Common Implementation Strategy for the Water Framework Directive

Environmental Quality Standards (EQS)

Substance Data Sheet

Priority Substance No. 29

Simazine

CAS-No. 122-34-9

Final version
Brussels, 15 January 2005

Disclaimer

This data sheet provides background information on the setting of the Environmental Quality Standard in accordance with Article 16 of the Water Framework Directive (2000/60/EC). The information was compiled, evaluated and used as outlined in the Manual [4] and has been discussed in a consultative process with the Expert Advisory Forum on Priority Substances and the Expert Group on Quality Standards. Furthermore, it has been peer-reviewed by the SCTEE [17]. The substance data sheet may, however, not necessarily represent the views of the European Commission.

New upcoming information was considered and included up to the date of finalisation of this data sheet. Information becoming available after finalisation of this document will be evaluated in the review process of priority substances according to Art. 16(4) of the Water Framework Directive. If necessary, the Environmental Quality Standard substance data sheets will then be revised in the light of technical and scientific progress.

1 Identity of substance

Priority Substance No: 29	Simazine
CAS-Number:	122-34-9
Classification WFD Priority List *:	WFD_PSR

* PS: priority substance; PHS: priority hazardous substance; PSR: priority substance under review according to Decision 2455/2001.

2 Proposed quality standards

2.1 Overall quality standards

Ecosystem	Quality Standard	Quality Standard "rounded values"	Comment
AA-QS all surface waters covered by the WFD	1 µg/l	**1 µg/l**	See 8.1.2 & 8.6
MAC-QS	4.2 µg/l	**4 µg/l**	See section 8.1.1

2.2 Specific quality standards

Protection Objective #	Quality Standard	Comment
Pelagic community (all types of surface waters covered by the WFD)	1 µg/l	see section 8.1
Benthic community (all types of sediments covered by the WFD)	3.4 µg/kg (wet wt) 15.5 µg/kg (dry wt)	tentative standard (EP method); see section 8.2
Predators (secondary poisoning)	No QS required	trigger values not met see section 8.3
Food uptake by man	304 µg/kg food corresponding conc. in water: 304 µg/l	see section 8.4
Abstraction of water intended for human consumption (AWIHC)	< 1 µg/l	A1-value for Σpesticides in CD 75/440/EEC; see section 8.5
Water intended for human consumption (WIHC)	0.1 µg/l	Drinking water standard set in CD 98/83/EC

If justified by substance properties or data available, QS for the different protection objectives are given independently for freshwater environments, transitional waters or coastal and territorial waters

3 Classification

R-Phrases and Labelling	Reference
Carc. Cat. 3; R40 - N; R50-53	[18]

4 Physical and chemical properties

Property	Value	Reference
Vapour pressure	2.94 x 10^{-6} Pa at 25 °C less than 10^{-5} Pa at 30 °C 1.5x 10^{-4} Pa	[1]
Henry's law constant	5.6 x 10^{-5} Pa m^3 /mol (at 22 °C)	[1]
Solubility in water	6.2 mg/l at pH 7 and 22 °C 5.29 mg/litre at 20 °C	[1]
Dissociation constant	PKa 1.62	[1]

5 Environmental fate and partitioning

Property	Value	Ref.
Hydrolytic stability (DT_{50})	DT50: 80 d at pH 4 and 25°C DT50: 44 d at pH 5 and 30°C DT50: >200 d at pH 7 and 50°C at environmentally occurring pHs and temperatures there was little degradation	[1]
Photostability (DT_{50}) (aqueous, sunlight, state pH)	Various studies on aqueous photolysis showed a wide range of DT50 values, for which there is no obvious explanation. Photodegradation is not generally considered a significant degradation pathway.	[1]
Readily biodegradable (yes/no)	not readily biodegradable	[1]
Degradation in Water/sediment -DT_{50} water - DT_{50} whole system	 12 – >77 d *ca.* 100 d	[1]
Mineralization		
Bound residue		
Distribution in water / sediment systems (active substance)	*ca.* 30% AR simazine in the sediment after *ca.* 28 days	[1]
Residues relevant to the aquatic environment	The significance of the data from the outdoor pond studies at various US sites is uncertain but the data does show that simazine degrades to hydroxysimazine and desethylsimazine in aqueous systems in the field Hydroxysimazine was detected at >10% AR on occasions in various studies but since these were sporadic, often divided between the water and sediment and the greatest level was 13% AR, this metabolite is not considered to be relevant.	[1]
Partition co-efficient (log P_{OW}) Koc	2.2 103 – 155 l/kg	[1] [7]
BCF (fish)	generally BCFs were ≈1 The risk of bioaccumulation is considered low	[1]

6 Effect data (aquatic environment)

For simazine, a risk assessment monograph in line with the provisions of Council Directive 91/414/EEC (placing of plant protection products on the market) is available [1]. However this report was finalized in 1996 and does not consider data that became available in the meantime. In order to make best use of all effect data available at present for the derivation of a water quality standard, it was therefore agreed at the workshop of the Expert Group on Quality Standards (12-16 May 2003, Brussels) that the United Kingdom in its competence as Rapporteur Member State for simazine shall perform an assessment of aquatic effect data that became available after finalisation of the monograph. It was further concluded that an attempt should be made to derive a quality standard proposal by means of statistical extrapolation (e.g. the species sensitivity distribution method) and compare the outcome of this approach with the standard assessment factor method.

Consequently, the UK Environment Agency has provided in October 2003 a "Report on Quality Standards for Atrazine and Simazine under the Water Framework Directive" [5]. This report analyses different data on simazine to determine long-term quality standards (AA-QS). Data sources used to produce a consolidated list of studies were the Alterra database[1] for simazine, data provided by the Fraunhofer-Insitiute (forwarded to FHI for the purpose of QS-setting by the United Kingdom, the Netherlands, France and Germany) and data evaluated and used in the simazine monograph [1]. Data and results / conclusions of the UK-report are presented in section 6.1 and Annexes 1 and 2 to this data sheet.

Data used in this data sheet are exclusively drawn from the simazine monograph [1] and the report provided by the UK Environment Agency [5].

6.1 Chronic toxicity to aquatic organisms

In this section the data analysis and SSD-based QS-proposals of the report provided by the UK Environment Agency [5] are summarized. This report analyses different data on simazine to determine long-term quality standards (AA-QS), using species sensitivity distributions (SSDs) and taking account of uncertainties. There were sufficient data to comply with the TGD's taxonomic group and minimum sample size requirements for the single species analyses and to establish SSDs. Underlying data and details of the SSDs set up with different data sets are collated in Annexes 1 (tables A1 & A2) and 2.

Based on the data shown in tables A1 & A2 of Annex 1, species sensitivity distributions (SSDs; Annex 2) were set up in the UK-report for several combinations of data, as follows:

1. The most sensitive data of all 19 species for that data are available (see Annex 1, Table A1)).

2. The most sensitive data for all 11 plant species (reflecting the herbicidal mode of action of simazine)

3. When more than one datum was available for the same endpoint and the same species a geometric mean was calculated (as recommended in the TGD) for all 19 species.

4. When more than one datum was available for the same endpoint and the same species a geometric mean was calculated (as recommended in the TGD) for the 11 plant species.

5. Only data in Table A1 for which full information on test duration and endpoint was available from the sources cited above. Again, there were two analyses for these data: one using the most

[1] Alterra Green World Research, NL-Wageningen

sensitive value when there were multiple results for the same species and endpoint, and one using the geometric mean of these values.

6. Only data that feature in the 1996 simazine monograph produced by the UK rapporteur under Council Directive 91/414/EEC and Regulation 3600/92 (Annex 1, Table 2).

7. A repeat of the analyses in 5 and 6 above using only plant species (algae and macrophytes) and removing data only reported as 'less than' values.

The ETX software developed by Van Vlaardingen et al. (2003) [6] was used for the SSD analyses.

Results are summarised in the UK-report [5] as follows:

HC5 values based on single species laboratory data ranged from 2.29 to 6.51 μg/L, a factor of just under 3, fitted a normal distribution, and did not differ substantially when logistic or triangular distributions were used. This gives confidence that model type and averaging of data did not have a major effect on the results and that an AF of 5 can cover these uncertainties. Use of an AF of 5 leads to QS that range from 0.459 to 1.3 μg/L, which is in close agreement with a QS of 0.5 μg/L based upon the *S. quadricauda* data (i.e., lowest NOEC in the data set divided by an assessment factor of 10, see table A1 in Annex 1). Limited mesocosm data suggest that measurable effects on assemblages are unlikely at 50 μg/L. No data were found to suggest that simazine has endocrine-disrupting effects similar to atrazine.

As regards the mesocosm data available [14, 15, 16], it is however evident from the monograph that these are not suitable for the purpose of quality standard setting because the studies "generally lacked detail and were carried out under environmental conditions of uncertain relevance for the notified uses" [1]. Consequently, in the monograph they are not considered sufficient to meet the requirements for microcosm/mesocosm data. Therefore, these studies are not considered for the purpose of quality standard setting in this data sheet.

6.2 Acute toxicity to aquatic organisms

Acute toxicity data for aquatic species are summarised in Section B.8.2 of the monograph [1]. Acute toxicity data were not subject to analysis in the UK-report [5].

Fish: Many of the studies for freshwater fish (including all those on the notified formulations) did not provide a specific LC50 value as this was greater than the highest concentration tested (highest nominal concentration was 100 mg as/l). Some studies did produce 96h LC50 values; these ranged from 42.33 to 164.4 mg as/l [both these limit values are from studies on zebrafish (*Brachydanio rerio*), using larvae and adults, respectively]. It should be noted that these LC50 values are above the solubility limit of simazine in water. It can be concluded that simazine is of low acute toxicity to fish. The 96h LC50 of 42.33 mg as/l for the larvae of zebrafish is used in the monograph for risk assessment [1].

Invertebrates: Studies on the active substance showed simazine to be of low toxicity to freshwater invertebrates, with EC50s for *Daphnia magna* and *Daphnia similis* of >100 and 457.62 mg as/l, respectively. An EC50 of >100 mg as/l is used in the monograph for risk assessment [1].

Algae/Plants: Studies showed simazine to be of high toxicity to freshwater algae. *Scenedesmus subspicatus* was the most sensitive species tested, with an E_bC_{50} value of 0.042 mg as/l from a study using the technical active substance. This value was used in the monograph for risk assessment [1]. In terms of simazine concentration, 'Gesatop 90 WG' (S. subspicatus 72 h EC50 0.059 mg/l) and 'Gesatop 500 SC' (S. subspicatus 72 h EC50 0.14 mg/l) were similar in toxicity to

the active substance tested alone. A study on the aquatic higher plant *Lemna gibba* gave an EC50 (based on frond growth) of 0.32 mg as/l.

Toxicity tests with algae/cyanobacteria resulting in significantly lower EC50 values than the lowest EC50 considered relevant in the simazine monograph have been reported in various documents provided by the Member States [7 - 12].

6.3 Toxicity to marine species

Some toxicity data have been submitted for various marine species. These data (see, e.g., table A1 in Annex 1) do not suggest that marine species are more sensitive to simazine than equivalent freshwater species. This observation is expected and in accordance with the fact that the toxic effects of simazine are due to its interference with the photosynthetic system (i.e. specific mode of action, target organisms are).

6.4 Risk to sediment dwelling invertebrates

Based on conclusions reached in section B.7.5.2 of the monograph [1] using the available sediment-water degradation data, it is concluded that significant exposure of sediment dwelling organisms is unlikely to occur.

6.5 Mammalian and avian toxicity data

Data presented in this section are drawn from the monograph [1].

Table 6.1: Mammal and bird oral toxicity data relevant for the assessment of non compartment specific effects relevant for the food chain (secondary poisoning)

Type of study	Species, test result	Ref.
Long-term toxicity to mammals	No information	
Acute dietary toxicity to birds	Japanese Quai: LD50 >2000 - > 5000 mg a.i. / kg bw Mallard Duck: LD50 >2000 – 4640 mg a.i. / kg bw	[1]
Reproductive toxicity to birds	No information	

6.6 Metabolites

In terms of exposure from spray drift, it has been concluded in the monograph [1] that in surface water simazine itself is the only environmentally significant residue. Hence, the risk to aquatic organisms from exposure to metabolites, where contamination is by spray drift, is considered low.

Desethylsimazine (G28279) is a product of soil degradation of simazine (see Section B.7 of [1]). This metabolite is relatively mobile and can constitute around 50% of the identified radioactively labeled material in the leachate of lysimeter studies (with the other ≈50% being parent compound). Therefore, there is a potential for this metabolite to contaminate surface waters through drainage. Data have been submitted which give LC/EC50 value for rainbow trout, *Daphnia magn*a, and *Scenedesmus subspicatus* of 17.2, >100 and 1.39 mg as/l, respectively. The risk to algae from exposure to desethylsimazine can be considered to be less than for simazine itself. No data were

submitted of the toxicity of this metabolite to aquatic higher plants. Given that this metabolite is of lesser toxicity to algae than the parent compound, it is also likely to be of lesser toxicity to aquatic higher plants. Hence, it is concluded that the risk to aquatic higher plants has been addressed by the risk assessment for the parent compound. [1]

6.7 Summary on endocrine disrupting potential

In the Communication from the Commission to the Council and the European Parliament on the implementation of the Community Strategy for Endocrine Disrupters, simazine is classified as a substance with evidence of endocrine disruption or evidence of potential ED [2].

However, in the risk assessment monograph [1] potential effects of simazine on endocrine regulation are not addressed and in the report provided by the UK Environment Agency it is stated that *"no data were found to suggest that simazine has endocrine-disrupting effects similar to atrazine"* [5].

Because there is apparently no concrete evidence available that simazine could affect endocrine regulation under field conditions this aspect is not further considered for the purpose of quality standard derivation in this data sheet.

7 Effect data (human health)

Data presented in this section are drawn from the monograph [1].

The lowest level at which any effect is found is 3.5 mg/kg/day, in the dog 52-week dietary study. The next lowest dose at which no effect is seen in a relevant parameter is 0.7 mg/kg/day in the same study. However, for the purposes of establishing an ADI the critical finding is considered to be carcinogenicity in Sprague-Dawley rats (malignant mammary tumours), found at levels as low as 5 mg/kg/day with a NOAEL at 0.5 mg/kg/day; this parameter was not explored in dogs and so the dog NOAEL is disregarded.

The mechanism of tumour formation has been explored in sufficient detail for a feasible mechanism to be postulated; this mechanism is non-genotoxic and a NOAEL has been determined. Further data appropriate to simazine indicate the contribution of a further mechanism (excess PRL secretion, not proven for atrazine) which is not applicable to man. An uncertainty factor of 100 is therefore considered adequate for the protection of the consumer.

ADI = 0.5 mg/kg/day / 100 = **0.005 mg/kg/day**.

Table 7.1: Summary human toxicology data [1]

	Value	Study	Safety factor
ADI	0.005 mg/kg/day	Carcinogenicity in Sprague-Dawley rats, found at levels as low as 5 mg/kg/day with a **NOAEL at 0.5 mg/kg/day**	100
Long term toxicity		The lowest level at which any effect is found is 3.5 mg/kg/day, in the dog 52-week dietary study. The next lowest dose at which no effect is seen in a relevant parameter is 0.7 mg/kg/day in the same study.	
Carcinogenicity		Treatment-related tumours were observed in Sprague-Dawley rats at levels as low as 5 mg/kg/day with a NOAEL at 0.5 mg/kg/day but are not considered relevant in humans **R40 "Possible risk of irreversible effects"** on the basis of carcinogenicity in rats. Simazine best fits category 3(a): well-investigated but for which the evidence of a tumour-inducing effect is insufficient for classification in Category 2. Additional experiments would not be expected to yield further relevant information with respect to classification	
Mutagenicity		Non-genotoxic	
Reproductive toxicity		No reproductive hazard	

8 Calculation of quality standards

In order to keep consistency with other legal frameworks (i.e. Council Directive 91/414/EC), the data used for the derivation of the simazine quality standards are exclusively drawn from the simazine monograph [1] and the consolidated database in the report provided by the UK Environment Agency [5].

In the case of simazine enough data are available to employ statistical extrapolation as a second supplementary approach to the standard assessment factor method in order to derive a quality standard proposal for the protection of the pelagic community.

Due to the specific mode of action demonstrated for simazine (interference with the photosynthetic system), difference of sensitivity between freshwater and marine species is not expected. This expectation is supported by comparison of toxicity test data for freshwater and marine organisms. Acute and long-term toxicity data for marine fish, mollusks and algae are cited in tables A1 and A2 of Annex 1. The data indicate that the sensitivity of marine species is comparable to that of freshwater species of the same taxonomic group. Algae are the most sensitive taxa and the lowest ecotoxicity value was reported for a freshwater species. As a consequence and in accordance with the TGD the freshwater and marine data may be pooled and further, the additional marine factor of 10 is not needed. It is therefore suggested to use the quality standard derived for freshwater also for the protection of the pelagic community in transitional, coastal and territorial waters.

Simazine metabolites are significantly less toxic than simazine itself [1] (see section 6.6 of this data sheet). It is therefore not necessary to consider these metabolites for the purpose of quality standard setting.

8.1.1 Quality standards for water derived by the assessment factor method

Annual average quality standard (AA-QS)

Freshwater algae (*Scenedesmus*) are the most sensitive species among the groups for which toxicity tests are available (see tables A1 and A2). In the UK-report an algae-study with

Scenedesmus quadricauda and a NOEC of 5 µg/l has been accepted for the consolidated database, which is lower than the lowest $NOEC_{algae}$ used in the monograph (*Scenedesmus subspicatus*, NOEC 11 µg/l). It is suggested to use the S. quadricauda NOEC as basis for the derivation of a AA-QS proposal.

Because long-term data are available for more than the minimum of 3 different taxonomic groups, the NOEC is divided by an assessment factor of 10 in order to derive the long term quality standard for surface water.

QS_{water} = 5 µg/l / AF (10) = 0.5 µg Simazine / l

The log Kow is only 2.18 and the water solubility is high. Thus the trigger criterion to calculate a corresponding $QS_{SPM.water}$ referring to the concentration of simazine in suspended particulate matter (SPM) is not met (see table 1a of [4]).

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

Acute toxicity data are available in the monograph [1] for a range of freshwater and saltwater organisms (fish, crustaceans, cyanobacteria, algae and higher plants). The lowest EC50 value is 42 µg simazine/l obtained with the alga species *Scenedesmus subspicatus*.

MAC-QS could be derived on the basis of this EC50 and the guidance given in the TGD on the effects assessment for intermittent releases (section 3.3.2 of part II of [3]). Because simazine is a herbicide with a specific mode of action and the most sensitive organism is a plant, it is deemed adequate in this case to only use a reduced assessment factor of 10 (instead of 100).

MAC-QS = 42 µg/l / AF (10) = 4.2 µg simazine / l

8.1.2 Quality standards for water derived by statistical extrapolation

Annual average quality standard (AA-QS)

In the UK-report [5] a range of different selections of single-species NOEC data were analysed by means of statistical extrapolation, i.e. calculating the 5-percentile of the data set assuming log-normal distribution. Results for the different SSDs do not differ that much (the 5-percentile cut-off values (≈ HC5) range from 2.3 to 6.4 µg/l; see section 6.1 and Annex 2).

As cyanobacteria, algae and higher plants are the most sensitive organisms (see table A1; simazine is a herbicide with a specific mode of action on the photosynthetic system), it should be considered to base the AA-QS on a SSD set up specifically with long-term NOEC data of the most sensitive organisms, i.e. primary producers (algae and higher plants). Respective calculations in the UK-report with data meeting the quality requirements for quality standard derivation (full report of study parameters such as study duration, effects observed, endpoint etc.) resulted in 5-percentile cut-off values of 3.9 µg/l if the most sensitive NOEC per species were used (Annex 2, figure 18) and 5.0 µg/l if the geometric means of the species NOECs serves as input data (Annex 2, figure 20). Because the latter data set is in agreement with the recommendation of the TGD to calculate geometric means in case more than one result for the same endpoint, effect and study duration is available for a species, this SSD is used as basis for the derivation of the AA-QS.

Using the ETX-software [6] (which is based on the statistical extrapolation method for calculating the 5-percentile of a log-normal distribution by Aldendberg and Jaworska [13]), it could be shown in

the UK-study that the data set is normally distributed (Anderson Darling goodness of fit = 0.193, p<0.1). The resulting sensitivity distribution for these primary producers single species NOECs (n=11) is shown in figure 1. The 5%-cut-off value (5%-COV ≈ HC5) is 5 μg/L, with a lower 95%-confidence limit of 1.49 μg/L and an upper confidence limit of 10.24 μg/L. [5]

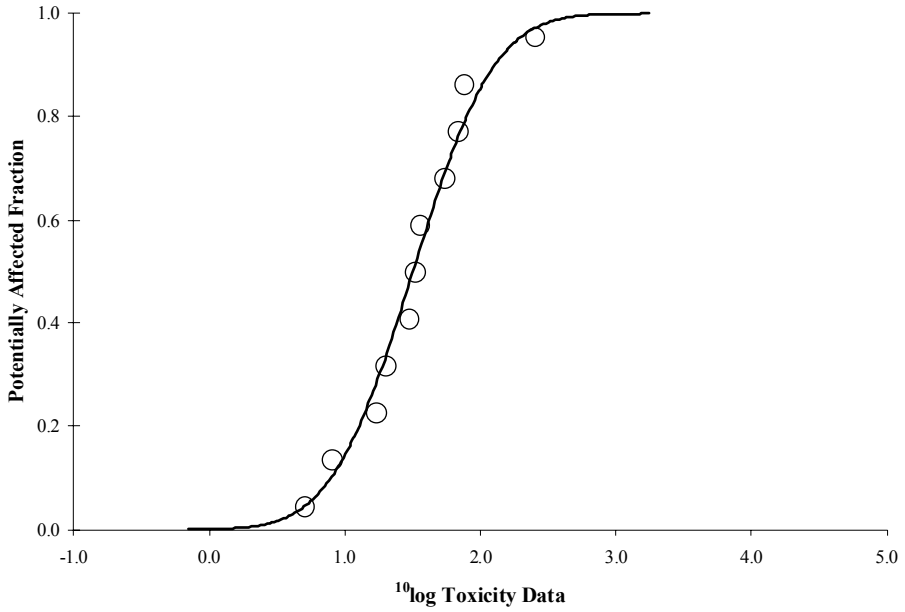

Figure 1: SSD for simazine based on geometric means of single species NOECs (primary producers only, input data see table A1)

For the derivation of the final PNEC (≈ quality standard) the TGD recommends to apply an additional assessment factor in the range of 5 – 1 on the 5%-COV, accounting for further uncertainties. With regard to the data available for simazine these uncertainties are:

1. *Statistical uncertainties around the 5th percentile:* The minimum species requirements of the TGD are not met (effects data for a second chordata species other than fish and an additional invertebrate species other than crustacean or insect are lacking). However, due to the specific mode of action of simazine with the photosynthetic apparatus, cyanobacteriae, algae and higher plants are the most sensitive species and these groups are covered by the SSDs. The factor between the SSD results (5%-cut off values) obtained with different data sets in the UK-report [5] is approximately 3 and the spread between the lower and the upper 95%-confidence limit of the SSD suggested as basis for the derivation of the QS_{water} in this data sheet is 7 and hence moderately high.
2. *Representativeness of the test systems for the water bodies to be covered by the QS:* The QS must be protective for all types of surface waters and communities that are addressed by the respective standard, as long as it is not possible to rule out that exposure to plant protection products may not occur in particular types of water bodies. This means that in the interpretation of studies an evaluation is necessary as to whether the test system can be considered representative for all water bodies that potentially are subject to plant protection product exposure. With regard to simazine, only single-species tests are available.

3. *Availability and test design of Higher Tier microcosm/mesocosm studies: Reliable m*icrocosm/mesocosm data are not available. 3 studies submitted in the context of the EU-risk assessment under CD 91/414/EEC were not considered sufficient to meet the requirement for microcosm/mesocosm data in the simazine monograph [1].

Taking account of the uncertainties addressed in points 1. – 3. above, an **assessment factor of 5**, in line with the assessment factor proposal made in the UK-study [5], is suggested to derive the QS.

$QS_{freshwater}$ = 5.0 µg/l / AF (5) = 1 µg simazine / l

The log Kow is only 2.18 and the water solubility is high. Thus the trigger criterion to calculate a corresponding $QS_{SPM.water}$ referring to the concentration of simazine in suspended particulate matter (SPM) is not met (see table 1a of [4]).

Because the AA-QS obtained by statistical extrapolation is based on the results of several single species studies with various primary producers, it is suggested to prefer the value obtained by this method over the figure obtained with the classical assessment factor approach taking only one figure, the most sensitive single species NOEC, into account.

8.2 Quality standard for sediment

The log Kow is only 2.18 and the water solubility is high. Thus the trigger criterion to calculate a $QS_{sediment}$ are normally not met (see table 1a of [4]). However, it is stated in the risk assessment monograph [1] that ca. 30% of applied simazine will be present in the sediment after 28 days.

Hence, it is deemed useful to derive an indicative value for sediment.

No data are available for sediment toxicity tests. According to the Manual (sections 4.3.2.3 & 4.3.2.4) [4] the $QS_{sediment}$ may be calculated using the equilibrium partitioning method in the absence of ecotoxicological data for sediment-dwelling organisms.

The equilibrium partitioning approach only considers uptake via the water phase. However, uptake may also occur via other exposure pathways like ingestion of sediment and direct contact with sediment. There is evidence from studies in soil that the proportion of the total dose remains low for chemicals with a log Kow up to 5. As the log Kow of simazine is only 2.18 exposure routes other than direct uptake via the water phase need not to be considered and the $QS_{sediment}$ is calculated as follows:

$$QS_{sed.wet\_weight}\ [mg.kg^{-1}] = \frac{Kp_{SPM\text{-}water}\ [3.88\ m^3/m^3]}{bulk\ density_{SPM.wet}\ [1{,}150\ kg/m^3]} * 1{,}000 * QS_{water}\ [mg/l]$$

with:

$K_{SPM\text{-}water}$ = f_{solid} (0.1) * Kp_{susp} (Koc (155) * foc (0.1) [l/kg]) / 1000 * RHO_{solid} (2500 kg/m^3) = 3.88 m^3/m^3 (sect 2.3.5 of [3])

bulk $density_{SPM.wet}$ = 1150 kg/m^3

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

QS_{water} = 0.001 mg/l

The TGD defines wet SPM as 90% vol/vol water (density 1 kg/l) and 10% vol/vol solids (density 2.5 kg/l), thus giving a wet density of (0.9 × 1) + (0.1 × 2.5) = 1.15 kg/l. The dry weight of solids is therefore 0.25 kg (per litre wet SPM) and thus the wet:dry ratio is 1.15/0.25 = 4.6.

This results in the following quality standards for sediment (wet and dry weight):

$QS_{sediment}$	3.4 µg/kg (wet wt)	15.5 µg/kg (dry wt)

The values derived by the EP-method should only be considered as tentative standards. In order to refine the quality standards for the sediment compartment long term tests conducted with benthic organisms are required. For the time being no reliable $QS_{sediment}$ can be derived.

8.3 Secondary poisoning of top predators

Since apparently no bioaccumulation occurs ($BCF_{fish} \approx 1$) and the log Kow is only 2.18, the calculation of a quality standard referring to the protection of top predators from secondary poisoning is not required (trigger value not met).

8.4 Quality standard referring to food uptake by humans

Simazine is classified as a carcinogen of category 3 but apparently shows no bioaccumulation ($BCF_{fish} \approx 1$). It therefore can be excluded that ingestion of food from aquatic environments could result in a significant uptake of simazine by humans.

The acceptable daily intake (ADI) for simazine was estimated in the risk assessment monograph (5 µg/kg bw/d).

In the Manual (section 4.3.2.6) [4] it is suggested that the ADI may not be exhausted for more than 10% by consumption of food originating from aquatic sources. For a person weighing 70 kg this results in an acceptable daily intake of 35 µg simazine per day.

The average fish consumption of an EU citizen is 115 g d-1 (TGD [3]). Thus, 115 g edible fish tissue (or seafood) must not contain more than 35 µg simazine.

$$\mathbf{QS_{hh.food}} = \frac{35\ \mu g\ Simazine}{115 g\ seafood\ consumption} * 1000\ g = \mathbf{304\ \mu g\ Simazine\ /\ kg\ seafood}$$

With a BCF of 1 the corresponding concentration in water is 304 µg/l.

8.5 Quality standard for drinking water abstraction

The imperative A1 value referring to drinking water abstraction by simple treatment is 1 µg/l for the total amount of pesticides (Council Directive 75/440/EEC). The drinking water standard (DWS) set in CD 98/83/EC is 0.1 µg/l for individual pesticides.

The DWS is a limit value never to be exceeded at the tap. The MAC-QS (ECO) derived for the protection of the freshwater community (cf. section 8.1) may therefore not suffice to allow for compliance with the DWS if only simple purification techniques (category A1 of CD 75/440/EEC, i.e. filtration and disinfection) are used for the abstraction of drinking water from surface water bodies according to Art. 7 of the WFD.

An assessment by experts in drinking water technology with regard to the question which fraction of the amount of simazine present in raw water can be removed by usual simple treatment procedures might be helpful. If the respective fraction were known, this figure could be used

together with the drinking water standard to set the maximum acceptable concentration in surface water bodies designated for the **a**bstraction of **w**ater **i**ntended for **h**uman **c**onsumption (AWIHC).

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

8.6 Overall quality standard

1 µg/l simazine may apply as overall annual-average quality standard (AA-QS) for all types of surface waters covered by the Water Framework Directive. If the drinking water standard is exceeded in areas designated for the abstraction of water intended for human consumption in accordance with Art. 7 of the WFD, specific measures need to be taken in order to guarantee compliance with the drinking water standard at the tap.

9 References

[1] UK Rapporteur Monograph, Council Directive 91/414/EEC: Simazine, Volumes 1-3 (Report and Proposed Decision of the United Kingdom made to the European Commission under Article 7(1) of Regulation 3600/92), Levels 1-4, Annexes A & B; December 1996.

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

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[18] ESIS: European Chemicals Bureau – ESIS (European Substances Information System), January 2005. http://ecb.jrc.it/existing-chemicals/ ⇒ tick ESIS button, then enter CAS or EINECS number of substance.

ANNEX 1: Consolidated data base – simazine aquatic toxicity [5]

Table A1: Simazine single species data [5]. References with a prefix 'n' refer to data on the Alterra database and 'cd Syngenta' refers to data supplied to Alterra by Syngenta. The left column highlights the data used for setting up the SSD on that the derivation of the AA-QS is based on. (Concentration = NOEC or equivalent)

Taxon	Species Latin Name	Effect	Duration (days)	Concentration (ug/l)	Reference	NOEC(or geom. mean) used for SSD (µg/l)
Vertebrate	*Carassius auratus*	-	365	2500	n86	
Vertebrate	*Lepomis macrochirus*	-	365	2500	n1527	
Vertebrate	*Morone saxatilis*		25	3000	CD Syngenta [80]	
Vertebrate	*Oncorhynchus mykiss*	Mortality	21	10000	CD Syngenta [891146]	
Vertebrate	*Oncorhynchus mykiss*	Mortality	21	700	CD Syngenta [1616]	
Vertebrate	*Oncorhynchus mykiss*	Mortality	28	8400	CD Syngenta [1907]	
Vertebrate	*Pimephales promelas*	-	120	1200	n3255	
Invertebrate	*Chironomus riparius*	Emergence	27	200	PSM-Datenbank	
Invertebrate	*Crassostrea virginica*	-	7	1000	n163	
Invertebrate	*Daphnia magna*	Reproduction	21	140	CD Syngenta [163]	
Invertebrate	*Daphnia magna*	Reproduction	21	36	CD Syngenta [163]	
Invertebrate	*Daphnia magna*	Reproduction	21	100	CD Syngenta [1617]	
Alga	*Anabaena flos-aqua*	Growth	5	20	CD Syngenta [164a]	20
Alga	*Chlamydomonas reinhardtii*	Growth	4	17	n7774	17
Alga	*Chlorococcus sp.*	Growth	14	8	Shuker et al. (1986)	8
Alga	*Chlorella pyrenoidosa*	Growth	5	52	n7791	29.73
Alga	*Chlorella pyrenoidosa*	Growth	5	17	Hiranpradit et al. (1992)	
Alga	*Navicula pelliculosa*	-	5	30	n2355	
Alga	*Navicula pelliculosa*	Growth	5	33	CD Syngenta [157]	33
Alga	*Scenedesmus quadricauda*	Growth	4	5	n9145	5
Alga	*Scenedesmus subspicatus*	Growth	3	11	CD Syngenta [164]	35.73
Alga	*Scenedesmus subspicatus*	Growth	3	64	CD Syngenta [1618]	
Alga	*Scenedesmus subspicatus*	Growth	3	21	CD Syngenta [941560]	
Alga	*Scenedesmus subspicatus*	Growth	3	44	CD Syngenta [1731]	

Taxon	Species Latin Name	Effect	Duration (days)	Concentration (ug/l)	Reference	NOEC(or geom. mean) used for SSD (µg/l)
Alga	*Scenedesmus subspicatus*	Growth	3	80	CD Syngenta [991597]	
Alga	*Scenedesmus subspicatus*	Growth	3	40	CD Syngenta [991597]	
Alga	*Raphidocellus subcapitata*	-	5	30	n3531	
Alga	*Raphidocellus subcapitata*	Growth	5	68	CD Syngenta [1579]	68
Alga	*Skeletonema costatum*	-	5	250	n3655	
Alga	*Skeletonema costatum*	Growth	5	250	CD Syngenta [154a]	250
Macrophyte	*Lemna gibba*	-	14	50	n1407	
Macrophyte	*Lemna gibba*	Frond number	14	54	CD Syngenta [1575]	54
Macrophyte	*Lemna minor*	Biomass	4	75	18093	75

Table A2: Simazine data taken from 91/414 monograph (1996) and used in reference [5]. (Concentration = NOEC or equivalent)

Taxon	Species Latin Name	Effect	Duration (days)	Concentration (ug/l)
Alga	*Scenedesmus subspicatus*	Growth	3	11
Alga	*Raphidocellus subcapitata*	Growth	5	69
Alga	*Anabaena flos-aquae*	Growth	5	20
Alga	*Navicula pelliculosa*	Growth	5	33
Alga	*Skeletonema costatum*	Growth	5	250
Macrophyte	*Lemna gibba*	Frond number	14	54
Vertebrate	*Oncorhynchus mykiss*	Growth	21	3200
Invertebrate	*Daphnia magna*	Reproduction	21	36
Invertebrate	*Ceriodaphnia dubia*	Reproduction	7	100

ANNEX 2:
Analysis of data in the report by the UK Environment Agency [5]

Analysis of single species tests for all taxa

Most sensitive NOEC used for the most sensitive endpoint

The most sensitive datum was a NOEC of 5 ug/L for 96-h growth of the alga *Scenedesmus quadricauda*. An AF of 10 applied to this datum would produce a QS of 0.5 ug/L. An Anderson-Darling Goodness of Fit test showed that the whole data set was normally distributed (AD GoF=0.69, p<0.05). The SSD (n=19) is shown in Figure 13. The HC5 was 2.293 ug/L, with an LCL of 0.587 ug/L and a UCL of 8.675 ug/L.

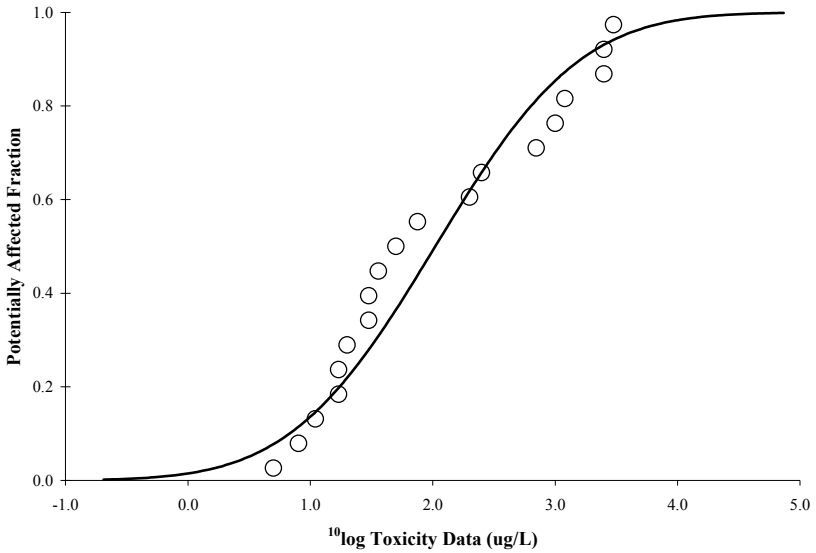

Figure 13. SSD for most sensitive data from single species laboratory tests with simazine (n=19).

Most sensitive NOEC for plant data

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.242, p<0.1). The SSD (n=11) is shown in Figure 14. The HC5 was 3.88 ug/L, with an LCL of 1.14 ug/L and a UCL of 7.93 ug/L.

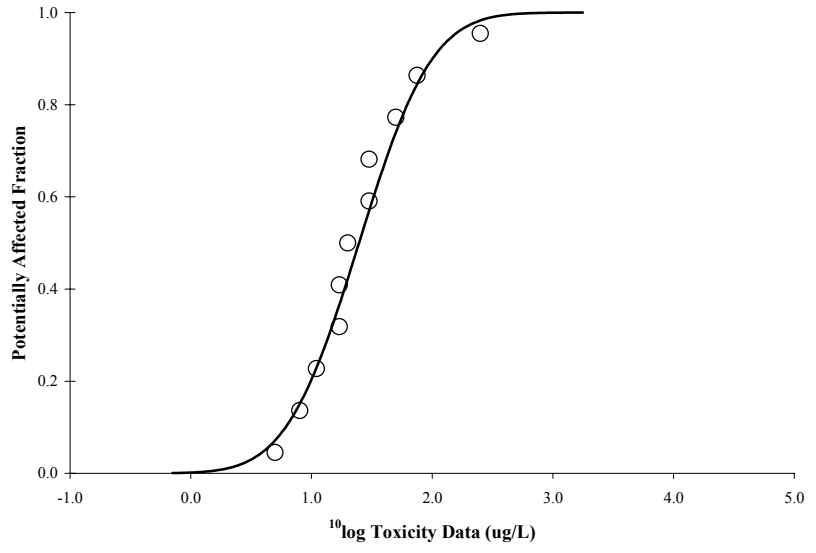

Figure 14 SSD for most sensitive data from single species laboratory plant (algae and macrophyte) tests with simazine (n=11).

Geometric mean NOEC used for the most sensitive endpoint

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.662, p<0.05). The SSD (n=19) is shown in Figure 15. The HC5 was 3.708 ug/L, with an LCL of 0.74 ug/L and a UCL of 10.12 ug/L.

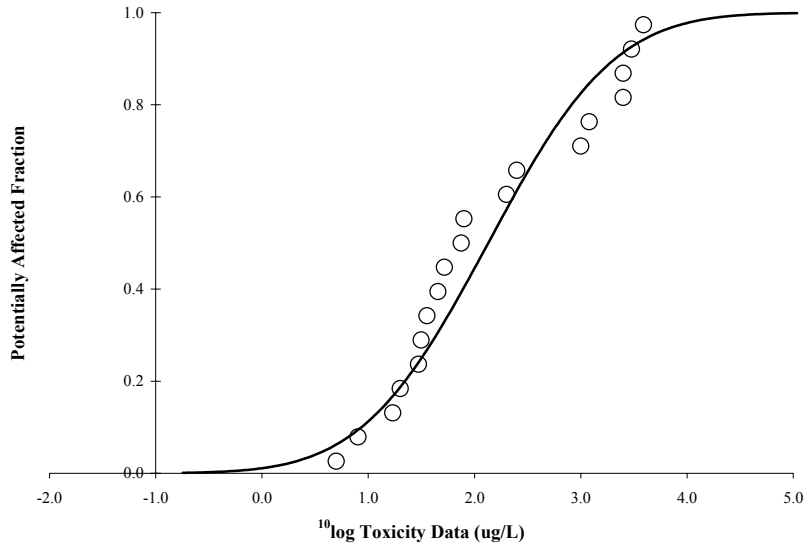

Figure 15 SSD for geometric mean data from single species laboratory tests with simazine (n=19).

Geometric mean NOECs for plant data

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.236, p<0.1). The SSD (n=11) is shown in Figure 16. The HC5 was 5.01 ug/L, with an LCL of 1.53 ug/L and a UCL of 10.04 ug/L.

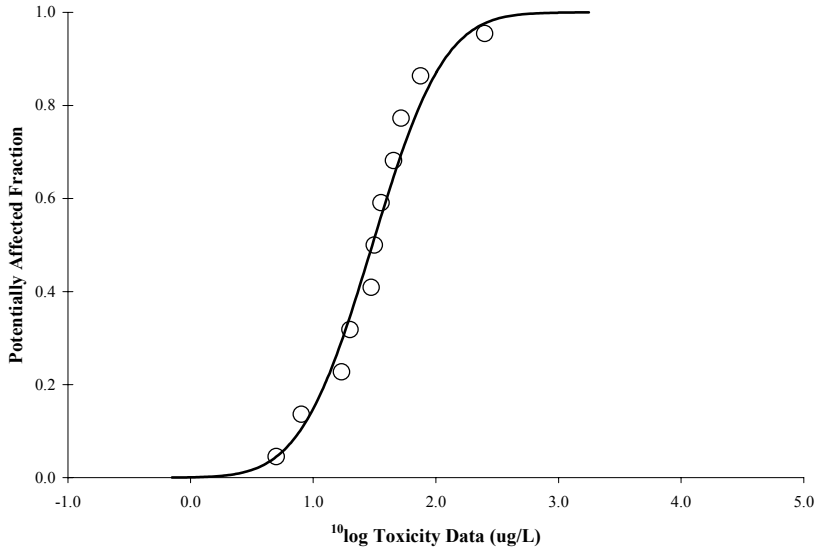

Figure 16 SSD for geometric mean data from single species plant (algae and macrophyte) laboratory tests with simazine (n=11).

Analysis of single species tests for which full data are available in Appendix 3

Most sensitive NOEC used for the most sensitive endpoint

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.232, p<0.1). The SSD (n=14) is shown in Figure 17. The HC5 was 3.81 ug/L, with an LCL of 1.04 ug/L and a UCL of 8.64 ug/L.

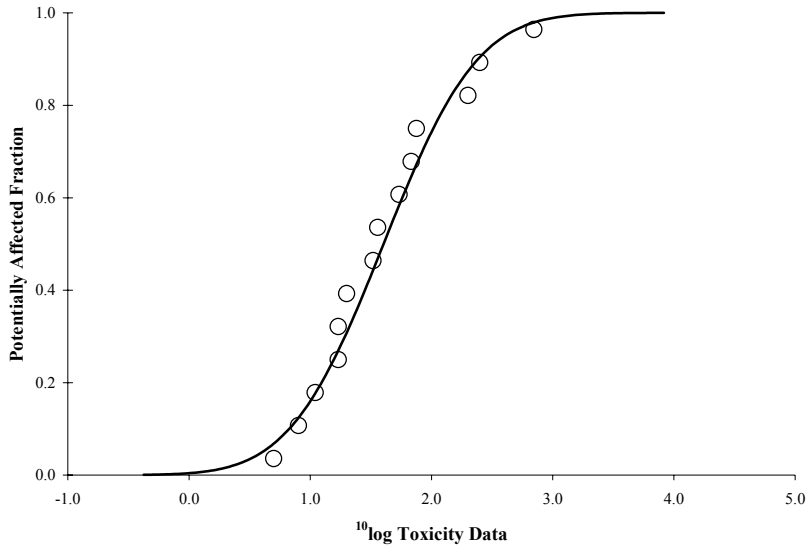

Figure 17 SSD for most sensitive data from single species laboratory tests with simazine (n=14).

Most sensitive NOEC for plant data

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.21, p<0.1). The SSD (n=11) is shown in Figure 18. The HC5 was 3.91 ug/L, with an LCL of 1.09 ug/L and a UCL of 8.26 ug/L.

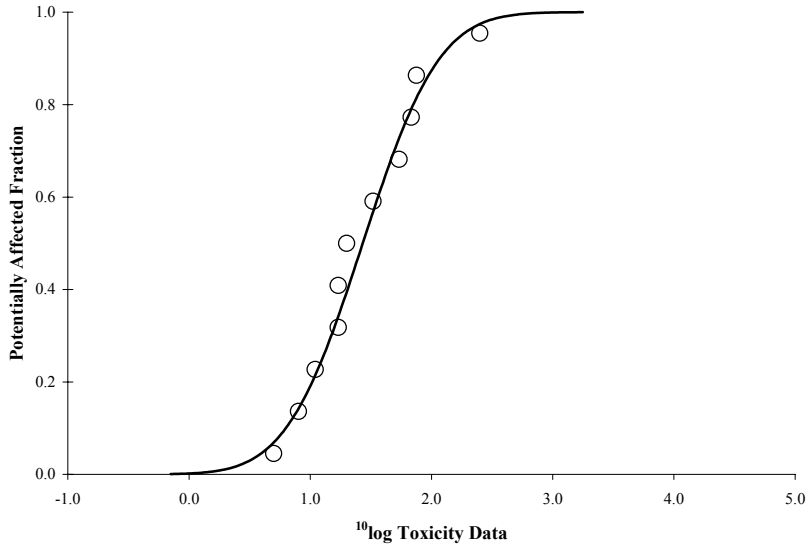

Figure 18 SSD for most sensitive data from single species laboratory tests with plants (algae and macrophytes) and simazine (n=11).

Geometric mean NOEC used for the most sensitive endpoint

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.46, p<0.1). The SSD (n=14) is shown in Figure 19. The HC5 was 3.43 ug/L, with an LCL of 0.74 ug/L and a UCL of 8.97 ug/L.

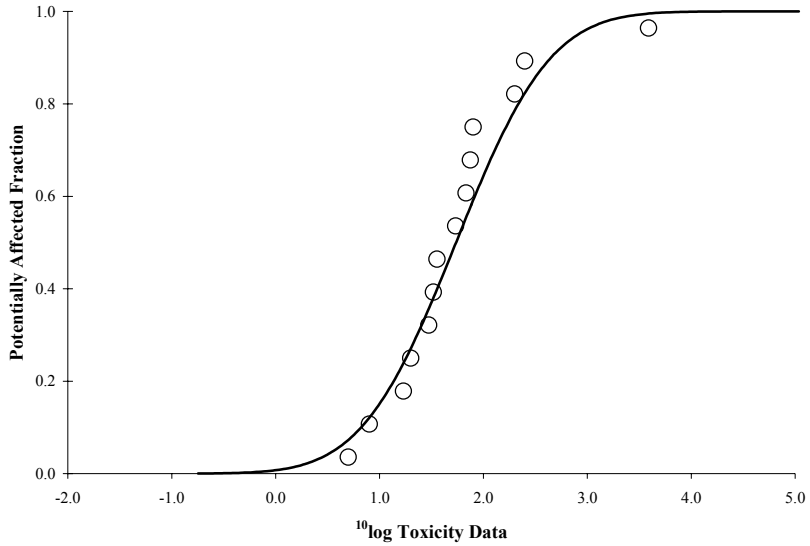

Figure 19 SSD for geometric mean data from single species laboratory tests with simazine (n=14).

Geometric mean NOECs for plant data

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.193, p<0.1). The SSD (n=11) is shown in Figure 20. The HC5 was 5.03 ug/L, with an LCL of 1.49 ug/L and a UCL of 10.24 ug/L.

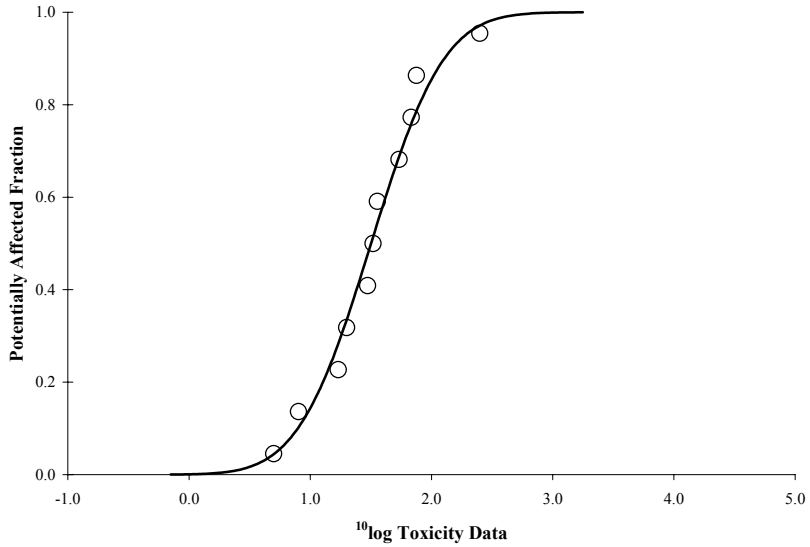

Figure 20 SSD for most sensitive data from single species laboratory tests with plants (algae and macrophytes) and simazine (n=11).

Analysis of single species tests in Appendix 4 (from 91/414 monograph)

Long-term toxicity data in the 1996 monograph for simazine (Appendix 4) do not comply with the requirements for number and diversity of data stated in the TGD. However, SSDs have been constructed for these data for comparison with those above. Multiple data for the same species and endpoints were not found in the monograph, so analyses are for all species and also for plants alone.

All species

An Anderson-Darling Goodness of Fit test showed that the data set was normally distributed (AD GoF=0.53, p<0.1). The SSD (n=9) is shown in Figure 21. The HC5 was 4.32 ug/L, with an LCL of 4.73 ug/L and a UCL of 14.38 ug/L.

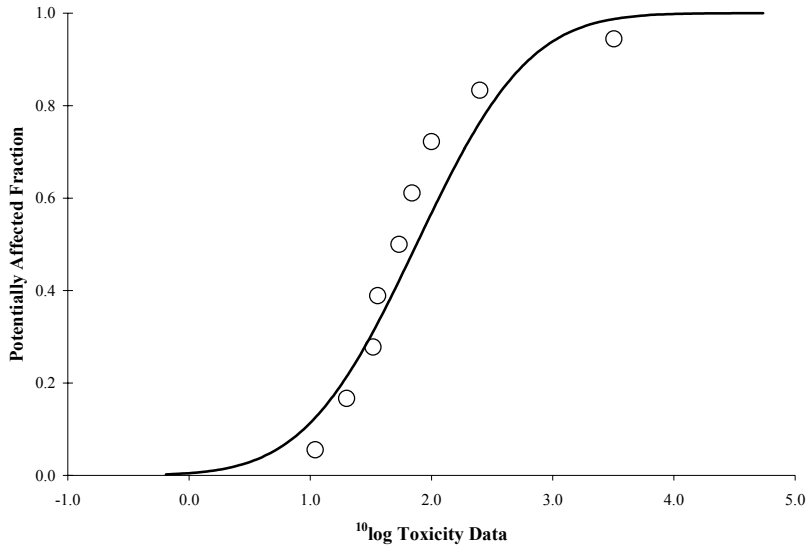

Figure 21 SSD for all data from 91/414 monograph for simazine (n=9).

Plants

An Anderson-Darling Goodness of Fit test showed that the data set (n=6) was normally distributed (AD GoF=0.201, p<0.1), although this test does not perform particularly well below n=8. The SSD is shown in Figure 22. The HC5 was 6.51 ug/L, with an LCL of 0.78 ug/L and a UCL of 16.83 ug/L.

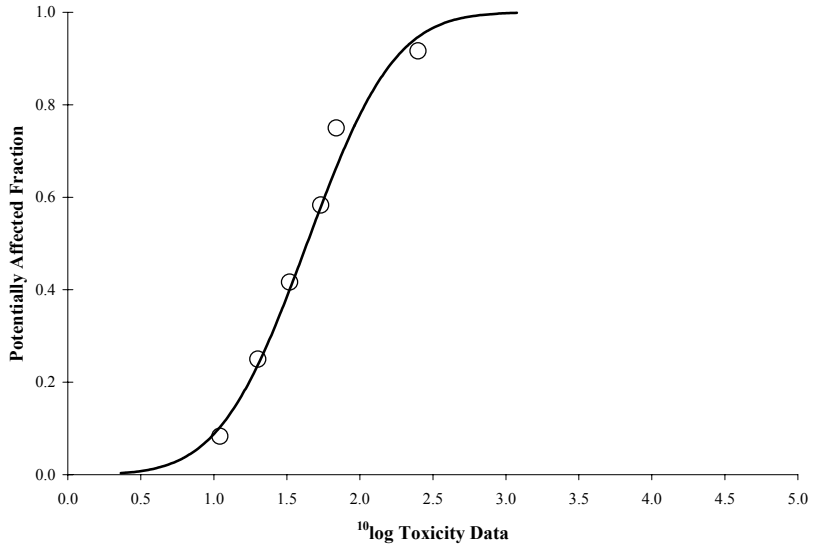

Figure 22 SSD for plant (algae and macrophyte) data from 91/414 monograph for simazine (n=6).