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SCIENTIFIC COMMITTEE ON PLANTS **SCP/SIMAZINE/002-Final**

OPINION OF THE SCIENTIFIC COMMITTEE ON PLANTS ON SPECIFIC QUESTIONS FROM THE COMMISSION CONCERNING THE EVALUATION OF SIMAZINE IN THE CONTEXT OF COUNCIL DIRECTIVE 91/414/EEC

(Opinion adopted by the Scientific Committee on Plants on 30/01/ 2003)

A. TITLE

OPINION OF THE SCIENTIFIC COMMITTEE ON PLANTS ON SPECIFIC QUESTIONS FROM THE COMMISSION CONCERNING THE EVALUATION OF SIMAZINE IN THE CONTEXT OF COUNCIL DIRECTIVE 91/414/EEC
(Opinion adopted by the Scientific Committee on Plants on 30/01/2003.)

B. TERMS OF REFERENCE

Simazine is a herbicide among the existing active substances selected in the first review list published in Commission regulation 3600/92. On the basis of the evaluation report established by the United Kingdom as Rapporteur Member State (RMS), the substance has been peer reviewed with Member State experts and consequently discussed with the 15 Member States in the working group "Plant Protection Products - Evaluation" of the Standing Committee on Plant Health.
The main problem identified during the review relates to the leaching potential of the active substances and their breakdown products. The Rapporteur has evaluated extensive modelling data and also monitoring data from several Member States and has identified use conditions, which are unlikely to lead to a contamination of groundwater. However, a consultation of the Scientific Committee on Plants appears necessary to have an additional, independent opinion on the following questions:

QUESTION 1: Can the Committee comment on the approach taken by the Rapporteur for the calculation of predicted environmental concentrations (PEC[1]) in groundwater ?

QUESTION 2: Does the Committee agree that the available monitoring data show that in large areas, application of simazine under the intended conditions (i.e. max. 0.75 kg a.s./ha in northern Member States and max. 1.0 kg a.s./ha in southern Member States on maize and sorghum in spring) will not result in concentrations of the active substance nor its breakdown products in excess to 0.1 μg/L in groundwater ?

C. OPINION OF THE COMMITTEE

Opinion on question 1:
The Rapporteur reported a number of studies for the calculation of PEC in groundwater but considered the first and higher tier FOCUS[2] modelling approaches reported on p. 56-59 of Addendum 4 to Annex B of September 2001 as most definitive. Therefore the Committee restricts its comments to these approaches.

The results of calculations of PEC in groundwater are very sensitive to the input parameters that describe the sorption and transformation of simazine and its metabolites in soil. Therefore the Committee's comments consist of an assessment of these input parameters.

[1] PEC: Predicted Environmental Concentration

[2] FOCUS: Forum for international Co-ordination of pesticide fate models and their USe

With respect to the first tier approach, the Committee accepts the sorption and transformation parameters for simazine and its de-ethylsimazine metabolite with exception of the K_{OC}[3] used for simazine. The Committee considers this K_{OC} too high, (which results in too low simulated concentrations in groundwater).

In the higher tier modelling approach increased sorption coefficients were used for simazine and de-ethylsimazine to take account of the phenomenon of increased sorption with time. The Committee does not accept these increased sorption coefficients because the measurement procedure was inappropriate and because the evidence for simazine was based on measurements with atrazine. In this modelling approach also shorter half-lives were used to describe enhanced transformation resulting from repeated applications. The Committee does not accept the shorter half-life of simazine because it is based on measurements in two soils only. The Committee accepts the shorter half-life of de-ethylsimazine because this is the same molecule as de-isopropylatrazine (see the Committee's answer to the question for atrazine). However, the Committee accepts the shorter half-life of de-ethylsimazine only for the FOCUS scenarios with pH above 6 because no evidence of enhanced transformation rates for soils with pH below 6 was presented.

As a result of the above considerations, the Committee does not accept the reported first and higher tier calculations of the environmental concentrations (PEC) in groundwater.

<u>Opinion on question 2:</u> The Committee considered the available evidence from one lysimeter study and of monitoring studies. The lysimeter study resulted in annual average concentrations of 0.08 µg/L for simazine and of 0.2 µg/L for de-ethylsimazine. The Committee cannot interpret this result because the reported rainfall was improbably high.
Results of a range of monitoring studies were available. However their reports in the monograph contained insufficient information on a) the simazine use pattern in the areas considered, b) the sampling strategy, and c) groundwater depths. The Committee considers the resulting interpretation problems so serious that they can even not be solved by considering the reduction in use rates proposed by the notifier. Therefore the Committee does not agree that available monitoring data demonstrate that concentrations of the active substance or its breakdown products will not exceed 0.1µg/l in groundwater.

[3] Koc : Organic carbon adsorption coefficient.

A. TITLE

REPORT OF THE SCIENTIFIC COMMITTEE ON PLANTS ON SPECIFIC QUESTIONS FROM THE COMMISSION CONCERNING THE EVALUATION OF SIMAZINE IN THE CONTEXT OF COUNCIL DIRECTIVE 91/414/EEC

B. TABLE OF CONTENTS

C. SOURCE DOCUMENTS MADE AVAILABLE TO THE COMMITTEE

1. SCP-SIMAZ 001: Terms of reference
2. SCP-SIMAZ 003: Monograph (DAR) and Proposed Decision of the United Kingdom made to the European Commission under Article 7(1) of Regulation 3600/92 ; Volume 1, December 1996.
3. SCP-SIMAZ 004: Addendum to Monograph, Volume 2, Annex A, list test and studies, December 1996.
4. SCP-SIMAZ 005: Addendum to Monograph, Volume 2, Annex A, list test and studies, April 1999.
5. SCP-SIMAZ 006: Addendum 2 to Monograph, Volume 3, Annex B, December 1996, Summary, scientific evaluation and assessment.
6. SCP-SIMAZ 007: Addendum 2 to Monograph, Volume 3, Annex B, February 2000.
7. SCP-SIMAZ 008: Addendum 2 to Monograph Volume 3, Annex B, February 2001, occurrence in groundwater.
8. SCP-SIMAZ 009: Addendum 3 to Monograph Volume 3, Annex B, March 2001, FOCUS groundwater.
9. SCP-SIMAZ 010: Addendum 4 to Monograph Volume 3, Annex B, September 2001.
10. SCP-ATRA 011: Report Syngenta, Basel, Egli, H & H-P Buser, 2002. Statement: EU review of atrazine and simazine-Proposal of safe use areas with regard to residues in ground- and surface water, 17 pp.
11. SCP-ATRA 012: Report Syngenta, Basel: Egli, H & H-P Buser, 2002. Position paper: EU review of atrazine and simazine- Comments to questions referred to SCP concerning the assessment of the risk of atrazine and simazine to groundwater, 16 pp.

D. SCIENTIFIC BACKGROUND ON WHICH THE OPINION IS BASED

I. Question 1:

Can the Committee comment on the approach taken by the Rapporteur for the calculation of predicted environmental concentrations (PEC) in groundwater?

Opinion on question 1:

The Rapporteur reported a number of studies for the calculation of PEC in groundwater but considered the first and higher tier FOCUS modelling approaches reported on p. 56-59 of Addendum 4 to Annex B of September 2001 as most definitive. Therefore the Committee restricts its comments to these approaches.

The results of calculations of PEC in groundwater are very sensitive to the input parameters that describe the sorption and transformation of simazine and its metabolites in soil. Therefore the Committee's comments consist of an assessment of these input parameters.

With respect to the first tier approach, the Committee accepts the sorption and transformation parameters for simazine and its de-ethylsimazine metabolite with exception of the K_{OC} used for simazine. The Committee considers this K_{OC} too high (which results in too low simulated concentrations in groundwater).

In the higher tier modelling approach increased sorption coefficients were used for simazine and de-ethylsimazine to take account of the phenomenon of increased sorption with time. The Committee does not accept these increased sorption coefficients because the measurement procedure was inappropriate and because the evidence for simazine was based on measurements with atrazine. In this modelling approach also shorter half-lives were used to describe enhanced transformation resulting from repeated applications. The Committee does not accept the shorter half-life of simazine because it is based on measurements in two soils only. The Committee accepts the shorter half-life of de-ethylsimazine because this is the same molecule as de-isopropylatrazine (see the Committee's answer to the question for atrazine). However, the Committee accepts the shorter half-life of de-ethylsimazine only for the FOCUS scenarios with pH above 6 because no evidence of enhanced transformation rates for soils with pH below 6 was presented.

As a result of the above considerations, the Committee does not accept the reported first and higher tier calculations of the environmental concentrations (PEC) in groundwater.

Scientific background on which the opinion is based

I.1. Introduction

Results of calculations of $PEC_{groundwater}$ depend strongly on the model-input parameters that describe sorption and transformation rate of the substances considered. Therefore the Committee analyses firstly the available information on these parameters before considering the different calculation approaches

I.2. Transformation

I.2.2. Soil metabolism in topsoils

Laboratory studies with aerobic soils showed that simazine transforms into de-ethylsimazine (DES) and hydroxysimazine (HS). The DES transformes further into dediethylsimazine (DDES). In studies with two soils, soil bound residues were 47 and 66% at the end of the studies and 8 to 19% evolved as $^{14}CO_2$ (the radioactive label must have been in the triazine ring although this was not reported). In these studies maximum percentages of 10-24% were reported for DES, 1-10% for DDES and 4-6% for HS. A study with another soil resulted in different percentages but the Committee agrees with the Rapporteur that this soil is less relevant (its pH was 8.7 which is very high).

The Rapporteur concluded that maximum levels of DES (and HS) did not exceed consistently 10% of the simazine dose both in laboratory and field experiments. The rapporteur concluded from this "that the metabolites in soil are not significant in the wider environmental context". The Committee analysed all reported field experiments in which DES was analysed. For in total 12 field experiments maximum percentage of DES were estimated assuming a dry bulk density of 1.3 kg/L: the percentages were <1, 2, 4, 4, 6, 9, 10, 11, 13, 17, 18, 19%. The three lowest percentages were based on studies in which only one sampling was carried out so these are no reliable maxima. In a thirteenth experiment DES remained below the detection limit but this was not specified. Given the results from these 13 field experiments, the Committee disagrees with the assessment of the Rapporteur of the maximum percentage DES and concludes that half of the relevant experiments show maximum percentage ≥ 10%.

In the first tier FOCUS modelling approach the notifier assumed that 75% of the simazine was transformed into DES. The Rapporteur considered this percentage plausible and appropriately justified (this percentage was based on the study in which a maximum percentage of DES of 24% was reported). The Committee considers this assessment of the formation of DES by the Rapporteur not consistent with the earlier conclusion of the Rapporteur that maximum levels of DES did not exceed consistently 10% of the simazine dose.

I.2.2. Transformation rates in topsoils

Laboratory studies on the transformation rate of simazine were reported for 20 soils (based on the monograph references Ellgehausen, 1985, Muller-Kallart, 1993 and Walker & Thompson, 1977). None of the studies were carried out at reference conditions (20^{o}C and a matric suction of 100 hPa). The Committee calculated these half-lives back to these reference conditions following FOCUS 2000 (p. 90 and 92) which resulted in an average half-life at reference conditions of 51 days.

Field persistence studies at seven sites in five EU countries showed that the simazine persistence in the field could be explained well from laboratory half-lives for all but one site (for this site the decline in the field was faster than expected on the basis of the laboratory studies). Thus the Committee did not further analyse the available field experiments for simazine and assumed that the laboratory half-lives can be used for assessment of simazine leaching.

Only one measurement of the transformation rate of DES was reported. The half-life at 25°C and at a matric suction of 330 hPa was 32 days. This corresponds with a half-life of 47 days at 20°C (using a Q_{10}[4] of 2.2 as recommended by FOCUS 2000, p. 92). The half-life at the reference condition could not be calculated back to the reference matric suction of 100 hPa because the soil texture was not reported. The correction factor (as derived from FOCUS, 2000, p. 90) ranges from 0.68 to 0.93 depending on the selected soil texture so the estimated half-life at reference conditions ranges from 32 to 44 days. At p. 61 of Addendum 4 to Annex B of the atrazine monograph, the Rapporteur briefly mentions three half-lives of de-isopropylatrazine in soil at reference conditions (24, 27 and 48 days). The studies from which these were derived were not summarized in the monograph (de-isopropylatrazine is the same molecule as DES).

I.3. Sorption

The monograph describes results of adsorption studies with simazine, DES, DDES and HS from eight literature references. Four of these references report Freundlich[5] exponents exceeding 1.0 for at least 50% of the isotherms. This is a strong indication of systematic errors because it is unlikely that Freundlich exponents of pesticide-soil isotherms exceed 1.0. Therefore results from these references are not further considered. One of the four remaining references measured simazine sorption at one concentration level only but for 18 soils. For five soils, the decrease in the concentration in the liquid phase was less than 10% which is insufficient for an accurate adsorption measurement; therefore the Committee ignored these results. The average K_{OC} of the remaining 13 soils was 96 L/kg and its range was 54-160 L/kg. The average K_{OC} of the remaining three references based on in total four soils was 102 L/kg and the K_{OC} range was 63-183 L/kg. In view of the similarity between these results the Committee considers the average K_{OC} of all acceptable studies as the best estimate (i.e. 98 L/kg). The average Freundlich exponent was 0.86 (based on measurements with these four soils from the remaining three references).

The Committee did thus not accept the adsorption measurements of DES reported in the simazine monograph. However, the Committee's assessment of the atrazine calculations resulted in K_{OC} values of 53, 55, 71 and 107 L/kg and an average Freundlich coefficient of 0.97 for de-isopropylatrazine which is the same molecule as DES.

I.4. Assessment of approaches for PEC-groundwater calculations

The Rapporteur reported a number of modelling studies including calculations for non-FOCUS scenarios. These calculations were carried out before the FOCUS groundwater scenarios had become available. The Committee restricted its assessment to the calculations with FOCUS scenarios because the Rapporteur considered these as most definitive (see p. 59 of Addendum 4 to Annex B of September 2001).

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[4] Q10: factor describing the increase of the transformation rate of pesticides in soil resulting from a temperature increase of 10°Celsius.

[5] The Freundlich exponent describes the curvature of the sorption isotherm. A value of 1.0 implies a linear isotherm and a value below 1.0 implies a continuously decreasing slope of the sorption isotherm.

The first study containing FOCUS scenario calculations is reported at p. 20-21 of Addendum 2 to Annex B (dated February 2001). The Rapporteur concludes that these calculations need to be repeated with different input parameters. Therefore the Committee did not assess these calculations.

The second study containing FOCUS scenario calculations is reported on p. 56 of Addendum 4 to Annex B of September 2001. These calculations are reported as "first tier modelling approaches" and were carried out with FOCUS PRZM[6] 1.1.1 using the sorption and transformation parameters shown in Table 1. Simazine was applied at a rate of 1.5 kg/ha to maize (pre-planting) every year for all FOCUS scenarios except Jokioinen where it was applied at the same rate to soil around bush berries and strawberries.

Table 1: Sorption and transformation parameters used in calculations with FOCUS PRZM 1.1.1 for the first tier modelling approach.

Substance	K_{OC} (L/kg)	Freundlich exponent	Half-life (d) at reference conditions	Percentage formed from simazine
Simazine	141	0.8	48	-
DES	57	0.95	27	75

The Committee does not accept the K_{OC} of simazine because it differs significantly from the average value of 98 L/kg that the Committee derived from the monograph. The Committee accepts the other sorption and transformation parameters. However, it considers the 75% formation of DES as a realistic worst-case value: this value is derived from the study with the highest maximum DES percentage (i.e. 24%).

The third study containing FOCUS scenario calculations is reported on p. 57-59 of Addendum 4 to Annex B of September 2001. These calculations are reported as "higher tier modelling approach" and were also carried out with FOCUS PRZM 1.1.1. The application rate and crops were the same as in the second study.

In this third study the same sorption parameters were used as in the second series but now the K_{OC} values increased with time as follows:
- an increase by a factor 1.3 at 7 days after application for simazine,
- an increase by a factor 1.7 at 1 day after application for DES.

The increase for simazine was extrapolated from atrazine and the increase for DES was identical to the value derived from de-isopropylatrazine (which is the same molecule as DES). As described in its assessment of the atrazine calculations, the Committee does not accept these increases for atrazine and de-isopropylatrazine and consequently does not accept them for simazine and DES either.

In this third study, shorter half-lives were used for simazine and DES. Their half-lives were decreased by a factor 2.3 to account for enhanced transformation. However, the only basis for this were experiments with two soils. The first experiment showed that simazine was mineralised faster to $^{14}CO_2$ in a soil with 12 previous applications of atrazine compared to soils that had not had atrazine and simazine applied. The magnitude of the enhancement was comparable to that measured for atrazine in this soil. The second experiment was a field experiment that showed a first-order half-life of simazine of 59

[6] PRZM: Pesticide Root Zone Model

days on a plot without previous simazine application and a half-life shorter than 46 days on a plot that had a history of simazine use of 12 years. The factor 2.3 was the same as used for atrazine and was also based on atrazine. However, the Committee considers these two studies insufficient to support the factor 2.3 for simazine as well.

The Committee agrees with the Rapporteur that there is sufficient evidence for enhanced transformation of DES for soils with pH above 6 (see the assessment for atrazine). However, the enhanced transformation was assumed to take place for all FOCUS groundwater scenarios whereas four of the nine FOCUS scenarios considered have pH values equal to or below 6 (Hamburg, Okehampton, Porto and Jokioinen). The Committee considers the pH to be part of the scenario definition and does therefore not accept use of enhanced transformation rates for these scenarios. The Committee accepts use of enhanced transformation rates of DES for the FOCUS scenarios Kremsmünster, Chateaudun, Piacenza, Thiva and Sevilla.

As a result of the above considerations the Committee does not accept the results obtained with the higher tier modelling approach in this third study.

II Question 2:

Does the Committee agree that the available monitoring data show that in large areas, application of atrazine and simazine under the intended conditions (i.e. max. 0.75 kg a.s./ha in northern Member States and max. 1.0 kg a.s./ha in southern Member States on maize and sorghum in spring) will not result in concentrations of the active substance nor its breakdown products in excess to 0.1 µg/L in groundwater ?

<u>Opinion on question 2:</u> The Committee considered the available evidence from one lysimeter study and of monitoring studies. The lysimeter study resulted in annual average concentrations of 0.08 µg/L for simazine and of 0.2 µg/L for de-ethylsimazine. The Committee cannot interpret this result because the reported rainfall was improbably high.
Results of a range of monitoring studies were available. However their reports in the monograph contained insufficient information on a) the simazine use pattern in the areas considered, b) the sampling strategy, and c) groundwater depths. The Committee considers the resulting interpretation problems so serious that they can even not be solved by considering the reduction in use rates proposed by the notifier. Therefore the Committee does not agree that available monitoring data demonstrate that concentrations of the active substance or its breakdown products will not exceed 0.1µg/l in groundwater.

<u>Scientific background on which the opinion is based:</u>

II.1. Introduction

The applied dosages indicated in the question are lower than those used in the past (e.g. about 1 to 3 kg/ha in northern Member States). The Committee expects that the concentrations in groundwater are directly proportional to the dosage of simazine and has used this assumption in its considerations.
To answer the question, the Committee summarizes below the relevant data on simazine leaching that were made available.

II.2. Lysimeter study with fallow soil

A lysimeter study was conducted with a fallow sandy loam soil in Germany. A simazine dose of 2.7 kg/ha was applied in May 1989. The depth of the lysimeter was 1.1 m. The organic carbon content of the soil was not reported. Annual rainfall was about 1500 mm in the first year and about 800 mm in the second year. In January 1990, 620 mm rainfall was reported which seems unrealistically high and thus may be an error whereas the rapporteur did not comment on this value. The percolated amount of water was 75 and 69 % of annual rainfall in the first and second year, respectively. This would be 1100 and 550 mm. However the Committee has no confidence in the rainfall reported for January 1990 and therefore does also not trust these 1100 mm. The annual average concentration of simazine was 0.08 μg/L in the first year and 0.02 μg/L in the second year. For DES these figures were 0.2 μg/L in the first year and less than 0.03 μg/L in the second year. The average concentration of DDES over the two-year period was 0.04 μg/L. The Committee cannot assess the significance of this experiment because of the rainfall problem and because the organic carbon content of the soil was not reported.

II.3. Monitoring studies

Table 1 summarises information in the monograph on groundwater monitoring in a number of member states.

Table 1. Summary of groundwater monitoring studies with simazine in different Member States. The percentages refer to the percentage of the samples that exceeded a concentration of 0.1μg/L. Empty cells in the table imply that no information was available about this item.

Country	Period	Total number of samples	Region(s)	Ground water sampling depth (m)	%>0.1 μg/L for simazine	%>0.1 μg/L for DES
Germany		4345			4	
Sweden		230			1	
Italy		1889			2	
Italy	1997	106	Northern Italy, maize growing regions		0	
UK		27658			1	
UK	1992-94				0.4-2	
Netherlands		3			0	
Netherlands	1985-1994	79	5 specified municipalities	0-20	5	
Netherlands	1985-1994	96	5 specified municipalities			0
Netherlands	1986-1997	150		'undeep'	6	
Netherlands	1986-1997	170		'deep'	0.6	

Netherlands	1995-1996	29			0	
Netherlands		314		0-6		29[A]
Netherlands		80		>6		0[B]
Belgium	1990	75	25 specified municipalities		0	
Belgium	1991-1996	4509			1	
Belgium	2000	250	Flanders		3	
France	1998	13	Landes	9-60	0	
France	1998	4	Landes			0

A) The percentage refers to the detection limit which was not specified but was presumably 0.1 μg/L. The 90th percentile of all positive samples (92) was 0.13 μg/L.
B) The percentage refers to the detection limit which was not specified but was presumably 0.1 μg/L.

No information was given on the use of simazine in the areas that were sampled and on the soil properties. No information was provided on the sampling strategy. For the Dutch study, in the period 1985-1994, the rapporteur reported that some information on simazine use pattern was provided but could not be interpreted because it was in Dutch.

Because of the limited information provided the Committee cannot use the results of the above monitoring studies in its answer to the question. For example it is not clear which percentage of the samples could have contained simazine or DES (so non-relevant[7] negatives are not excluded) and to which extent non-agricultural uses like industrial weed control or point source contamination influenced the result (so non-relevant positives are not excluded either).

II. 4. Extrapolation from atrazine monitoring studies

The notifier provided the SCP with a document "EU review of atrazine and simazine - Comments to questions referred to SCP concerning the assessment of the risk of atrazine and simazine to groundwater". The notifier suggested that concentrations of simazine in groundwater and surface water would be lower than for atrazine after similar use in a given region because the K_{OC} of simazine would be lower than that for atrazine. Thus results of monitoring studies with atrazine could be used for assessment of simazine leaching. The Committee disagrees with this conclusion based on the following arguments:

1. The Committee's assessment of K_{OC} values resulted in an average value of 98 L/kg for simazine and of 107 L/kg for atrazine.
2. Leaching to groundwater is also strongly influenced by the transformation rate in soil.

The Committee found an average half-life of simazine at reference conditions of 51 days whereas the notifier reported a median value of atrazine of 30 days (not including soils that showed accelerated transformation; see opinion on atrazine).

[7] "non-relevant" refers to non-relevant groundwater samples for monitoring studies, in the context of this opinion it is not related to the term "non-relevant metabolite".

REFERENCE

FOCUS (2000) FOCUS groundwater scenarios in the EU review of active substances. Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference SANCO/321/2000 rev.2, 202 pp.

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