC 100	1
<i>Daphnia magna</i>	immobility	48h	EC ₅₀ >1	2
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96h	LC ₅₀ > 100	1
<i>Bluegill sunfish</i>	mortality	96h	LC ₅₀ > 100	1
<i>Lepomis macrochirus Bluegill</i>	mortality	96h	LC ₅₀ > 10	2
<i>Oncorhynchus mykiss</i>	mortality	96h	LC ₅₀ > 10	2
<i>Oncorhynchus mykiss</i>	growth	21d	NOEC>250	1

¹⁾ Effect concentration basis for calculation of former PNEC. Test substance purity 95.4%.

²⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0013 mg/L and NOEC of 0.0005mg/L. Since the acute/chronic ratio is low, a PNEC based on long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.0013 mg/L is divided by a factor of 100, which results in a PNEC of 0.000013 mg/L.

Revised EQS calculation according to EU-harmonised methodology (4)

There is chronic data available for three trophic levels. The most sensitive of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0013 mg/L and NOEC of 0.0005mg/L. Dividing the lowest NOEC of 0.0005 mg/L by an assessment factor of 10, results in a PNEC of 0.00005 mg/L.

1.3 Bioaccumulation and persistence

Thifensulfuron methyl is not expected to bioaccumulate. In water the primary degradation occurs rapidly mainly by photolysis, DT₅₀ 97-125h. In water/sediment studies the herbicide mainly remains in the water phase. DT₅₀ for primary degradation is 2-2.3 weeks. In water the following metabolites are formed: *thifensulfuron acid* and *2-acid-3-sulfonamide*.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.00005 mg/L the proposed EQS/water quality objective for *thifensulfuron methyl* is 0.00005 mg/L.

1.5 Comments

Thifensulfuron methyl is not volatile. Low K_{oc}-value and high water solubility indicate mobility in soil allowing the substance to leach through the soil profile. *Thifensulfuron methyl*

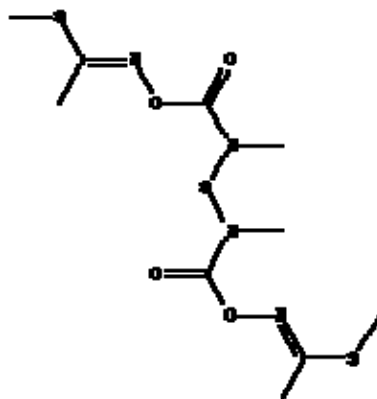
is degraded rapidly in soil into metabolites. Neither of the studied metabolites; *thifensulfuron acid*, IN-L225, *2-acid-3-sulfonamid*, IN-L223/1, *O.desmethyl thifen. acid*, IN-JZ789, and *triazine acid*, IN-V7160, show high toxicity towards aquatic organisms.

1.6 Literature

- (1) European Commission Peer Review Programme. *Thifensulfuron Monograph, 1996*. Rapporteur Member State: France, addendum included.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Jenny Kreuger et al., 2003. Bekämpningsmedel i vatten från typområden, åar och I nederbörd under 2002. Årsrapport till det nationella programmet för miljöövervakning av jordbruksmark, delprogram pesticider. Sveriges lantbruksuniversitet, Avdelningen för vattenvårdslära, Uppsala.
- (4) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Thiodicarb

Thiodicarb is an insecticide and molluscicide. It acts primarily as an ingestion or stomach toxicant with some complementary contact activity. The substance is in Sweden used against snails in cultivation of oleiferous plants and cereals. *Thiodicarb* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *thiodicarb* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *thiodicarb*.

		Reference
CAS-No.	59669-26-0	1
Empirical formula	C ₁₀ H ₁₈ N ₄ O ₄ S ₃	1
Molecular weight [g/mol]	354.5	1
Solubility in water [mg/kg]	0.022 at 25°C	1
pKa	not relevant	1
Vapour pressure [Pa]	2.7 × 10 ⁻³ at 25°C	1
Log P _{ow}	1.62	1
Henry's law constant [Pa×m ³ /mol]	4.3 × 10 ⁻² at 25°C	1

1.2 Toxicity to aquatic organisms

The toxicity of *thiodicarb* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *thiodicarb*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	96h, static	E _r C ₅₀ 120 NOEC 3.2	1
<i>Selenastrum capricornutum</i>		96h, static	E _r C ₅₀ 94.5 NOEC 1.6	2
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, flow-through	EC ₅₀ 0.027	1
<i>Mydopsis bahia</i>	mortality	96h, flow-through	LC ₅₀ 0.026 ²⁾	2
<i>Mydopsis bahia</i>	mortality	96h, flow-through	LC ₅₀ 0.029	2
<i>Mydopsis bahia</i>	mortality	96h, flow-through	LC ₅₀ 0.075	2
<i>Crassostrea virginica</i>	mortality	96h, flow-through	LC ₅₀ 1	1
<i>Crassostrea virginica</i>	mortality	96h, flow-through	LC ₅₀ 0.45 ¹⁾	2
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.009	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 1.4	1
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 1.5	2
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 2.7	2
<i>Salvelinus fontinalis</i>	mortality	96h, static	LC ₅₀ 4.45	2
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 3.3	2
<i>Cyprinodon variegatus</i>	mortality	96h, flow-through	LC ₅₀ 0.53	2
<i>Pimephales promelas (early life stage)</i>	growth	35d, flow-through	NOEC 0.025	1

¹⁾ Test performed on substance with purity <90%. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 94.5%

The most sensitive (acute effects) of the tested species was *Mydopsis bahia*, with a LC₅₀ of 0.026 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.026 mg/L is divided by a factor of 100, which results in a PNEC of 0.00026 mg/L.

The toxicity of *methomyl* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *methomyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	72h, static	EC ₅₀ 94	1
<i>Scendesmus subspicatus</i>	growth rate	72h, static	EC ₅₀ 100	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.017	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.0016 ¹⁾	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, semi-static	EC ₅₀ 0.62	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 99%

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.0016 mg/L. Short term studies are available from three trophic levels. However chronic toxicity has only been tested for crustaceans. An assessment factor of 100 is therefore used for calculation of

the predicted no effect concentration. Hence, the PNEC for the metabolite *methomyl* is calculated to 0.000016 mg/L.

1.3 Bioaccumulation and persistence

Thiodicarb is not expected to bioaccumulate. The log P_{ow} is low, 1.62, and therefore no fish bioaccumulation study has been carried out. *Thiodicarb* hydrolyses at environmentally relevant pH to one major metabolite (>10%); *methomyl*, which is stable to further hydrolysis. *Thiodicarb* is hydrolysed within a DT_{50} of 30.8 days. In water/sediment systems, *thiodicarb* is degraded with a half-life of less than 1 hour. The DT_{50} for *methomyl* was calculated as 21 and 29 hours in the two systems. Distribution between water and sediment has not been reported due to rapid degradation.

1.4 Proposed water quality objective

Thiodicarb

Since PNEC is 0.00026 mg/L, the proposed water quality standard for *thiodicarb* is 0.0003 mg/L.

Methomyl

Since PNEC is 0.000016 mg/L, the proposed water quality standard for *methomyl* is 0.00002 mg/L.

1.5 Comments

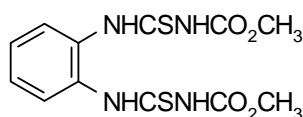
Both *thiodicarb* and its metabolite *methomyl* are expected to be mobile in soil. However due to rapid degradation the risk for leaching through the soil profile to surface- and ground waters is considered to be low.

1.6 Literature

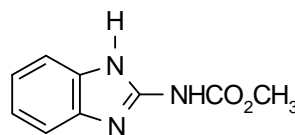
- (1) European Commission Peer Review Programme. *Thiodicarb Monograph*, 2003. Rapporteur Member State: United Kingdom.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Thiophanate-methyl and carbendazim

Thiophanate-methyl is a benzimidazole precursor. Intended use is to control fungus in fruit cultivation and cereals. The metabolite *carbendazim* formed in the plant is the actual toxicant, a systemic fungicide. *Thiophanate-methyl* is under evaluation within the framework of EU Dir. 91/414. *Carbendazim* is no longer in use in Sweden, banned 1998. *Carbendazim* is under evaluation within the framework of EU Dir. 91/414.



Thiophanate-methyl



Carbendazim

1.1 Physico-chemical properties

Physico-chemical properties of *thiophanate-methyl* are summarised in table 1.1.

Table 1.1.1: Physico-chemical properties of *thiophanate-methyl*.

		Reference
CAS-No.	23564-05-8	1
Empirical formula	C ₁₂ H ₁₄ N ₄ O ₄ S ₂	1
Molecular weight [g/mol]	342.4	1
Solubility in water [mg/kg]	20 at pH 4-7.5, 20 °C	1
pKa	7.28	1
Vapour pressure [Pa]	9.5 × 10 ⁻⁶	1
Log P _{ow}	1.5	1
Henry's law constant [Pa×m ³ /mol]	8.1 × 10 ⁻⁵	1

Table 1.1.2: Physico-chemical properties of *carbendazim*.

		Reference
CAS-No.	10605-21-7	1
Empirical formula	C ₉ H ₉ N ₃ O ₂	1
Molecular weight [g/mol]	191.2	1
Solubility in water [mg/kg]	29 at pH 4 8 at pH 7 7 at pH 8, 24 °C	1
pKa	4.2	1
Vapour pressure [Pa]	9 × 10 ⁻⁵ at 20 °C 1.3 × 10 ⁻³ at 20 °C	1
Log P _{ow}	1.38 at pH 5 1.51 at pH 7 1.49 at pH 9	1
Henry's law constant [Pa×m ³ /mol]	3.6 × 10 ⁻³	1

1.2 Toxicity to aquatic organisms

The toxicity of *tiophanate-methyl* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *tiophanate-methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Chlorella vulgaris</i>	biomass growth rate	96 h, static	E _b C ₅₀ 1.0 E _r C ₅₀ 1.8 NOEC 0.25	1
Higher aquatic plants				
<i>Lemna gibba</i>		14 d, static	EC ₅₀ >4.7 NOEC 4.7	2
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48 h, flow-through	EC ₅₀ 5.4	1, 2
<i>Daphnia carinata</i>		48 h, static	EC ₅₀ 12.7	1
<i>Daphnia magna</i>	reproduction	21 d, semi-static	NOEC 0.18 ¹⁾	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96 h, static	LC ₅₀ 58	2
<i>Cyprinodon variegatus</i>	mortality	96 h, flow-through	LC ₅₀ 17	2
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ >41	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, flow-through	LC ₅₀ 11.0	1
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 1.0	1
<i>Oncorhynchus mykiss</i>	mortality	28 d, flow-through	NOEC 0.32	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97.6%

The most sensitive (acute effects) of the tested species was *Onchorhynchus mykiss*, with a LC₅₀ of 1.0 mg/L. The most sensitive species towards chronic toxicity was *Daphnia magna* with a NOEC of 0.18 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest LC₅₀ of 1.0 mg/L is divided by a factor of 100, which results in a PNEC of 0.01 mg/L.

The toxicity of *tiophanate-methyl* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *carbendazim*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>		72 h, static	EC ₅₀ 1.3 NOEC 0.5	3
<i>Selenastrum capricornutum</i>		72 h, static	EC ₅₀ 7.7 NOEC 2.5	3
<i>Scenedesmus subspicatus</i>		72 h, static	EC ₅₀ 420 NOEC 10	3
<i>Chlorella pyrenoidosa</i>		72 h, static	EC ₅₀ 0.34	3
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.35	2,3
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.39	3

<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.15	3
<i>Daphnia magna</i>	immobilisation	48 h, static	EC ₅₀ 0.19	3
<i>Mysidopsis bahia</i>	immobilisation	96 h, static	LC ₅₀ 0.098	2
<i>Daphnia magna</i>		21 d, semi-static	NOEC 0.0015	3
<i>Daphnia magna</i>	reproduction	21 d, semi static	NOEC 0.025	3
<i>Daphnia magna</i>	reproduction	21 d, semi static	NOEC >0.01	3
<i>Daphnia magna</i>		21 d, static-renewal	NOEC 0.0031	2
<i>Daphnia magna</i>	immobility	21 d, static-renewal	NOEC 0.027	3
<i>Mysidopsis bahia</i>		28 d, flow-through	NOEC 0.025	2
Molluscs				
<i>Crassostrea virginica</i>	shell deposition	96 h, flow-through	EC ₅₀ >1.2	2
Fish				
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ 0.019	2
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ 0.010	2
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ 0.012	2
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ 0.0074	2
Geometric mean value				2
<i>Ictalurus punctatus</i>	mortality	96 h, static	LC ₅₀ 0.011 ¹⁾	
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.65	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.37	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.32	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.15	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.83	3
Geometric mean value				3
<i>Oncorhynchus mykiss</i>	mortality	96 h, static	LC ₅₀ 0.39	
<i>Pimephales promelas</i>	mortality	96 h, static	LC ₅₀ >10	2
<i>Lepomis macrochirus</i>	mortality	96 h, flow-through	LC ₅₀ >1.9	2
<i>Oncorhynchus mykiss</i>	mortality	96 h, semi-static	LC ₅₀ 0.98	3
<i>Cyprinus carpio</i>	mortality	96 h, static	LC ₅₀ 0.44	3
<i>Oncorhynchus mykiss</i>	behaviour mortality	21 d, flow-through	NOEC 0.003 NOEC 0.018	3
<i>Oncorhynchus mykiss</i>	survival	79 d, flow-through	NOEC 0.011	3

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 99%

The most sensitive (acute effects) of the tested species was *Ictalurus punctatus*, with an EC₅₀ of 0.011 mg/L (geometric mean value). Since the acute/chronic ratio is low, a PNEC based on the long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest EC₅₀ of 0.011 mg/L is divided by a factor of 100, which results in a PNEC of 0.00011 mg/L.

1.3 Bioaccumulation and persistence

Neither *tiophanate-methyl* nor *carbendazim* are expected to bioaccumulate. Hydrolysis is pH-dependent, in acid environment the substance is stable and very persistent whilst in neutral and alkaline solutions hydrolysis is much faster. The major degradation product is *carbendazim* (1). *Carbendazim* is stable towards hydrolysis (3). In water/sediment systems *carbendazim* degrades with in a DT₅₀ of 6-11 days in water phase and 16-74 days in the whole system.

1.4 Proposed water quality objective

Thiophanat-methyl

Since PNEC is 0.01 mg/L, the proposed water quality standard for *tiophanate-methyl* is 0.01 mg/L.

Carbendazim

Since PNEC is 0.00011 mg/L, the proposed water quality standard for *carbendazim* is 0.0001 mg/L.

1.5 Comments

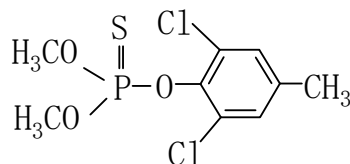
Tiophanate-methyl has a medium to high mobility in soil, but is rapidly degraded (pH dependent process) (1). Since the transformation product *carbendazim* is biological active, a WQO is established for *carbendazim*. The substance is mainly remained in water phase only 0.5% is partitioned into the sediment. No relevant metabolites have been reported.

1.6 Literature

- (1) European Commission Peer Review Programme. *Tiophanate-methyl Monograph*, 1997. Rapporteur Member State: Germany.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) European Commission Peer Review Programme. *Carbendazim Monograph*, 1997. Rapporteur Member State: Germany.

1. Tolclofos-methyl

Tolclofos-methyl inhibits the motility of zoospores of phycomycetous fungi. The fungicide is not systemic in plants. It is intended for use in winter cereals and seed treatment before seeding potatoes. *Tolclofos-methyl* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *tolclofos-methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *tolclofos-methyl*.

		Reference
CAS-No.	57018-04-9	1
Empirical formula	C ₉ H ₁₁ Cl ₂ O ₃ PS	1
Molecular weight [g/mol]	301.12	1
Solubility in water [mg/kg]	0.708 at 20°C	1
pKa	Not applicable	1
Vapour pressure [Pa]	8.77 × 10 ⁻⁴ at 20°C	1
Log P _{ow}	4.56	1
Henry's law constant [Pa×m ³ /mol]	0.37 at 20°C	1

1.2 Toxicity to aquatic organisms

The toxicity of *tolclofos-methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *tolclofos-methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scendesmus subspicatus</i>	growth rate	72h, static	E _r C ₅₀ >1.1 NOEC 0.22	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 48	1
<i>Daphnia magna</i>	growth and reproduction	21d, flow-through	NOEC 0.026	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ >0.72	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 0.69	1
<i>Onchorhynchus mykiss</i>	hatch ability fry survival, growth	97d, flow-through	NOEC 0.012 ¹⁾	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 97.6%

The most sensitive of the tested species was *Onchorhynchus mykiss*, with a NOEC of 0.012 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *tolclofos-methyl* is calculated to 0.0012 mg/L.

1.3 Bioaccumulation and persistence

Tolclofos-methyl is expected to bioaccumulate, due to high Log P_{ow} and BCF 670 (whole fish). *Tolclofos-methyl* is not prone to hydrolysis under environmental conditions. *Tolclofos-methyl* declined relatively rapidly in the water phase with a DT₅₀ of 0.9 to 1.6 days. Much of this decline was due to partitioning to sediment 49 to 73% after 3 to 7 days. Degradation in sediment occurs with a DT₅₀ of 19 - 27 days. The metabolite *DM-TM* was the sole metabolite detected in significant quantities in both water and sediment, occurring at respective maximums of 11 and 13 %. The metabolite degraded at a similar rate in both water and sediment with a DT₅₀ of 27 to 43 days. The metabolite is not toxic towards aquatic organisms.

1.4 Proposed water quality objective

Since PNEC is 0.0012 mg/L, the proposed water quality standard for *tolclofos-methyl* is 0.001 mg/L.

1.5 Comments

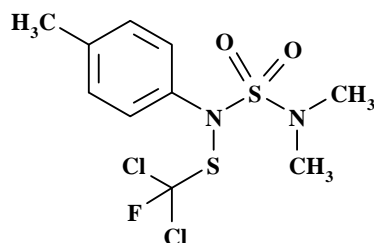
Tolclofos-methyl is solid in soil, however the metabolite is mobile and may leach through the soil profile. Due to the partition into sediment a complementary quality objective is recommended.

1.6 Literature

- (1) European Commission Peer Review Programme. *Tolclofos-methyl Monograph, 2003*. Rapporteur Member State: Sweden.

1. Tolyfluanid and DMST

Tolyfluanid is a multi site inhibitor interfering at many locations in the metabolism of fungi. Intended use in, among other crops, fruit, cabbage, leak, potatoes and beets. *Tolyfluanid* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *tolyfluanid* are summarised in table 1.1.

Table 1.1.1: Physico-chemical properties of *tolyfluanid*.

		Reference
CAS-No.	731-27-1	1
Empirical formula	C ₁₀ H ₁₃ Cl ₂ FN ₂ O ₂ S ₂	1
Molecular weight [g/mol]	347.3	1
Solubility in water [mg/kg]	0.9 at 20°C	1
Vapour pressure [Pa]	2 x 10 ⁻⁴	1
Log P _{ow}	3.9	1
Henry's law constant [Pa×m ³ /mol]	7.7 x 10 ⁻²	1

1.2 Toxicity to aquatic organisms

The toxicity of *tolyfluanid* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *tolyfluanid*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Scendesmus subspicatus</i>	growth rate	72h, static	E _r C ₅₀ >1 NOEC >1	1
<i>Pseudo-kirchneriella subcapitata</i>		72h, static	E _r C ₅₀ >5 ¹⁾ NOEC >0.5 ¹⁾	1
Crustaceans				

<i>Daphnia magna</i>	immobility	48, flow-through	EC ₅₀ 0.19	1
<i>Daphnia magna</i>	immobility	48, static	EC ₅₀ 0.69	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.1	1
<i>Daphnia magna</i>	reproduction and survival	21, semi-static	NOEC 0.061 ¹⁾	1
Microcosm				
<i>Daphnia magna</i>	population abundance	35d, static	NOEC 0.032 ¹⁾ NOEAEC 0.18 ¹⁾	1
Mesocosm				
Zooplankton, macro invertebrates, emergent insects	population and abundance	56, static	EAC 0.046 ¹⁾ NOEC 0.01 ¹⁾ NOEAEC 0.099 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96, flow-through	LC ₅₀ 0.016 ^{1,2)} (nominal conc.)	1
<i>Onchorhynchus mykiss</i>	mortality	96, static	LC ₅₀ 0.045 (nominal conc.)	1
<i>Leuciscus idus</i>	mortality	96, static	LC ₅₀ 0.055 (nominal conc.)	1
<i>Lepomis macrochirus</i>	mortality	96, static	LC ₅₀ 0.066 ¹⁾ (nominal conc.)	1
<i>Poecilia reticulata</i>	mortality	96, static	LC ₅₀ 0.092 ¹⁾ (nominal conc.)	1
<i>Brachudanio rerio</i>	mortality	96, static	LC ₅₀ 0.051 ¹⁾ (nominal conc.)	1
<i>Pimephales promelas</i>	mortality	96, static	LC ₅₀ 0.043 ¹⁾ (nominal conc.)	1
<i>Onchorhynchus mykiss</i>	growth	21d, flow-through	NOEC 0.0098 (nominal conc.)	1
<i>Onchorhynchus mykiss</i>	growth	21d, flow-through	LC ₅₀ 0.0093 ¹⁾ (nominal conc.)	1
Microcosm				
<i>Onchorhynchus mykiss</i>	growth rate	28, static	NOEC 0.044 ¹⁾	1
Mesocosm				
<i>Onchorhynchus mykiss</i>	growth rate	35d, static	NOEC 0.06 ¹⁾	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity 90%

The most sensitive (acute effects) of the tested species was *Onchorhynchus mykiss*, with a LC₅₀ of 0.016 mg/L and NOEC 0.0093 mg/L. Since the acute/chronic ratio is low, a PNEC based on long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest LC₅₀ of 0.016 mg/L is divided by a factor of 100, which results in a PNEC of 0.00016 mg/L.

Table 1.2.2: Aquatic ecotoxicity data of *DMST*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudo-kirchneriella subcapitata</i>	growth rate	72h, static	E _r C ₅₀ 71 NOEC 10	1
Crustaceans				

<i>Daphnia magna</i>	immobilisation	48h, static	EC ₅₀ 31	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 5.6	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ >35	1
<i>Onchorhynchus mykiss</i>	growth	21d, semi-static	NOEC 10	1
<i>Fathead minnow, early life stage</i>	behaviour and morphology	32d, flow-through	NOEC >10	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive (acute effects) of the tested species was *Daphnia magna*, with a LC₅₀ of 31 mg/L and NOEC 5.6 mg/L. Since the acute/chronic ratio is low, a PNEC based on long term data does not guarantee appropriate protection against acute effects, hence the PNEC is based on acute toxicity data. The lowest LC₅₀ of 31 mg/L is divided by a factor of 100, which results in a PNEC of 0.31 mg/L.

1.3 Bioaccumulation and persistence

Log P_{ow} 3 for *tolyfluanid* indicates risk for bioaccumulation. However, BCF is 74, therefore the substance is not considered to bioaccumulate. Due to increased hydrolytic qualities, the metabolite has even lower potential for bioaccumulation. The hydrolysis of *tolyfluanid* is dependent on pH and temperature: it is most rapid in alkaline conditions and high temperatures. In water/sediment systems *tolyfluanid* is transformed into metabolites within DT₅₀ of 1.4-6 h in water phase and 2.6-5 h in sediment. The main metabolite *DMST*, which is distributed evenly between water and sediment, is more stable; DT₅₀ 20-75 days in water phase and DT₅₀ 34-77 days in sediment. Because *tolyfluanid* is rapidly transformed into *DMST*, a separate water quality objective for the metabolite is established.

1.4 Proposed water quality objective

Tolyfluanid

Since PNEC is 0.00016 mg/L, the proposed water quality standard for *tolyfluanid* is 2×10^{-4} mg/L.

DMST

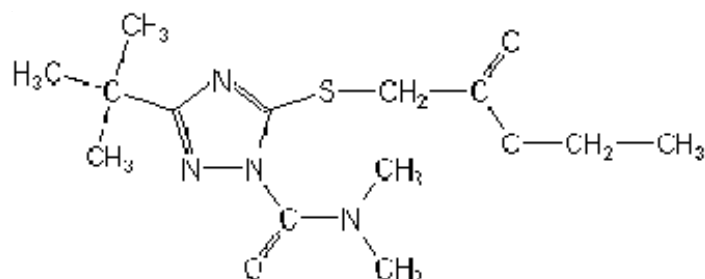
Since PNEC is 0.31 mg/L, the proposed water quality standard for *DMST* is 0.3 mg/L.

1.5 Literature

- (1) European Commission Peer Review Programme. *Tolyfluanid Monograph*, 2003. Rapporteur Member State: Finland.

1. Triazamate and metabolite II

Triazamate is an insecticide used as protection against aphids in sugar beets, potatoes, peas and beans. The insecticide primary acts as a stomach poison, but also via contact action. *Triazamate* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *triazamate* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *triazamate*.

		Reference
CAS-No.	112143-82-5	1
Empirical formula	C ₁₃ H ₂₂ N ₄ O ₃ S	1
Molecular weight [g/mol]	314.4	1
Solubility in water [mg/kg]	443 pH 7 at 20°C	1
pKa	Not relevant at pH 2.7 to 10	1
Vapour pressure [Pa]	1.3 × 10 ⁻⁴ at 25°C	1
Log P _{ow}	2.56 at pH 5.7 and 21°C	1
Henry's law constant [Pa×m ³ /mol]	4.5 × 10 ⁻⁵	1

1.2 Toxicity to aquatic organisms

The toxicity of *triazamate* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *triazamate*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudo-kirchneriella subcapitata</i>	growth rate	72h, static	E _r C ₅₀ >400 NOEC 38	1
<i>Pseudo-kirchneriella subcapitata</i>	growth rate	72h, static	E _r C ₅₀ 0.69 ¹⁾ NOEC 1.0 ¹⁾	1
Crustaceans				

<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.048	1
<i>Daphnia magna</i>	immobility	48h, flow-through	EC ₅₀ 0.014	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.38	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.0035 ²⁾	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 0.0085 ¹⁾	1
<i>Daphnia magna</i>	reproduction	21d, flow-through	NOEC 0.0012 ³⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 0.43	1
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ 1.0	1
<i>Lepomis macrochirus</i>	mortality	96h, static	LC ₅₀ 0.53	1
<i>Lepomis macrochirus</i>	mortality	96h, flow-through	LC ₅₀ 0.88	1
<i>Onchorhynchus mykiss</i>	mortality	96h, semi-static	LC ₅₀ 0.62 ¹⁾	1
<i>Pimephales promelas</i>	growth	33d, flow-through	NOEC 0.03	1

¹⁾ Test performed on preparation, triazamate 140 g a.s./L EW (triazamate 140g/L). Value expressed as active substance.

²⁾ Solution acidified to pH6.

³⁾ Effect concentration basis for calculation of PNEC. Test substance purity 96.6%

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.0012 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for triazamate is calculated to 0.00012 mg/L.

The toxicity of *metabolite II* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *metabolite II*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Daphnia magna</i>	immobilisation	48h, static	EC ₅₀ 0.35 ¹⁾	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static-renewal	LC ₅₀ 10	1

¹⁾ Effect concentration basis for calculation of PNEC.

The most sensitive of the tested species was *Daphnia magna*, with an EC₅₀ of 0.35 mg/L. Only two trophic levels are tested in short term studies, hence not fulfilling the database set. However, compared to studies with the active ingredient, the studies are considered to cover the most sensitive organism, here *Daphnia magna*. Therefore an assessment factor of 1000 is used for calculation of the predicted no effect concentration. Hence, the lowest EC₅₀ of 0.35 mg/L is divided by a factor of 1000, which results in a PNEC of 0.00035 mg/L.

1.3 Bioaccumulation and persistence

Triazamate is not expected to bioaccumulate. BCF are estimated for triazamate and its metabolites, none exceed 100, trigger value for bioaccumulation. Triazamate is hydrolysed,

more rapidly at neutral and basic pH values. Four major hydrolysis metabolites were formed; *metabolite II*, X, XVII and XI. In water/sediment systems, pH >7, *triazamate* is rapidly degraded in the water phase, DT₅₀ of 3.6-7.2 hours. However some of the metabolites are more persistent; *metabolite II*, X and XVII degrade within a DT₅₀ of 94, 1.3 and 118 days respectively. Additionally an unknown metabolite has been found, metabolite A. *Triazamate* and its metabolites are mainly kept in water phase. Based on available ecotoxicity data, only *metabolite II* is considered to be relevant: toxic towards *Daphnia magna* and more persistent than parent compound. Therefore a separate water quality objective is proposed for *metabolite II*.

1.4 Proposed water quality objective

Triazamate

Since PNEC is 0.00012 mg/L, the proposed water quality standard for *triazamate* is 1×10^{-4} mg/L.

Metabolite II

Since PNEC is 0.00035 mg/L, the proposed water quality standard for *metabolite II* is 3×10^{-4} mg/L.

1.5 Comments

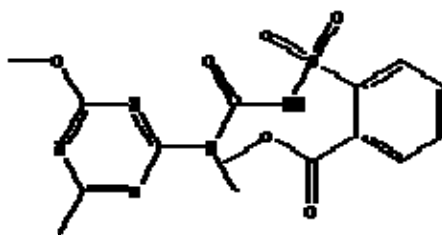
Metabolites IX, XIII, XV and *XIX* formed in soil, have potential to leach through the soil profile and reach both surface- and ground waters. *Triazamate* is rapidly degraded in soil; leach is therefore not relevant. *Triazamate* is not expected to volatilise.

1.6 Literature

- (1) European Commission Peer Review Programme. *Triazamate Monograph*, 2003. Rapporteur Member State: United Kingdom.

1. Tribenuron methyl

Tribenuron methyl is a sulfonylurea herbicide, intended for use in cereals and pasture. The mode of action is inhibition of the plant enzyme acetolactate synthase. The inhibition leads to rapid cessation of shoot and root cell division and growth. *Tribenuron methyl* has been evaluated within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *tribenuron methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *tribenuron methyl*.

		Reference
CAS-No.	101200-48-0	1
Empirical formula	C ₁₅ H ₁₇ N ₅ O ₆ S	1
Molecular weight [g/mol]	395.4	1
Solubility in water [mg/kg]	48.9 at 20° pH 5 2040 at 20° pH 7 18300 at 20° pH 9	1
pKa	4.7	1
Vapour pressure [Pa]	5.2×10 ⁻⁸	1
Log P _{ow}	2.6 at pH 5 0.78 at pH 7 0.3 at pH 9	1
Henry's law constant [Pa×m ³ /mol]	3×10 ⁻²	1

1.2 Toxicity to aquatic organisms

The toxicity of *tribenuron methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *tribenuron methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Chlorella fusca vacuolata</i>	growth	24h	EC ₅₀ 0.08	2
Aquatic plants				
<i>Lemna gibba</i>	frond number	14d	EC ₅₀ 0.0043 ¹⁾ NOEC 0.001 ²⁾ nominal	1
Crustaceans				

<i>Daphnia magna</i>	immobility	48h	EC ₅₀ >894	1
<i>Daphnia magna</i>	immobility	96h	EC ₅₀ 720	2
<i>Daphnia magna</i>	growth	21d	NOEC 120	1
Fish				
<i>Oncorhynchus mykiss</i>	mortality	96h	LC ₅₀ 738	1
<i>Lepomis macrochirus</i>	mortality	96h	EC ₅₀ >1000	1
<i>Oncorhynchus mykiss</i>	growth	21d	NOEC 560	1

¹⁾ Effect concentration basis for calculation of former PNEC. Test substance purity 92.6%.

²⁾ Effect concentration basis for calculation of revised PNEC.

Former water quality objective calculation

The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0043 mg/L and a NOEC of 0.001 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.0043 mg/L is divided by a factor of 100, which results in a PNEC of 4.3×10⁻⁵ mg/L.

Revised EQS calculation according to EU-harmonised methodology (3)

There is chronic data available for three trophic levels. The most sensitive of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0043 mg/L and a NOEC of 0.001 mg/L. Dividing the lowest NOEC of 0.001 mg/L by an assessment factor of 10, results in a PNEC of 0.0001 mg/L.

1.3 Bioaccumulation and persistence

Tribenuron methyl has a low P_{ow}, 0.3-2.6, depending on pH, and is therefore not expected to bioaccumulate. In water *tribenuron methyl* degrades through hydrolytic cleavage, more rapidly at acidic conditions. In water/sediment systems the degradation occurs with a DT₅₀ of 13-31 days in the water phase, and 17-32 days for the whole system. The major degradation products (exceeding 10%) in water are *triazine amine*, *acid sulfonamide* and *saccarin*. The metabolites are found mainly in water phase except *triazine amine* which partitions into sediment. Studies indicate that metabolites formed in water/sediment system are not more toxic to aquatic organisms than the parent compound.

1.4 Proposed EQS/water quality objective

Since PNEC is 0.0001 mg/L., the proposed EQS/water quality objective for *tribenuron methyl* is 0.0001 mg/L.

1.5 Comments

Tribenuron methyl is rapidly transformed in aerobic soil (DT₅₀ 12 days) to the metabolites *triazine amine*, *acid sulfonamide* and *saccarin*. *Triazine amine* degrades fairly rapid (DT₅₀ 30 days), while *acid sulfonamide* and *saccarin* degrade more slowly, DT₅₀ 165 days and 131

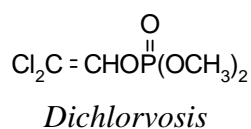
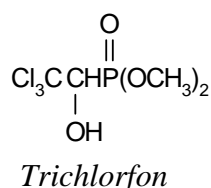
days. *Tribenuron methyl* may leach through the soil profile. Leach potential is increased in alkaline soils. *Tribenuron methyl* is not volatile.

1.6 Literature

- (1) European Commission Peer Review Programme. *Tribenuron methyl Monograph*, 2003. Rapporteur Member State: Sweden.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Lepper; P., 2005. *Manual on the Methodological Framework to Derive Environmental Quality Standards for Priority Substances in accordance with Article 16 of the Water Framework Directive (2000/60/EC)*. Fraunhofer-Institute, Germany.

1. Trichlorfon and dichlorvos

Trichlorfon is an organophosphorous insecticide, intended for use in, among other crops; beets, strawberries and cultivation of fruit. The main metabolite is *dichlorvos*, which is a stronger acting acetylcholine esterase inhibitor than *trichlorfon*. Therefore a separate water quality objective has been established for *dichlorvos*. *Dichlorvos* is an organophosphorous insecticide/acaricide no longer in use in Sweden (not for field use after 1980).



1.1 Physico-chemical properties

Physico-chemical properties of *trichlorfon* are summarised in table 1.1.1.

Table 1.1.1: Physico-chemical properties of *trichlorfon*.

		Reference
CAS-No.	52-68-6	2
Empirical formula	C ₄ H ₈ Cl ₃ O ₄ P	2
Molecular weight [g/mol]	257.3	2
Solubility in water [mg/kg]	123 000 at 15°C 154 000 at 25°C	2
Vapour pressure [Pa]	2.1×10 ⁻⁴ at 20°C 5.0×10 ⁻⁴ at 25°C	2
Log P _{ow}	0.52	2
Henry's law constant [Pa×m ³ /mol]	4.4×10 ⁻⁷ at 20°C	4

Physico-chemical properties of *dichlorvos* are summarised in table 1.1.2.

Table 1.1.2: Physico-chemical properties of *dichlorvos*.

		Reference
CAS-No.	62-73-7	4
Empirical formula	C ₄ H ₇ Cl ₂ O ₄ P	4
Molecular weight [g/mol]	221.0	4
Solubility in water [mg/kg]	10 000 at 20°C 18 000 at 25°C	1 4
Vapour pressure [Pa]	1.6 at 20°C 2.1 at 25°C	1 4
Log P _{ow}	1.5 1.9	1 4
Henry's law constant [Pa×m ³ /mol]	2.58 × 10 ⁻²	4

1.2 Toxicity to aquatic organisms

The toxicity of *trichlorfon* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *trichlorfon*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Simocephalus serrulatus</i>		48 h, static	LC ₅₀ 0.00070	3
<i>Daphnia pulex</i>		48 h, static	EC ₅₀ 0.00070	3
<i>Penaeus duorarum</i>		48 h, flow-through	LC ₅₀ 0.00036	3
<i>Daphnia magna</i>		48 h	EC ₅₀ 0.00092	1
<i>Daphnia magna</i>	survival reproduction growth	21 d, flow-through	NOEC 0.000025	1
		21 d, flow-through	NOEC 0.0000057	
		21 d, flow-through	NOEC 0.0000086	
<i>Daphnia magna</i>		21 d, flow-through	NOEC 0.0000056	1
Fish				
<i>Salmo salar</i>		96 h, static	LC ₅₀ 0.3	3
<i>Oncorhynchus mykiss</i>		96 h	LC ₅₀ 1.6	1
<i>Oncorhynchus mykiss</i>		96 h, static	LC ₅₀ 0.43	3
<i>Oncorhynchus clarki</i>		96 h, static	LC ₅₀ 0.38	3
<i>Lepomis macrochirus</i>		96 h, static	LC ₅₀ 0.23	3
<i>Lepomis macrochirus</i>		96 h	LC ₅₀ 2.1	1
<i>Ictalurus punctatus</i>		96 h, static	LC ₅₀ 0.88	3
<i>Ictalurus melas</i>		96 h, static	LC ₅₀ 0.52	3
<i>Salvelinus fontinalis</i>		96 h, static	LC ₅₀ 0.24	3
<i>Salvelinus namaycush</i>		96 h, static	LC ₅₀ 0.55	3
<i>Pimephales promelas</i>		96 h, static	LC ₅₀ 7.9	3
<i>Micropterus salmoides</i>		96 h, static	LC ₅₀ 3.4	3
<i>Oncorhynchus mykiss</i>		21 d, flow-through	NOEC 0.07	3

¹⁾ Effect concentration basis for calculation of PNEC. Test substance of technical quality with unknown purity.

The most sensitive of the tested species was *Daphnia magna*, with a NOEC of 0.0000056 mg/L. Short and long term studies are available from two trophic levels, fish and crustaceans, but available studies on algae are not fully reliable. Supportive studies suggest, though, that algae are less sensitive to trichlorfon than fish and crustaceans. This can also be expected from the mode of action, and experience from other organophosphorous insecticides confirms that algae are the more tolerant to these compounds; Therefore an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for trichlorfon is calculated to 5.6×10^{-7} mg/L.

The toxicity of *dichlorvos* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *dichlorvos*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Crustaceans				
<i>Simocephalus serrulatus</i>	immobility	48 h, static	EC ₅₀ 0.00026	3
<i>Gammarus lacustris</i>	immobility	96 h, static	EC ₅₀ 0.00050	3
<i>Daphnia pulex</i>	immobility	48 h, static	EC ₅₀ 0.000066	3
<i>Mysidopsis bahia</i>	immobility	96 h, flow-through	EC ₅₀ 0.019	3
<i>Mysidopsis bahia</i>	reproduction	28 d, flow-through	NOEC 1.4 × 10 ⁻⁶ ¹⁾	3
Mollusca				
<i>Crassostrea virginica</i>	shell deposition	96 h, flow-through	EC ₅₀ >1.0	3
<i>Crassostrea virginica</i>	shell deposition	96 h, flow-through	EC ₅₀ 89	3
Fish				
<i>Oncorhynchus clarki</i>	mortality	96 h, static	LC ₅₀ 0.17	3
<i>Salvenius namaycush</i>	mortality	96 h, static	LC ₅₀ 0.19	3
<i>Pimephales promelas</i>	Mortality	96 h, static	LC ₅₀ 12	3
<i>Lepomis macrochirus</i>	Mortality	96 h, static	LC ₅₀ 0.87	3
<i>Cyprinodon variegates</i>	Mortality	96 h, flow-through	LC ₅₀ 7.4	3
<i>Oncorhynchus mykiss</i>	Growth	61 d, early life-stage, flow-through	NOEC 0.0052	3
<i>Cyprinodon variegates</i>	Growth	34 d, early life stage, flow-through	NOEC 0.96	3

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98%.

The most sensitive of the tested species in short-term tests was *Daphnia pulex*, with an EC₅₀ of 0.000066 mg/L. The only available long-term data from the same trophic level is generated from the salt-water species *Mysidopsis bahia* with a NOEC of 0.0000014 mg/l. Short and long-term studies are available from two trophic levels, fish and crustaceans, but available studies on algae are not fully reliable. Supportive studies suggest, though, that algae are less sensitive to dichlorvos than fish and crustaceans. This can also be expected from the mode of action, and experience from other organophosphorous insecticides. Because of the difference in short-term toxicity between *Daphnia* (EC₅₀ 0.000066 mg/l) and *Mysidopsis* (EC₅₀ 0.019 mg/l) an assessment factor of 10 is not sufficient, and therefore a factor of 50 is applied for calculation of the predicted no effect concentration. Hence, the PNEC for dichlorvos is calculated to 2.8 × 10⁻⁸ mg/L.

1.3 Bioaccumulation and persistence

Neither *trichlorfon*, nor *dichlorvos*, is expected to bioaccumulate. Breakdown is mainly due to hydrolysis and increases with increasing pH; at 25°C half-life has been determined to 104 days at pH 5, 34 hours at pH 7 and 31 minutes at pH 9. Degradation in soil is usually rapid with half-lives ranging from a couple of days to a few weeks, but may be delayed in cold,

acidic environment. The main metabolite formed at pH>5 is *dichlorvos*. Breakdown of *dichlorvos* is hydrolytic as well as microbial, but stable towards photolysis. Degradation is pH-dependent faster in alkaline media. In lakes and rivers at neutral pH, half-life is reported to be approximately 4 days (1). At pH < 5, *desmethyl-dichlorvos* is the major breakdown product. The breakdown of metabolites is mainly microbial. Other significant metabolites are *dichloroacetic acid*, *dichloroethanol* and *trichloroacetaldehyde*. Studies covering the toxicity of metabolites are missing and ought to be supplemented.

1.4 Proposed water quality objective

Trichlorfon

Since PNEC is 5.6×10^{-7} mg/L, the proposed water quality objective for substance is 6×10^{-7} mg/L.

Dichlorvos

PNEC is 2.8×10^{-8} mg/L, the proposed water quality objective for *dichlorvos* is therefore 3×10^{-8} mg/L.

1.5 Comments

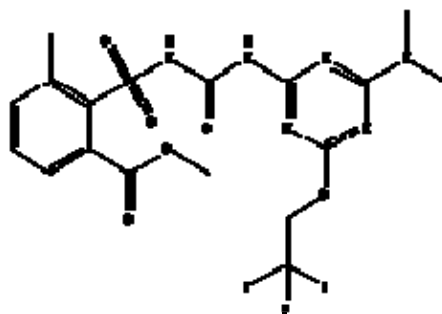
Dichlorvos may reach surface- and groundwater through the soil profile (1).

1.6 Literature

- (1) Centre for Substances and Risk assessment (CSR), 1998, RIVM, The Netherlands
- (2) Karin Hanze, 1990, *Ekotoxikologisk utvärdering av triklorfon*, National Chemicals Inspectorate, Sweden
- (3) Pesticide Ecotoxicity Database, 2001, Environmental Fate and Effects Division of Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.
- (5) Howard, P.H., 1991, Handbook of Environmental Fate and Exposure Data for Organic Chemicals, Vol. 3: Pesticides. Lewis Publishers, Chelsea MI, p. 251-258.

1. Triflusulfuron methyl

Triflusulfuron methyl is a sulfonylurea herbicide. It inhibits the enzyme acetolactase synthase. The herbicide is intended for use in sugar beets.



1.1 Physico-chemical properties

Physico-chemical properties of *triflusulfuron methyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *triflusulfuron methyl*.

		Reference
CAS-No.	126535-15-7	1
Empirical formula	C ₁₇ H ₁₉ F ₃ N ₆ O ₆ S	1
Molecular weight [g/mol]	492.4	1
Solubility in water [mg/kg]	1 at pH 3 and 25°C 2.7 at pH 5 110 at pH 7 11000 at pH 9	1
pKa	4.4	1
Vapour pressure [Pa]	<1.33 ×10 ⁻⁵	1
Log P _{ow}	14.8 at pH 5, 25°C 3 at pH 7 0.86 at pH 9	1
Henry's law constant [Pa×m ³ /mol]	6.5 ×10 ⁻⁵ at pH 3, 25°C 2.4×10 ⁻³ at pH 5 0.6 ×10 ⁻⁵ at pH 7 5.0 ×10 ⁻⁷ at pH 9	1

1.2 Toxicity to aquatic organisms

The toxicity of *triflusulfuron methyl* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *triflusulfuron methyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Higher aquatic plants				

<i>Lemna minor</i>	Frond number	14d, static	EC ₅₀ 0.009 NOEC 0.0025	1
<i>Lemna gibba</i>		14d, static	EC ₅₀ 0.0028 ¹⁾ NOEC 0.0013	2
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 460	1
<i>Daphnia magna</i>		48h, static	EC ₅₀ 960	2
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 11	1
Fish				
<i>Lepomis macrochirus</i>	mortality	96h, static	EC ₅₀ 760	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ 730	1
<i>Cyprinus carpio</i>	mortality	96h, static	EC ₅₀ >880	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	EC ₅₀ 960	2
<i>Onchorhynchus mykiss</i>	growth	21d, flow-through	NOEC >210	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98.7%

Supporting data on algae are available, but results not listed because the tests exceed optimal exposure duration time. The most sensitive (acute effects) of the tested species was *Lemna gibba*, with an EC₅₀ of 0.0028 mg/L and a NOEC of 0.0013 mg/L. Since the acute/chronic ratio is low and does not guarantee appropriate protection against acute effects, the PNEC is based on acute toxicity data. Hence, the lowest EC₅₀ of 0.0028 mg/L is divided by a factor of 100, which results in a PNEC of 0.000028 mg/L.

Table 1.2: Aquatic ecotoxicity data of *triazine amine*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	biomass	96h, static	E _b C ₅₀ 170	1
<i>Selenastrum capricornutum</i>	biomass	96h, static	E _b C ₅₀ 68.6 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 324	3
Fish				
<i>Pimephales promelas</i>	behaviour	96h, static	EC ₅₀ 139	3

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 98.4%

The most sensitive (acute effects) of the tested species was *Selenastrum capricornutum*, with an EC₅₀ of 68.6 mg/L. Since only acute toxicity data is available, an assessment factor of 1000 is used, for protection against chronic effects. The lowest EC₅₀ of 68.6 mg/L is divided by a factor of 1000, which results in a PNEC of 0.0686 mg/L.

1.3 Bioaccumulation and persistence

Triflusalufuron methyl is not expected to bioaccumulate, due to low log P_{ow} in neutral and alkaline pH. No bioaccumulation studies have been performed. Hydrolysis of *triflusalufuron methyl* is pH dependent; DT₅₀ 3.7 at pH 5, DT₅₀ 32 at pH 7 and DT₅₀ 37 at pH 9. The

degradation has been studied in two water/sediment systems; moving water at pH 7.4-8.1 and static water at pH 7.8-8.3. At equilibrium the distribution of the substance was 52-65% in water and 28-44% in sediment. Time of degradation in water/sediment was 18-21 days in static water and 30-39 days in moving water. Several major (>10%) metabolites are formed during degradation; free acid of *triflusulfuron methyl*, *methyl saccharin* and *triazine amine*, which was further metabolised to *N-desmethyl triazine amine*.

1.4 Proposed water quality objective

Triflusulfuron methyl

Since PNEC is 0.000028 mg/L, the proposed water quality standard for *triflusulfuron methyl* is 3×10^{-5} mg/L.

Triazine amine

Since PNEC is 0.0686mg/L, the proposed water quality standard for *triazine amine* is 0.07 mg/L.

1.5 Comments

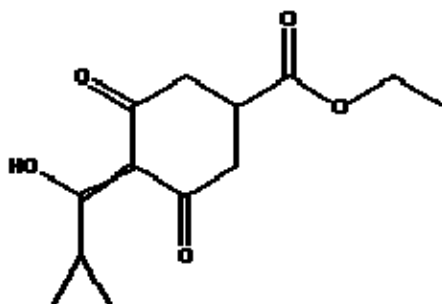
Thifensulfuron methyl, as well as its metabolites, is very mobile in soil, and can reach surface- and ground waters via leaching through the soil profile.

1.6 Literature

- (1) Bard J., 1995. *Ecotoxicological evaluation of the herbicide triflusulfuron methyl*. Nässja Ekotoxkonsult.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.
- (3) Nurmi E., 1996. *Addendum to the ecotoxicological evaluation of the herbicide triflusulfuron methyl*. Finnish environment agency.
- (4) Tomlin, C., 2000. *The Pesticide Manual, 12th edition*. British Crop Protection Council.

1. Trinexapac and its metabolite trinexapac-acid

Trinexapac-ethyl is taken up by leaves and shoots and inhibits the biosynthesis of gibberellins. *Trinexapac-ethyl* is intended for use in rye to shorten the plant. *Trinexapac-ethyl* has been evaluated/is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *trinexapac-ethyl* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *trinexapac-ethyl*.

		Reference
CAS-No.	95266-40-3	1
Empirical formula	C ₁₃ H ₁₆ O ₅	1
Molecular weight [g/mol]	252.3	1
Solubility in water [mg/kg]	1.1 at pH 3.5, 25 °C 2.8 at pH 4.9 10.2 at pH 5.5 21.1 at pH 8.2	1
pKa	4.57 at 20 °C	1
Vapour pressure [Pa]	2.16 × 10 ⁻³ at 25°C	1
Log P _{ow}	1.5 at pH 5 -0.29 at pH 6.9 -2.1 at pH 8.9	1
Henry's law constant [Pa×m ³ /mol]	5.4 × 10 ⁻⁴	1

1.1 Toxicity to aquatic organisms

The toxicity of *trinexapac-ethyl* to aquatic organisms is summarised in table 1.2.1.

Table 1.2.1: Aquatic ecotoxicity data of *trinexapac-ethyl*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Pseudokirchneriella subcapitata</i>	growth rate	72h, static	EC ₅₀ 60 NOE _r C 9.4	1
<i>Anabaena flos-aquae</i>	growth rate	96h, static	EC ₅₀ 25.7 NOE _r C 25	1

Aquatic plants				
<i>Lemna gibba</i>	biomass	7d, semi-static	EC ₅₀ 8.8 NOEC 2.3	1
<i>Lemna gibba</i>		7d, static	EC ₅₀ 0.19 NOEC 0.018 ¹⁾	2
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, semi-static	EC ₅₀ >142.5	1
<i>Daphnia magna</i>	growth, reproduction	21d, flow-through	NOEC 11	1
<i>Daphnia magna</i>	growth, reproduction	21d, flow-through	NOEC 2.4	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, semi-static	LC ₅₀ 68	1
<i>Cyprinodon variegatus</i>	mortality	96h, static	LC ₅₀ 180	2
<i>Lepomis macrochirus</i>	mortality	96h, semi-static	LC ₅₀ >130	1
<i>Cyprinus carpio</i>	mortality	96h, semi-static	LC ₅₀ 57	1
<i>Ictalurus punctatus</i>	mortality	96h, semi-static	LC ₅₀ 35	1
<i>Pimephales promelas</i>	growth	35d, flow-through	NOEC 0.41	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 92.2%

The most sensitive of the tested species was *Lemna gibba*, with a NOEC of 0.018 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *trinexapac-ethyl* is calculated to 0.0018 mg/L.

The toxicity of *trinexapac-acid* to aquatic organisms is summarised in table 1.2.2.

Table 1.2.2: Aquatic ecotoxicity data of *trinexapac-acid*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Anabaena flos-aquae</i>	growth rate	96h, static	EC ₅₀ 17.5 NOEC 12.5	1
<i>Microcystis aeruginosa</i>	growth rate	72h, static	EC ₅₀ 72 NOEC 32	1
<i>Navicula pelliculosa</i>	growth rate	96h, static	EC ₅₀ >100 NOEC >100	1
Aquatic plants				
<i>Lemna gibba</i>	biomass	7d, static	EC ₅₀ 1.5 NOEC 0.30 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ >100	1
Fish				
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ >100	1
<i>Cyprinus carpio</i>	mortality	96h, flow-through	LC ₅₀ >100	1

¹⁾ Effect concentration basis for calculation of PNEC. Test substance purity 99%

The most sensitive of the tested species was *Lemna gibba*, with a NOEC of 0.3 mg/L. Acute toxicity at three trophic levels has been tested. However chronic toxicity has only been studied for primary producers. Therefore an assessment factor of 100 is used for calculation of

the predicted no effect concentration. Hence, the PNEC for *trinexapac-ethyl* is calculated to 0.003 mg/L.

1.2 Bioaccumulation and persistence

Trinexapac-ethyl is not expected to bioaccumulate. *Trinexapac-ethyl* is stable towards hydrolysis at pH 5 and 7. At pH 9, *Trinexapac-ethyl* is hydrolysed with in a DT₅₀ of 10.9 days. Degradation has been studied in two water/sediment systems. The DT₅₀ was 3.4-4.9 days in water phase and 3.8-5.2 days in sediment. However the substance remains mainly in water phase. One major metabolite, exceeding 10%, was formed; *trinexapac-acid*. The metabolite was studied in the same water/sediment systems as parent compound. It was degraded slightly slower, with a DT₅₀ of 11-13 days in water phase and 12-14 days in sediment phase.

1.3 Proposed water quality objective

Trinexapac-ethyl

Since PNEC is 0.0018 mg/L, the proposed water quality standard for *trinexapac-ethyl* is 0.002 mg/L.

Trinexapac-acid

PNEC is 0.003 mg/L, the proposed water quality standard for *trinexapac-acid* is 0.003 mg/L.

1.4 Comments

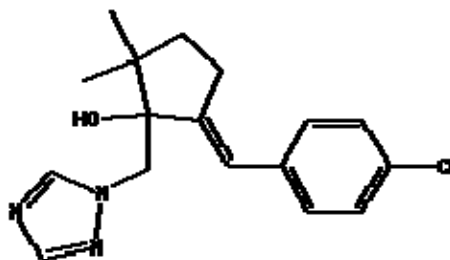
A separate water quality objective has been set for the metabolite *trinexapac-acid*.

1.5 Literature

- (1) European Commission Peer Review Programme. *Trinexapac-ethyl Monograph, 2003*. Rapporteur Member State: The Netherlands.
- (2) Pesticide Ecotoxicity Database, 2001. Environmental Fate and Effects Division of the Office of Pesticide programs, U.S.EPA, Washington, D.C.

1. Triticonazole

Triticonazole is a systemic fungicide, inhibiting the sterol biosynthesis pathway. The fungicide is intended for use as seed treatment in cereals. *Triticonazole* is under evaluation within the framework of EU Dir. 91/414.



1.1 Physico-chemical properties

Physico-chemical properties of *triticonazole* are summarised in table 1.1.

Table 1.1: Physico-chemical properties of *triticonazole*.

		Reference
CAS-No.	131983-72-7	1
Empirical formula	C ₁₇ H ₂₀ ClN ₃ O	1
Molecular weight [g/mol]	317.8	1
Solubility in water [mg/kg]	9.3 at pH 7.3-8.7 and 20 °C	1
pKa	Not relevant	1
Vapour pressure [Pa]	< 1 × 10 ⁻⁶ at 50 °C	1
Log P _{ow}	3.29 at 20 °C	1
Henry's law constant [Pa×m ³ /mol]	< 3.8 × 10 ⁻⁵	1

1.2 Toxicity to aquatic organisms

The toxicity of *triticonazole* to aquatic organisms is summarised in table 1.2.

Table 1.2: Aquatic ecotoxicity data of *triticonazole*.

Species	End-point	Exposure duration	Result [mg as/L]	Reference
Algae				
<i>Selenastrum capricornutum</i>	growth rate	96h, static	E _r C ₅₀ >1 NOEC >1	1
<i>Scenedesmus subspicatus</i>	growth rate	72h, static	E _r C ₅₀ 8.6 ¹⁾	1
Crustaceans				
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 9	1
<i>Daphnia magna</i>	immobility	48h, static	EC ₅₀ 6.9	1
<i>Daphnia magna</i>	reproduction	21d, semi-static	NOEC 0.092	1
Fish				
<i>Onchorhynchus</i>	mortality	96h, semi-static	LC ₅₀ >10	1

<i>mykiss</i>				
<i>Onchorhynchus mykiss</i>	mortality	96h, flow-through	LC ₅₀ >3.6	1
<i>Lepomis macrochirus</i>	mortality	72h, flow-through	LC ₅₀ >8.9	1
<i>Onchorhynchus mykiss</i>	mortality	96h, static	LC ₅₀ 8.0 ¹⁾	1
<i>Onchorhynchus mykiss</i>	growth	28d, flow-through	NOEC 0.01 ²⁾	1

¹⁾ Test performed on preparation. Value expressed as active substance.

²⁾ Effect concentration basis for calculation of PNEC. Test substance purity not known.

The most sensitive of the tested species was *Onchorhynchus mykiss*, with a NOEC of 0.01 mg/L. Since both short and long term studies are available, and three trophic levels have been tested, an assessment factor of 10 is used for calculation of the predicted no effect concentration. Hence, the PNEC for *triticonazole* is calculated to 0.001 mg/L.

1.3 **Bioaccumulation and persistence**

Triticonazole is not expected to bioaccumulate. Although Log P_{ow} exceeds 3, considered as high, BCF is rather low 72-94. The time and route of degradation has been studied water/sediment system. The substance dissipates into the sediment, distribution after 105 days 8.9% in water and 70.9% in sediment. No metabolites exceed 10%.

1.4 **Proposed water quality objective**

Since PNEC is 0.001 mg/L, the proposed water quality standard for *triticonazole* is 0.001 mg/L.

1.5 **Comments**

Triticonazole is not very mobile in soil, Koc 504. However during degradation in soil several metabolites are formed which are more mobile and may reach ground- and surface water via leaching through the soil profile. According to toxicity tests, these metabolites are low toxic towards aquatic organisms. No major metabolites were formed in water or sediment. *Triticonazole* dissipates into the sediment. Therefore an additional quality objective for sediment is recommended.

1.6 **Literature**

- (1) European Commission Peer Review Programme. *Triticonazole Monograph*, 2003. Rapporteur Member State: Austria.