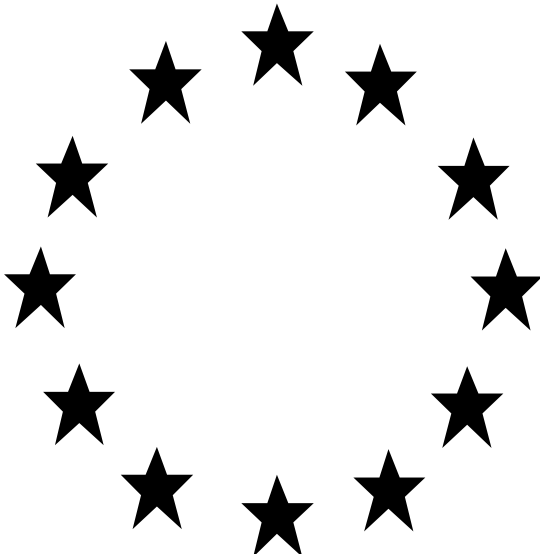

Final addendum to the

Additional Report

- public version -

Additional risk assessment provided by the rapporteur Member State Greece for the existing active substance

TRIFLURALIN

according to the Accelerated Resubmission Procedure laid down in Commission Regulation (EC) No. 33/2008

May 2009

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Council Directive 91/414/EEC

TRIFLURALIN

Addendum 1 to Additional Report to the DAR

Summary, Scientific Evaluation and Assessment

May 2009

Report and Proposed Decision of Hellas
made to the European Commission under Article 8 of 91/414/EEC

HELLENIC MINISTRY OF RURAL DEVELOPMENT AND FOOD
GENERAL DIRECTORATE OF PLANT PRODUCTION
DIRECTORATE OF PLANT PROTECTION
DEPARTMENT OF PESTICIDES
Hippokratous 3-5,
10164 Athens
Hellas

VOLUME 3
ANNEX B

RAPPORTEUR MEMBER STATES SUMMARY, EVALUATION AND ASSESSMENT OF THE DATA AND INFORMATION SUBMITTED

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VOLUME 3

B.8 ENVIRONMENTAL FATE AND BEHAVIOUR

The notifier has re-worked the aquatic degradation kinetics to produce a new system DT_{50} for sediment. This was derived from the existing water/sediment studies (Yon, D.A., 1993a &1993b, *see DAR*) by following the FOCUS kinetics guidance and is described in report GHE-P-12080. The rework of the FOCUS Step 3 and 4 analysis is described in amended report GHE-P-12083 for the soil incorporated uses. The notifier has also generated two reports, GHE-P-12081 and GHE-P-12082, to address GW contamination using appropriate input values. These RMS has provided all four reports in this Addendum.

B.8.1.2 RATE OF DEGRADATION

B.8.1.2.1a Laboratory studies - Aerobic degradation at 20°C

The following individual DT50's (Washbrooke, 1976 and Graper, L.K., 1989) were normalized to pF2 using a Walker coefficient of 0.7 and subsequently averaged:

Soil type	Moisture (MWHC)	Temperature, °C	DT_{50} (days)
Speyer 2.1	40%	22	136
Speyer 2.2	40%	22	356
Sandy loam	75%	22	154
Loam	75%	22	81
Clay loam	75%	22	179
		Geomean, 22°C:	**161**
		Geomean, 22°C, pF 2:	**115**
		Geomean, 20°C, pF 2:	**135**

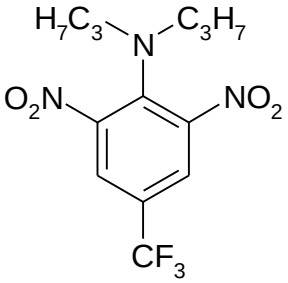
B.8.4 FATE AND BEHAVIOUR IN WATER (Annex IIA 7.2.1; Annex IIIA 9.2.1, 9.2.3)

B.8.4.3.2 Degradation in water/sediment systems

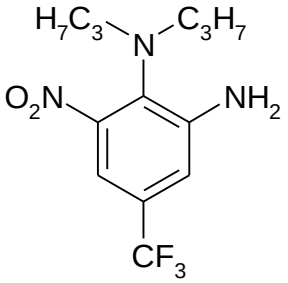
Yon, D.A., "Modeling the kinetics of the degradation of trifluralin in laboratory sediment-water test systems", Report No.: GHE-P-12080, 2009. Not published
Objective: To re-calculate a trifluralin DT_{50} for sediment by following the FOCUS kinetics guidance
GLP: Not applicable

1. Introduction

In support of the Annex I re-submission for trifluralin in the EU, according to directive 91/414/EEC, it is necessary to provide data on the kinetics of formation and decline of the parent and major metabolites in water sediment test systems according to the FOCUS guidance on degradation kinetics (Ref. 1). This allows assessment of the likelihood of accumulation of these compounds in water and sediment to be made. The data also allows further modelling to assess the likelihood of contamination of surface water by trifluralin and its major metabolite TR-4.



Trifluralin (MW 335.3)



Metabolite TR-4
(MW 305.2)

In the Dow AgroSciences dossier submitted to the rapporteur member state (Greece) in April 2002, data were presented regarding the behaviour of trifluralin in a core guideline laboratory study (Ref. 2) conducted in the EU in two sediment-water test systems maintained under aerobic conditions. In accordance with the test guideline, this study was conducted with spiking of the water layer. Additional data are also available in a supplementary study (Ref. 3) which was conducted with sediment spiked residues of trifluralin (mimicking a run-off loss). The data from both of these studies have been re-evaluated in accordance with FOCUS.
Data on the amounts of parent and metabolite in the various test systems were evaluated using the kinetic modelling tool KINGUI (Ref. 4) developed by Bayer CropScience to implement the findings of the FOCUS workgroup on degradation kinetics into a simple modelling tool. The tool is freely available and can be provided upon request. With KINGUI a model is defined as a number of compartments that interact together simultaneously. The degradation of each compartment may be single first order (SFO) or more complicated. All models are described in detail in the FOCUS guidance on degradation kinetics (Ref. 1).

2. Modelling tools and data used

2.1 Input Data.

Input data were derived from the data presented in two Dow AgroSciences reports (Ref. 2 and 3). The studies were conducted in the EU on three different water sediment test systems. The experimental details are summarised below.

Ref. no	Test system	Site	Sediment Texture	Country	Specifics of experimental design
2	1	Neuenkleusheim, Ople	Clayey sand	Germany	Based on BBA guideline study design where the air-flow was passed just over the water surface. Conducted using a sediment layer of 2-2.5 cm covered with *ca* 6 cm of associated water. Water layer treated directly with trifluralin.
2	2	Neuenkleusheim, Ople	Loamy clay	Germany	
3	3	Sediment – Borstel Water – Wenne at Berg	Loamy sand	Germany	Sieved sediment was treated directly with trifluralin, mixed, added to the incubation unit to 2-2.5 cm depth and then covered with *ca* 6 cm of water. Air-flow was passed just over the water surface.

A summary of the water-sediment system properties of the various test sites is presented in Table 1.

Individual test units were taken for analysis at intervals up to 56 days (test system 1 and 2) and 100 days (test system 3). Radioactivity in the water and sediment phases was extracted and analysed. Radioactivity in the volatile traps was also determined. The results for test system 1 and 2 show rapid movement of radioactivity

from the water phase into the sediment with concurrent formation of low levels of metabolite TR-4 plus polar metabolites (data not shown in the table) and high levels of ^{14}C in the volatile traps (assumed to be trifluralin). Test system 3 (sediment spiked) shows that trifluralin remains in the sediment layer then degrades to TR-4 plus polar metabolites. Build up of ^{14}C in the volatile traps is not as extensive as with the water spiked test systems. A summary of the distribution results is presented in Tables 2 and 3. Data are presented for trifluralin and TR-4 in both the water and sediment phases of the test systems. The amount of non-extractable residue (NER) and volatiles determined at each timepoint are also shown. Finally, a row of data called "Total triflu + volatiles" has also been added for each timepoint and this is the sum of the trifluralin residues in the water and sediment and volatile traps.

2.2 KINGUI Model (v1.1).

The package is built on a MATLAB runtime engine (The MathWorks, Natick, Massachusetts, USA), allowing to it to be freely distributed to users. The package includes an intuitive graphical user interface (GUI) which allows definition of complex degradation pathways, import of experimental data via text files and extensive graphical and statistical output of results. Differential equation numerical solutions and parameter optimisation are implemented with MATLAB implementations of Runge-Kutta and the Levenberg-Marquardt algorithms, respectively.
With KINGUI, models are constructed conceptually using the input screen shown below, which shows how the various components are related. Complex models can be built quickly and easily and no programming skills are needed. All calculated model values (rate constants, initial amounts, formation fractions, goodness of fit statistics) are presented as tables and graphs.
The goodness of fit of a model to measured data is shown by a number of indices which are automatically calculated by the software including χ^2 error (%, as recommended by FOCUS) , model efficiency (EF) and coefficient of determination (R^2). All of these indices are presented in the tabular output from the software.

2.3 Degradation schemes.

The data were evaluated in two different ways. In the first instance a simple model was developed that only considered the rate of degradation of the total trifluralin residue. This was calculated by adding trifluralin residues in the water and sediment and volatile traps at each time point and subjecting the data to a simple single first order decline model. The degradation scheme is shown in Figure 1 and has parent degrading to a sink compartment only. Only single first order (SFO) kinetics were considered in this analysis.

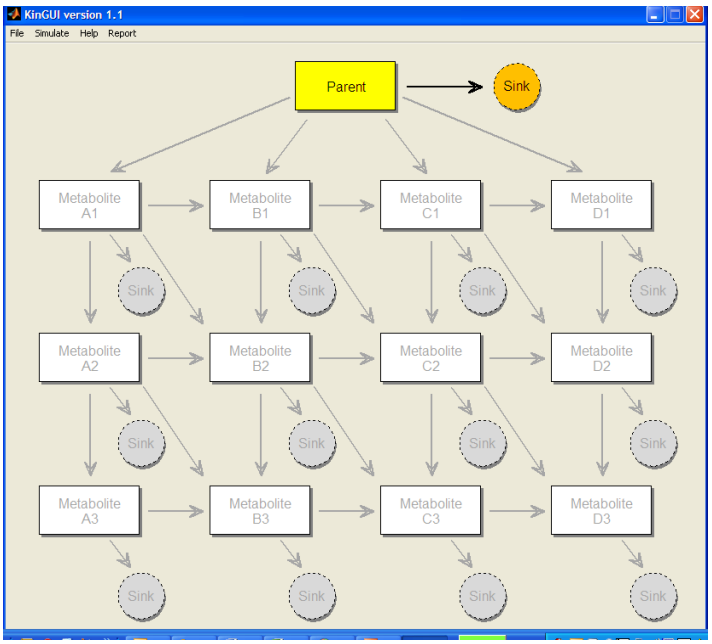


Figure 1: Input screen for the KINGUI software programme for SFO degradation of total trifluralin residues.

After this simple analysis, a more complicated compartment model was constructed with trifluralin degrading to metabolite TR-4, volatilising from the test system and also moving to the sink (bound residues). All processes in this model were SFO. The model is shown in Figure 2.

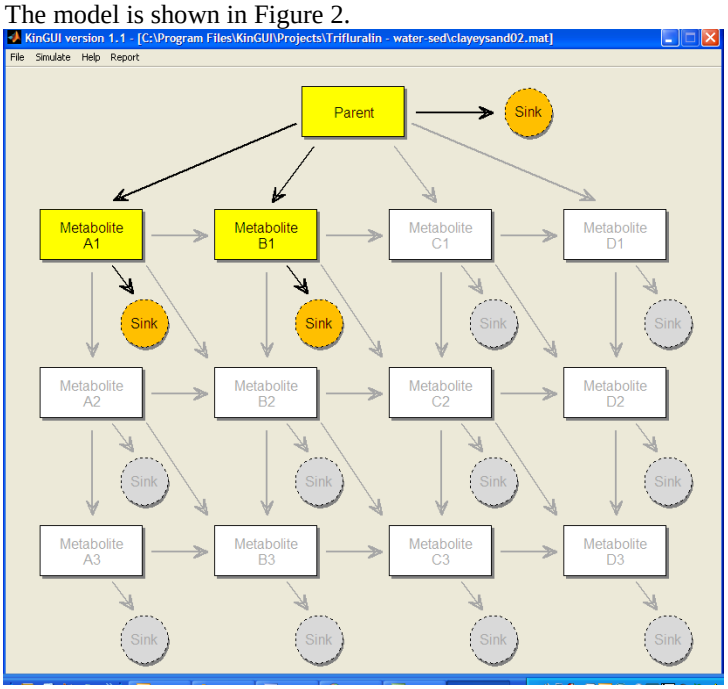


Figure 2: Input screen for the KINGUI software programme for SFO degradation of total trifluralin residues..

In thus above scheme trifluralin (parent) degrades to metabolite TR-4 (Metabolite A1) and also to the sink, but also moves to compartment B1 to represent volatile losses. The degradation rate of compartment B1 is set = 0 (no degradation). Furthermore, in these simulations the last timepoint for the volatile loss component was removed as volatiles would not be expected to decrease as there is no degradation modelled.

2.4 Output Data.

Output Tables and Graphs from the KINGUI programme for the various stages of the evaluation are presented in Appendix 1 and 2.
DT50 values for the various degradation process were taken directly from the KINGUI output files and are summarised in Table 4 and 5.

3. Results

3.1 Degradation kinetics of total trifluralin residues in the water sediment systems.

In this analysis the trifluralin residues in the water and sediment and volatile traps at each time point and subjecting the data to a simple single first order decline model (see Figure 1 in section 2.3). Output for the various data sets evaluated are presented in Appendix 1 in both tabular and graphical form and the goodness of fit of the models and validity of the results is also assessed in Appendix 3 (Table A3-1). The findings are summarised in Table 4 along with the optimised parameters for the models and show that the results from all three test systems are considered valid and the fit of the model is good (χ^2 error <15%). The degradation DT50 values for the total trifluralin residues range from 20 – 106 days.

For the purposes of further exposure modelling, the worst case value of 106 days will be used for the degrading compartment (sediment).

3.2 Compartment modelling of trifluralin and metabolites in the water sediment systems.

In this analysis the residues of trifluralin and metabolite were subjected to compartment modelling as described in Figure 2 in section 2.3. Output for the various data sets evaluated are presented in Appendix 2 in both tabular and graphical form and the goodness of fit of the models and validity of the results is also assessed in Appendix 3 (Table A3-2). The findings are summarised in Table 5 along with the optimised parameters for the models.

The findings show that for parent degradation the results from all three test systems are considered valid and the fit of the model is good (χ^2 error <15%). The DT50 values for the degradation of trifluralin residues range from 4.1 – 17 days.
The degradation rate and formation values calculated for metabolite TR-4 were not considered valid based on statistical tests, however, the visual fit was reasonably good (although there were very few data points). The resulting DT50 values for the metabolite were in the range 13.2 – 78.6 days and the formation fractions varies between 0.05 and 0.49.
The rate constant for degradation of volatile residues was set = zero (no degradation) so statistics could not be calculated. The formation fraction values for volatiles were considered valid for two of the test systems (1 and 2) with values of 0.85 and 0.67 respectively. These indicate that volatilization was a significant and rapid mechanism for dissipation of trifluralin from water sediment test systems where residues are spiked directly to the water column.
The DT50 for the volatilization process in these two test systems is equivalent to 4.8 and 8.0 days respectively.
The volatilization rate for test system 3 is not considered valid but the value is 210.5 days which is consistent with sediment spiking and strong sorption of residues to the sediment.

4. CONCLUSIONS

Data from two water sediment studies conducted by Dow AgroSciences have been re-evaluated according to the FOCUS guidance on degradation kinetics. The two studies differ in that in first study, the two water sediment test systems were spiked in the water phase and in the second study, the test system was spiked in the sediment (mimicking a run-off loading). A total of three water sediment test systems were evaluated.
Data on the amounts of parent and metabolite TR-4 in the various test systems were evaluated using the kinetic modelling tool KINGUI developed by Bayer CropScience to implement the findings of the FOCUS workgroup on degradation kinetics into a simple modelling tool. The tool is freely available and can be provided upon request. With KINGUI a model is defined as a number of compartments that interact together simultaneously. The degradation of each compartment may be single first order (SFO) or more complex. All models are described in detail in the FOCUS guidance on degradation kinetics.
The data were evaluated in two different ways. In the first instance a simple model was developed that only considered the rate of degradation of the total trifluralin residue (total trifluralin residues in the water and sediment and volatile traps). A more complicated compartment model was also assessed with trifluralin degrading to metabolite TR-4, volatilising from the test system and also moving to the sink (bound residues).
The findings for the "total trifluralin residues" show that the results from all three test systems are considered valid and the fit of the model is good an all cases (χ^2 error <15%). The degradation DT50 values for the total trifluralin residues range from 20 – 106 days. For the purposes of further exposure modelling, the worst case value of 106 days will be used for the degrading compartment (sediment).
The findings for the compartment modelling for trifluralin and metabolites show that the results for parent are considered valid in all cases. The DT50 values for the degradation of trifluralin residues range from 4.1 – 17 days, but this is largely dissipation as volatile levels are significant.
The results for metabolite TR-4 are not considered valid on statistical grounds although the visual fit of the model to the data is reasonably good. The resulting DT50 values for the metabolite were in the range 13.2 – 78.6 days and the formation fraction varies between 0.05 and 0.49.
The formation fraction values for volatiles were considered valid for two of the test systems (1 and 2) with values of 0.85 and 0.67 respectively. These indicate that volatilization was a significant and rapid mechanism for dissipation of trifluralin from water sediment test systems where residues are spiked directly to the water column. The DT50 for the volatilization process in these two test systems is equivalent to 4.8 and 8.0 days respectively.

REFERENCES

1. Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration. The final report of Workgroup on Degradation Kinetics of FOCUS, EC Document Reference SANCO/10058/2005 version 2.0, June, 2006.

2. Yon, D.A. (1993): Determination of the aquatic degradation of trifluralin.
Dow AgroSciences, unpublished report no. GHE-P-3024 (9 March 1993). Ref. K40.

3. Yon, D.A. (1993): Supplementary study for the determination of the aquatic degradation of trifluralin. Dow AgroSciences, unpublished report no. GHE-P-3023 (8 March 1993). Ref. K41.

4. KINGUI test version 1.1, developed by Bayer Technology Services for Bayer CropScience (2006). User interface for kinetic evaluations.

Table 1: Summary of water-sediment test system properties.

Sediment type (quoted BBA classification)	**Clayey sand[2]**	**Loamy clay[2]**	**Loamy sand**
Test system	1	2	3
Sediment			
Textural analysis (%)			
Sand	75	29	68
Silt	8	16	25
Clay	17	55	7
Textural classification (UK)	Sandy loam	Clay	Sandy loam
pH	7.1	6.7	5.7
Organic matter (%)[1]	0.3	3.1	2.6
Organic carbon (%)	0.2	1.8	1.5
Total nitrogen (mg/kg)	0.5	2.0	--
Total phosphorous (mg/kg)	0.3	0.2	--
Dry weight (% w/w dry soil)	81	67	--
Parameter taken at time of sampling			
Redox potential (U_H, mV)	221	490	--
Smell	Odourless	Odourless	--
Associated water			
pH	7.5	7.2	7.9
Parameter taken at time of sampling			
Redox potential (U_H, mV)	517	522	351
O_2 content (mg/L)	$\geq$ 12	$\geq$ 12	12
Conductivity (mS/m)	21	21	18
Temperature (°C)	13.2	3.7	5.2
Smell, appearance	Odourless, clear	Odourless, clear	Odourless, clear

[1] *Calculated as organic carbon x 1.724*
[2] *Associated water was sampled on two occasions & used for both sediment types*
-- Details not available in report

Table 2: Distribution of trifluralin and metabolites in water-sediment test systems 1 and 2.

Sampling interval/ sample type		Radioactive components (% AR)							
		Clayey sand				Loamy clay			
		Triflur-alin	**TR-4**	NER	Volatiles	Triflur-alin	TR-4	NER	Volatiles
0 d	Aq.	9[1]	-	-	-	3[1]	-	-	-
	Sed.	94	-	-	-	108	-	-	-
	Total	***103***	***-***	***3***	***≤1***	***111***	***-***	***4***	***≤1***
Total triflu + volatiles		**103**				**111**		-	-
6 h	Aq.	11	-	-	-	3[1]	-	-	-
	Sed.	76	-	-	-	89	-	-	-
	Total	***87***	***-***	***2***	***2***	***92***	***-***	***5***	***2***
Total triflu + volatiles		**89**				**94**			
3 d	Aq.	4[1]	-	-	-	2[1]	-	-	-
	Sed.	47	-	-	-	67	-	-	-
	Total	***51***	***-***	***2***	***42***	***69***	***-***	***4***	***25***
Total triflu + volatiles		**93**				**94**			
7 d	Aq.	3[1]	-	-	-	2[1]	-	-	-
	Sed.	38	-	-	-	47	-	-	-
	Total	***41***	***-***	***6***	***63***	***49***	***-***	***9***	***51***
Total triflu + volatiles		**104**				**100**			
14 d	Aq.	3[1]	-	-	-	1[1]	-	-	-
	Sed.	12	-	-	-	16	9	-	-
	Total	***15***	***4***	***˜ı***	***72***	***17***	***9***	***11***	***57***
Total triflu + volatiles		**87**				**74**			
30 d	Aq.	2[1]	-	-	-	1[1]	-	-	-
	Sed.	6	1	-	-	6	7	-	-
	Total	***8***	***1***	□	***77***	***7***	***7***	***13***	***62***
Total triflu + volatiles		**85**				**69**			
56 d	Aq.	4[1]	-	-	-	1[1]	-	-	-
	Sed.	2	3	-	-	1	4	-	-
	Total	***6***	***3***	***26***	***60***	***2***	***4***	***26***	***53***
Total triflu + volatiles		**66**				**55**			

All figures are mean of duplicate samples

[1] *Not analysed, assumed to be all parent material*

Table 3: Distribution of trifluralin and metabolites in water-sediment test system 3.

Sampling interval		Radioactive components (% AR)			
		Triflur-alin	**TR-4**	NER	Volatiles
0 d	Aq.	2			
	Sed.	98	-		
	Total	***100***	***-***	***4***	***ND***
Total triflu + volatiles		**100**			
6 h	Aq.	3	-		
	Sed.	97	-		
	Total	***100***	***-***	***3***	***ND***
Total triflu + volatiles		**100**			
3 d	Aq.	2	-		
	Sed.	90	-		
	Total	***92***	***-***	***1***	***5***
Total triflu + volatiles		**97**			
7 d	Aq.	2	-		
	Sed.	83	-		
	Total	***85***	***-***	***5***	***7***
Total triflu + volatiles		**92**			
14 d	Aq.	2	-		
	Sed.	69	1		
	Total	***71***	***1***	***9***	***6***
Total triflu + volatiles		**77**			
28 d	Aq.	2	-		
	Sed.	16	16		
	Total	***18***	***16***	***28***	***5***
Total triflu + volatiles		**23**			
100 d	Aq.	3	-		
	Sed.	4	2		
	Total	***7***	***2***	***52***	***6***
Total triflu + volatiles		**13**			

[1] *Not analysed, assumed to be all parent material*
[2] *Assumed to comprise numerous minor components*

Table 4: Summary of results from the analysis of "Total Trifluralin" residues.

Parameter	Test systems		
	Clayey sand	Loamy clay	Sandy loam
X^2 error (%)	5.2077	6.6419	10.8276
k_{deg} (d^{-1})	0.0065	0.0124	0.0342
Degradation DT50 (d)	106.4	56.1	20.3
Data considered valid?	Y	Y	Y

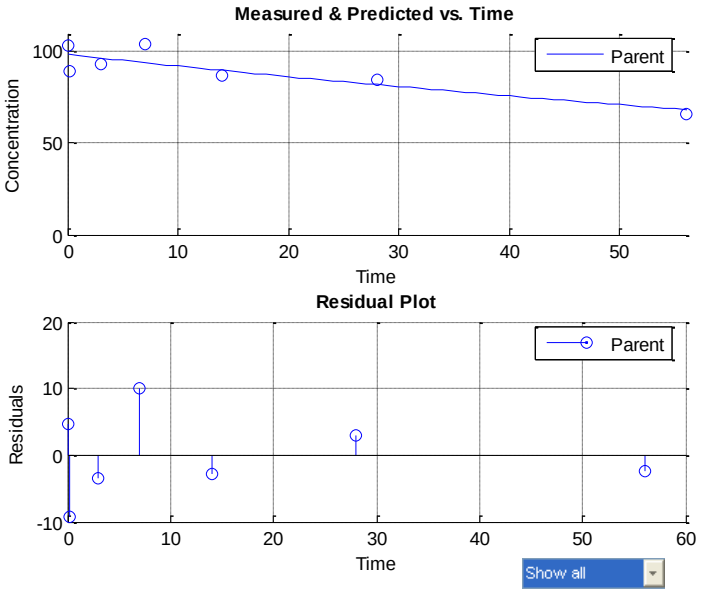
Table 5: Summary of results from the analysis of Trifluralin compartment model.

Parameter	Test systems		
	Clayey sand	Loamy clay	Sandy loam
Degradation rate constants			
Parent			
X^2 error (%)	13.1801	8.4941	9.7399
k_{deg} (d^{-1})	0.17	0.1292	0.0408
DT50 (d)	4.1	5.4	17.0
Data considered valid?	y	y	y
TR-4			
X^2 error (%)	NaN	5.9716	NaN
k_{deg} (d^{-1})	0.0088	0.0269	0.0524
DT50 (d)	78.6	25.8	13.2
Data considered valid?	n	n	n
Volatiles			
X^2 error (%)	9.2074	11.3922	48.2248
k_{deg} (d^{-1})	0.0000	0.0000	0.0000
DT50 (d)	Infinite	Infinite	Infinite
Data considered valid?	y	y	y
Formation fractions			
TR-4			
FF_A1	0.0484	0.1275	0.4929
Data considered valid?	n	n	n
Volatiles			
FF_B1	0.8508	0.6683	0.0807
Data considered valid?	y	y	n

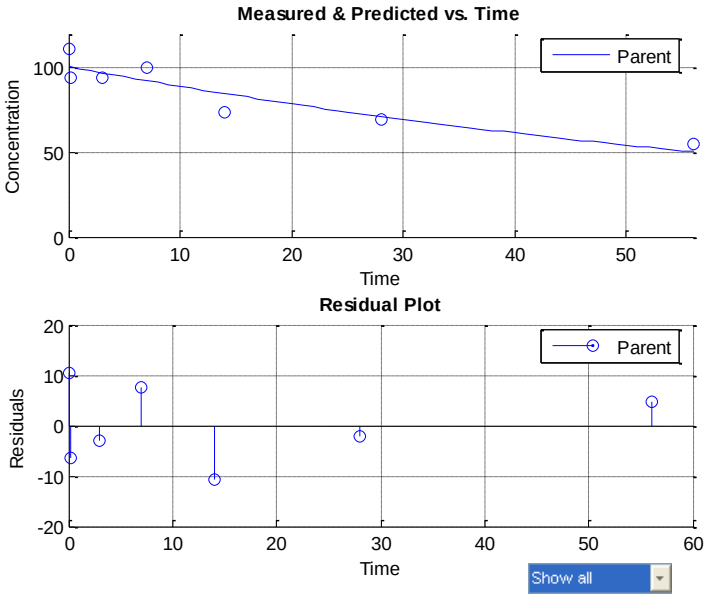
APPENDIX 1

Graphic results for SFO model analysis of "total trifluralin" residues in water sediment systems.

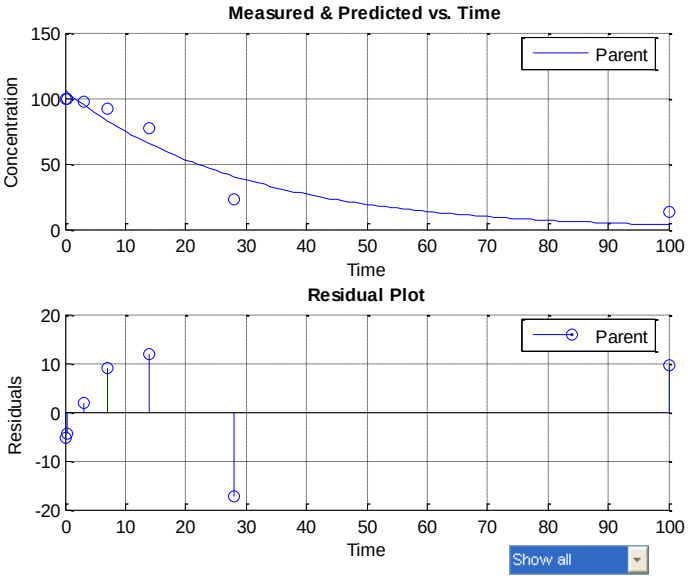
a) Test system 1; Clay sand.



b) Test system 2; Loamy clay.



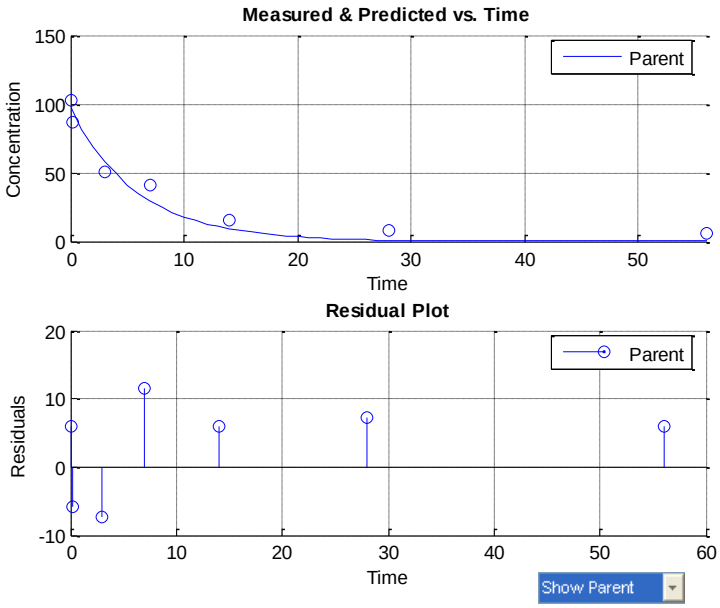
c) Test system 3; Loamy sand.



APPENDIX 2

Graphic results for SFO model analysis for trifluralin compartment model for residues in water sediment test systems.

a) Test system 1; Clay sand.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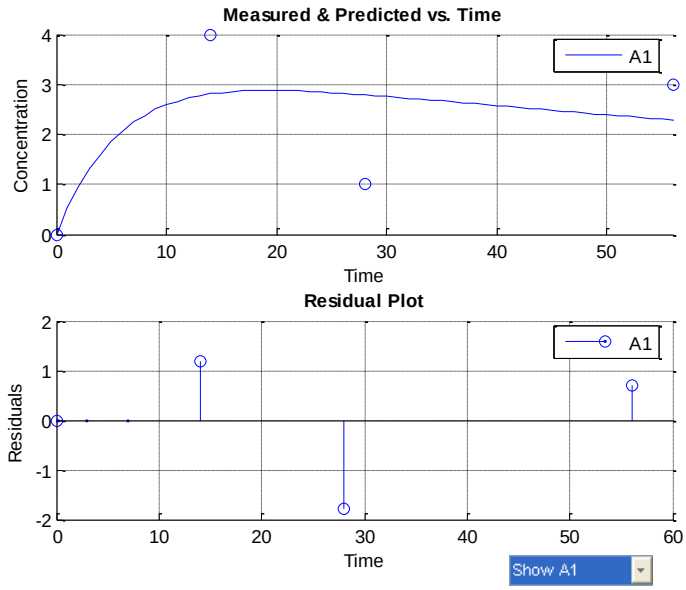
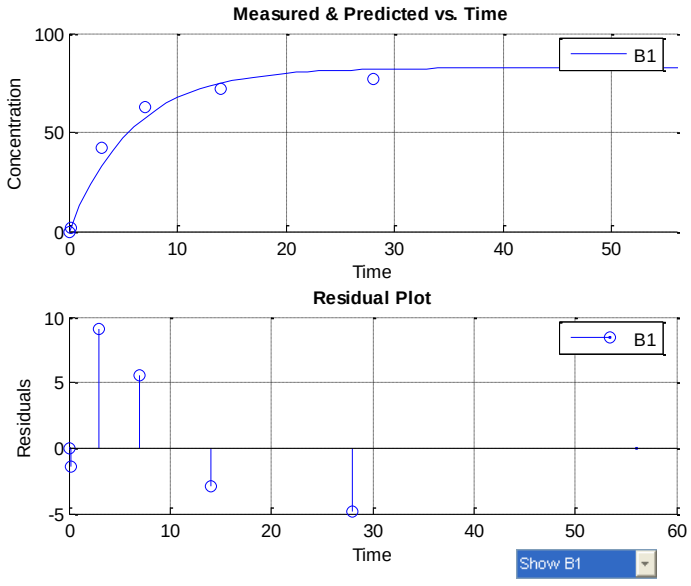
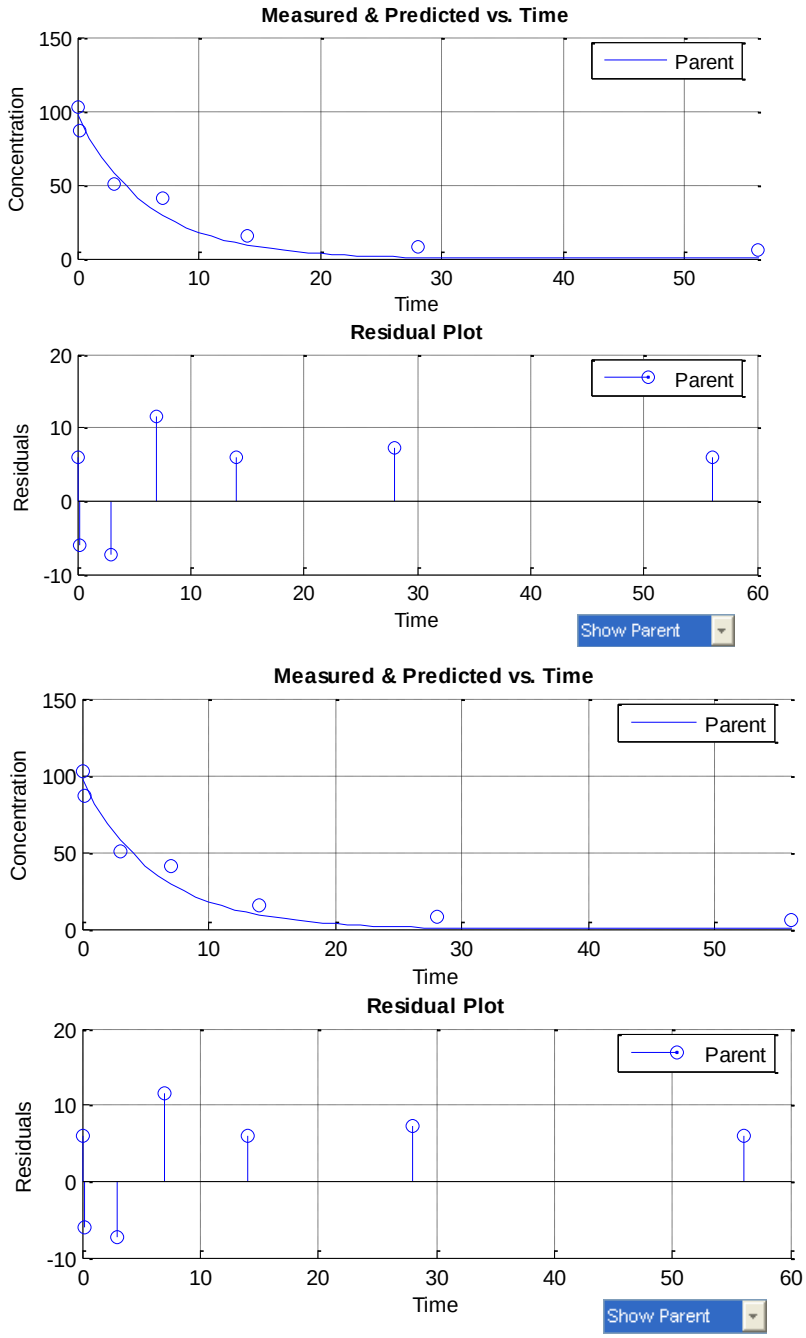
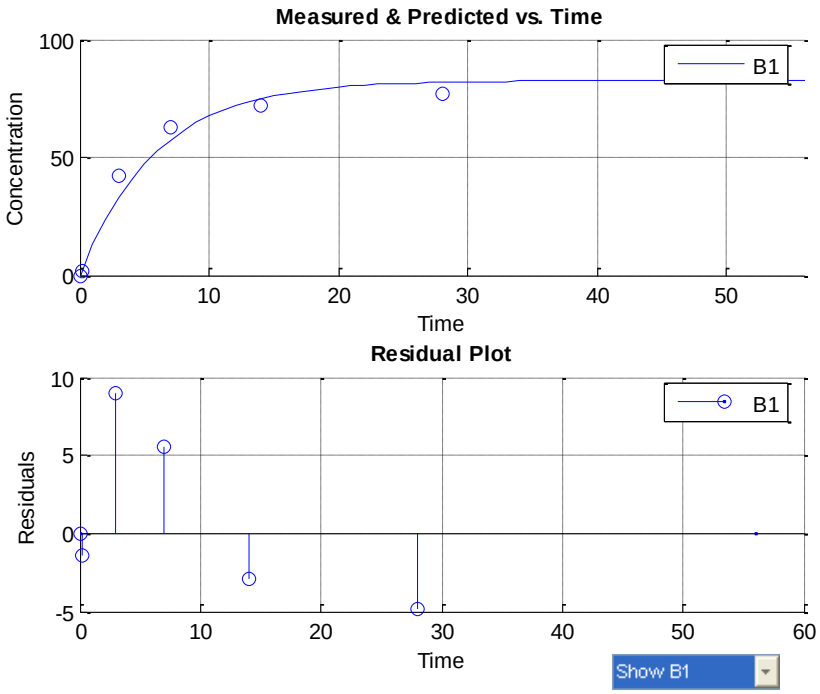
Parent
Concentration
Time
Residual Plot
Parent
Residuals
Time
Show Parent


Measured & Predicted vs. Time
A1
Concentration
Time
Residual Plot
A1
Residuals
Time
Show A1

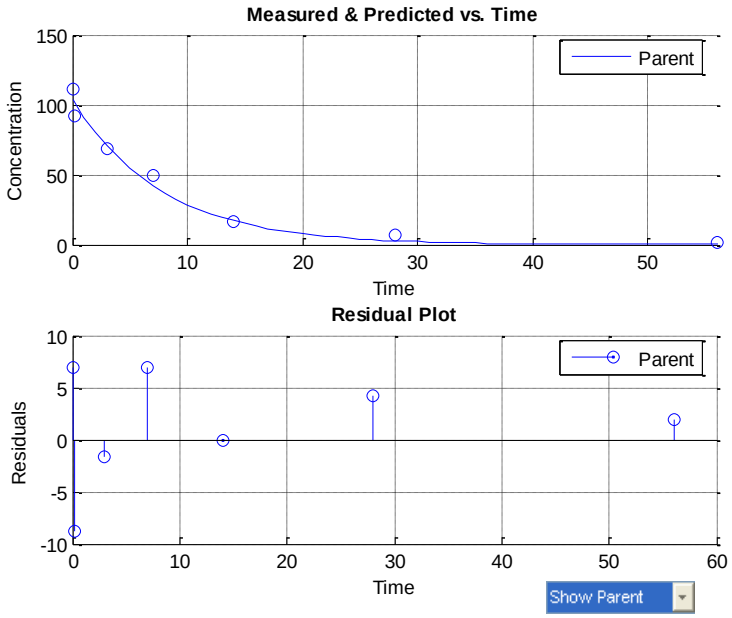

Measured & Predicted vs. Time
B1
Concentration
Time
Residual Plot
B1
Residuals
Time
Show B1

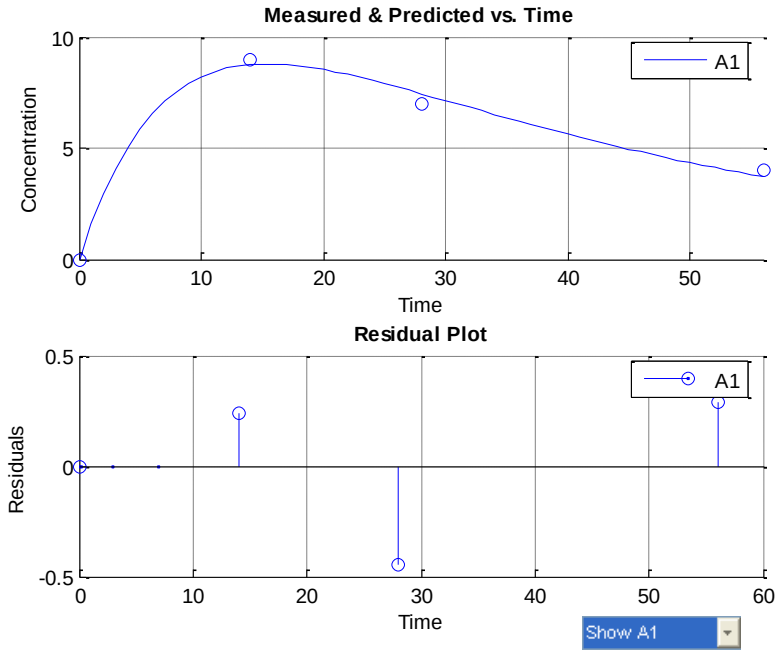
b) Test system 1; Clay sand – remove 28d timepoint for metabolite TR-4.

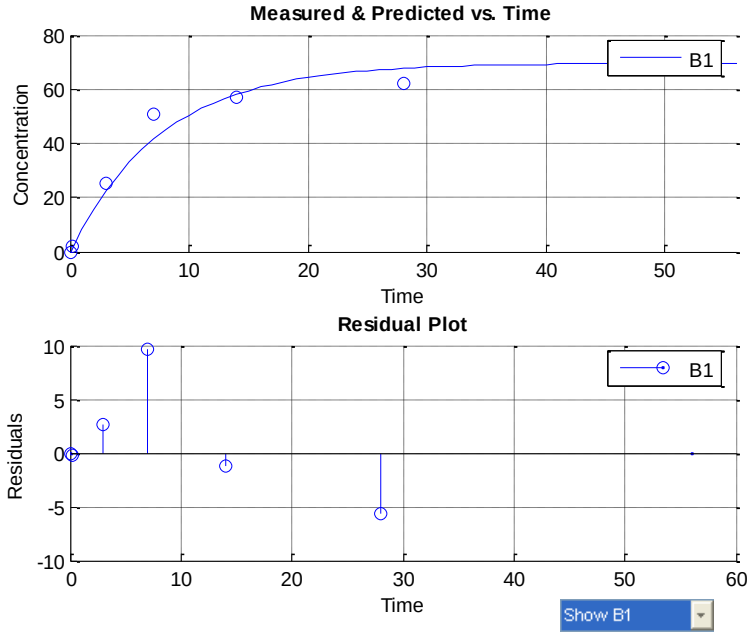




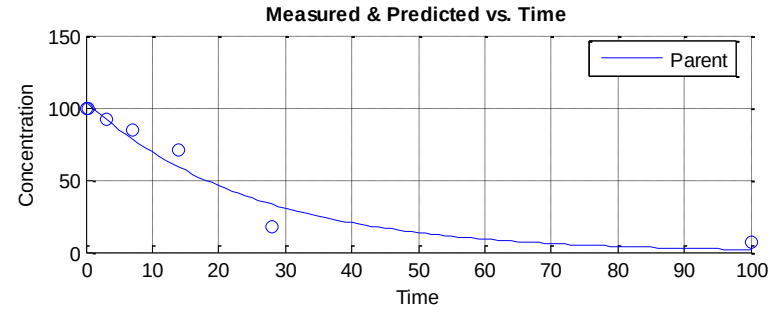
c) Test system 2; Loamy clay.







d) Test system 3; Sandy loam.


Measured & Predicted vs. Time
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Time
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150
0
10
20
30
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70
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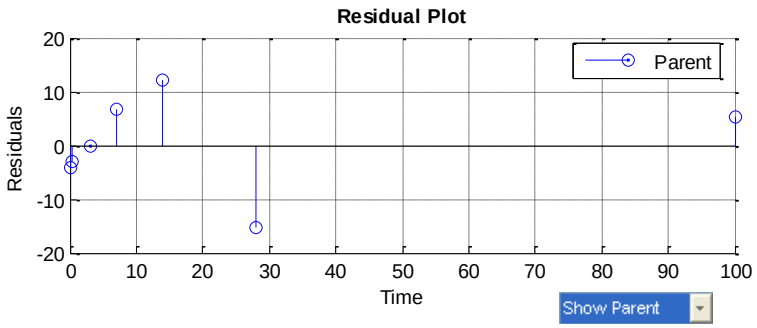
90
100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Parent
Residuals
Time
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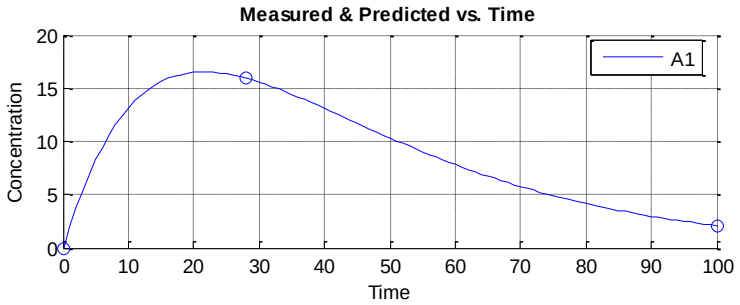
Measured & Predicted vs. Time
A1
Concentration
Time
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60
70
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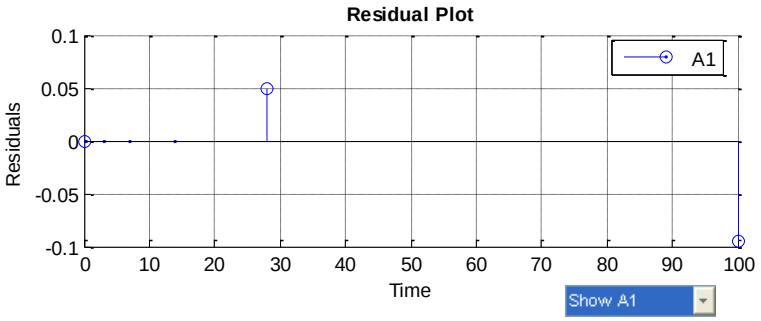
90
100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A1
Residuals
Time
Show A1
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90
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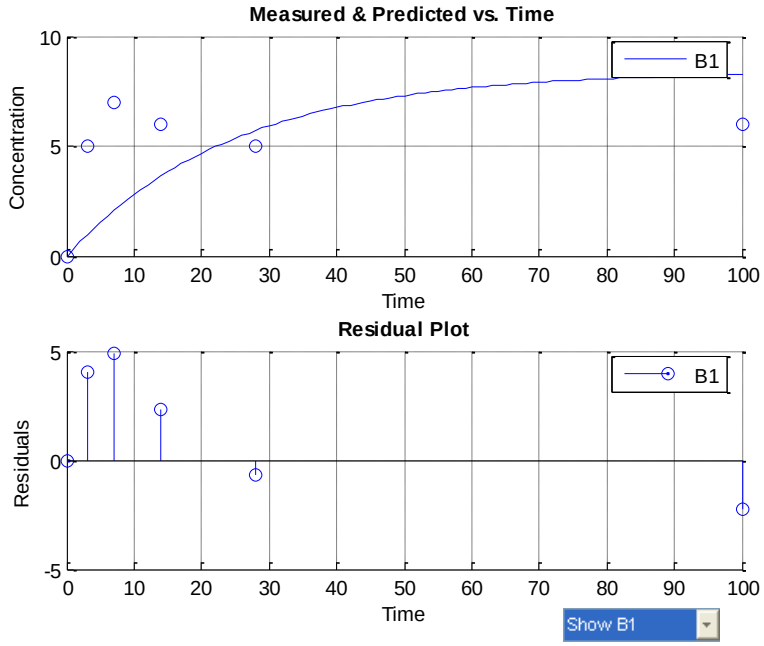
Measured & Predicted vs. Time
Concentration
Time
B1
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50
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70
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90
100

Residual Plot
Residuals
Time
B1
Show B1
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APPENDIX 3

Assessment of goodness of fit and validity of results for trifluralin modelling.

Table A3-1: Assessment of results for SFO model analysis for "total trifluralin" residues (section 3.1).

Parameter	Test systems		
	Loamy clay	Clayey sand	Sandy loam
$\chi 2$ error (%)	6.6419	5.2077	10.8276
R^2	0.8485	0.7552	0.9237
stdev/estimated value	0.218	0.277	0.246
LCL < 0	n	n	n
T <0.05	y	y	y

The results show that the χ^2 error is low in all cases which is less than the guidance value of <15% error set by FOCUS as an acceptable limit. The standard deviation of the estimates as a fraction of the estimate is also small (<0.3 in all cases) and in no cases is the lower confidence limit less than zero. Finally, "t" is less than 0.05 in all cases so the estimates are considered significant. Therefore, the data from these calculations are all considered valid.

Table A3-2: Assessment of results for compartment model analysis for trifluralin and its metabolites (section 3.2).

Parameter	Tests systems		
	Clayey sand	Loamy clay	Sandy loam
Degradation rate constants			
Parent			
$\chi 2$ error (%)	13.1801	8.4941	9.7399
R^2	0.9761	0.9849	0.9478
stdev/estimated value	0.1276	0.0944	0.1446
LCL < 0	n	n	n
T <0.05	y	y	y
Metabolite TR-4 (A1)			
$\chi 2$ error (%)	NaN	5.9716	NaN
R^2	0.9995	0.9927	1
stdev/estimated value	8.1364	1.4647	2.3492
LCL < 0	y	y	y
T <0.05	n	n	n
Volatiles (B1)			
$\chi 2$ error (%)	9.2074	11.3922	48.2248
R^2	0.9775	0.9684	0.2564
stdev/estimated value	value fixed	value fixed	value fixed
LCL < 0	--	--	--
T <0.05	--	--	--
Formation fractions			
Metabolite TR-4 (A1)			
stdev/estimated value	2.2417	0.7820	1.7486
LCL < 0	y	y	y
Volatiles (B1)			
stdev/estimated value	0.1527	0.1606	3.5960
LCL < 0	n	n	y

The results for the compartment analysis show that for the parent compound, the χ^2 error is low in all cases and is less than the guidance value of <15% error set by FOCUS as an acceptable limit. The standard deviation of the estimates as a fraction of the estimate is also small (<0.15 in all cases) and in no cases is the lower confidence limit less than zero. Finally, "t" is less than 0.05 in all cases so the estimates are considered significant. Therefore, the data from these calculations for the degradation of triflualin are all considered valid. The results for metabolite TR-4 show that χ^2 error could not be calculated in two cases (probably due to the lack of data points for this metabolite). The ratio of standard deviation to the estimated value for both the rate

constant and formation fraction are > 1 in all cases indicating unacceptable confidence limits and, finally, the lower confidence limit is less than zero in all cases. Based on this assessment the data for data for TR-4 are not considered valid.
The results volatile components (degradation rates set = 0, ie no degradation) show that χ^2 error was <15% for test systems 1 and 2 but was 48% for test system 3. The latter tests system was sediment spiked and had significantly less volatile loss. The standard deviation and confidence limits for the rate constant were not calculated becuase the values was fixed at zero. The ratio of standard deviation to the estimated value for the formation fraction are < 1 for test system 1 and 2 indicating acceptable confidence limits and, finally, the lower confidence limit are also less than zero for systems 1 and 2. Based on this assessment the data (formation fraction and rate of formation) for volatile components from test systems 1 and 2 are considered valid.

B.8.6 PREDICTED ENVIRONMENTAL CONCENTRATIONS IN SURFACE WATER AND IN GROUND WATER (PECsw, PECgw) (Annex IIIA 9.2.3, 9.2.1)

B.8.6.1 Predicted Environmental Concentrations in Surface Water and Sediment

Reeves, G., "THE PREDICTED ENVIRONMENTAL CONCENTRATIONS OF TRIFLURALIN AND METABOLITES USING THE FOCUS SURFACE WATER TOOLS AND SCENARIOS FOR CRITICAL GOOD AGRICULTURAL PRACTICE – SUPPLEMENTARY ANALYSIS", report nuber GHE-P-12083, 2009, not published

Objective: To estimate the PEC_{sw} values for trifluralin and metabolites.
Guidelines: FOCUS Surfacewater Scenarios.
GLP: No (modelling study)

1. Introduction

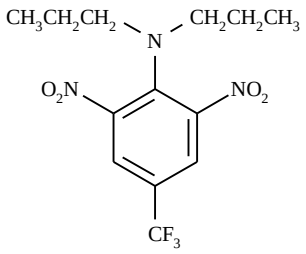
This report provides supplementary data to modelling work previously carried out as described in GHE-P-11836[(1)], with the intention of addressing open points in the Evaluation Table (April 2009) for trifluralin in support of the Annex I resubmission. This current report, as well as GHE-P-11836, should be read as companion reports.

Trifluralin is the active substance in TREFLAN herbicides which are registered for the control of grass and broad-leaved weeds in a wide range of field crops. To support Annex I inclusion under Directive 91/414/EEC, a study has been carried out to model the predicted environmental concentration for trifluralin and its metabolites in EU surface waters. This was following the pre-emergence use of TREFLAN herbicides in cotton, winter oilseed rape and sunflowers according to GAP. The modelling was carried out using the FOCUS surface water scenarios [(2)].

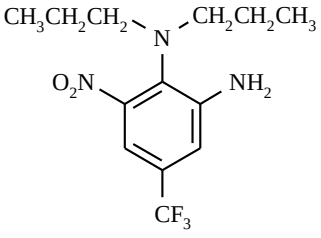
The modelling was conducted within the Field Exposure and Effects group of Dow AgroSciences, European Development Centre, 2nd Floor, 3 Milton Park, Abingdon, Oxon., OX14 4RN, UK.

2. MODELLING INFORMATION

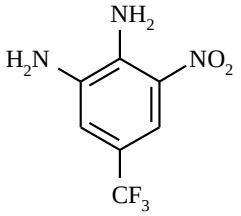
2.1 Test Items



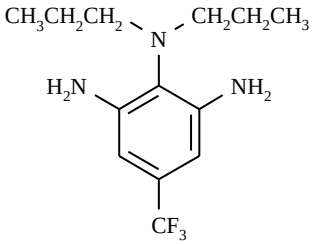
Trifluralin



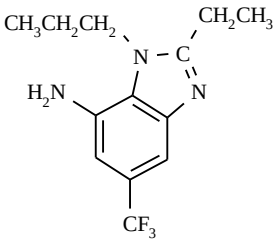
Metabolite TR-4



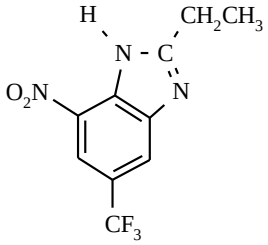
Metabolite TR-6



Metabolite TR-7



Metabolite TR-14



Metabolite TR-15

Metabolites TR-4, TR-7 and TR-14 were identified in the water sediment studies at 16.0% AR, 14.2% AR and 29.5% AR respectively. TR-6 and TR-15 are major aqueous photolysis products and were found at 50.4% AR and 31.5% AR respectively.

2.2 Overview FOCUS Surface Water Tools

The FOCUS surface water models are a series of four stepwise procedures for calculating predicted environmental concentrations in surface water (PECsw) and sediment (PECsed) at the "edge of field scale". The process starts with simple calculations based on worst-case assumptions (Steps 1 and 2) and proceeds to more complex evaluations based on realistic combinations of cropping, soil, weather, field topography and water body characteristics (Steps 3 and 4).

2.3 Steps 1 and 2

STEPS 1-2 in FOCUS (version 1.1) calculates PECsw and PECsed values using a Microsoft Visual Basic program. The calculations assume a field:water body ratio of 10:1 and a water depth of 30 cm overlying sediment of 5 cm depth with sorption only occurring in the top 1 cm of sediment. The sediment has an organic carbon content of 5% and bulk density of 0.8 kg/L. Pesticide input is based on "worst-case" assumptions of spray drift, run-off, erosion and/or drainage. The compound specific input values required for the calculations are molecular weight, water solubility, DT_{50} (in soil and sediment/water), Koc, number of applications, application interval and application rate. Drift values have been calculated at the 90th percentile from BBA data assuming default "no spray zones" depending on the crop.

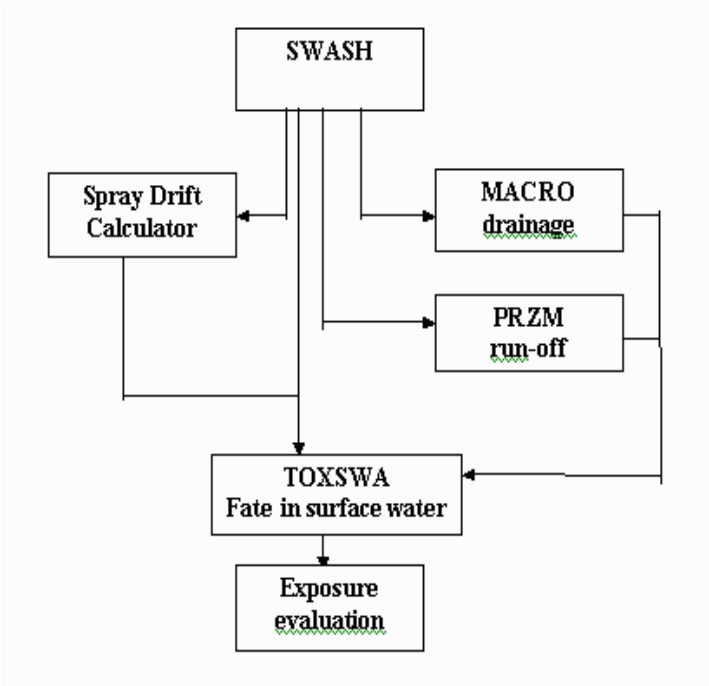
At Step 1, inputs from spray drift, run-off, erosion and/or drainage are evaluated as a single loading to the water body and "worst-case" water and sediment concentrations are calculated. The combined run-off/erosion and drainage input to the water body is set at 10% of the application rate and this is distributed instantaneously between water and sediment at the time of loading according to the Koc of the compound.

At Step 2, loadings are refined as a series of individual applications, each resulting in drift to the water body, followed by a run-off/erosion/drainage event occurring four days after the last application. The magnitude of the loading is based upon the region of use (Northern or Southern Europe), season of application and crop interception.

2.4 Step 3

For Step 3, ten realistic worst-case scenarios with respect to surface water vulnerability have been defined, which are representative of the range of agriculture in the EU. Each FOCUS scenario is defined as either a “drainage” (D) or “runoff” (R) scenario depending on which of these is the main hydrological process by which water will reach nearby surface water. Each scenario is characterised by a set of weather, soil and crop parameters. Three different types of water bodies (pond (p), ditch (d) and stream (s)) were also identified and one or two of these water bodies is associated with each scenario. For each water body, the distance from the treated crop to the water is dependent on the crop type and is fixed to default values at Step 3 in order to calculate drift loadings. Inputs from drainage and runoff/erosion and subsequent fate and distribution in the water body are calculated using simulation models.

The Step 3 modelling process is summarised in the following scheme:



SWASH is a software shell created to prepare the input data and link the runs of the various models at Step 3. SWASH does not perform any model simulations, but encompasses a number of individual tools and models involved in the Step 3 calculations. Its main functions are to maintain a central pesticide properties database and prepare input for the MACRO, PRZM and TOXSWA models. SWASH also provides an overview of crop and water body combinations in each scenario, the extent of each scenario and the versions of each model installed including its shell and database. The spray drift calculator (v1.1) embedded in the SWASH shell provides the drift loading for the TOXSWA model based on application rate, number of applications per season, crop type, water body and the distance

between the crop and water body. The versions of the models used in this report were SWASH v2.1, MACRO v4.4.2, PRZM v1.1.1 and TOXSWA v2.2.1.

The leaching model MACRO calculates drainage inputs to surface water bodies for the six Step 3 scenarios where drainage is a significant input. The model simulates pesticide movement through both macropore flow and bulk matrix flow. The movement of water through the soil matrix is described using Richards' equation and solute transport is described with the convection-dispersion equation. Solute movement in the macropores is assumed to be dominated by mass flow. Mass exchange between the flow domains is calculated using approximate first-order expressions based on an effective diffusion path length. Sorption is described with a Freundlich isotherm, with the sorption sites partitioned between the two domains. Degradation is calculated using first-order kinetics.

The Pesticide Root Zone Model (PRZM) calculates runoff and erosion loadings into surface water bodies for four of the Step 3 surface water scenarios. PRZM is a one-dimensional, dynamic, compartmental model that simulates chemical movement in unsaturated soil systems within and immediately below the root zone. The model has hydrologic (flow) and chemical transport components to simulate runoff, erosion, plant uptake, leaching, decay, foliar washoff, and volatilisation. Pesticide transport and fate processes include advection, dispersion, molecular diffusion, and soil sorption.

TOXSWA describes the behaviour of pesticides in the water body (ditch, pond or stream) at the edge-of-field scale following input from drift, drainage and runoff/erosion. It calculates pesticide concentrations in the water and sediment layers based on transport, transformation, sorption and volatilisation. In the water layer, pesticides are transported by advection and dispersion, while in the sediment, diffusion is also included. The transformation rate covers the combined effects of hydrolysis, photolysis and biodegradation. Sorption to suspended solids and to sediment is described by the Freundlich equation. Pesticides are transported across the water-sediment interface by diffusion.

2.5 Step 4

At Step 4, further refinement of the exposure calculations can be carried out if the risk assessments using Step 3 scenarios show that there is a potential risk to aquatic organisms. The guidance given by FOCUS is very general for Step 4 but the types of procedure that can be used are (i) further refinement of pesticide input parameters for the Step 3 models, (ii) label mitigation measures such as buffer zones, or (iii) modification of the Step 3 scenarios (e.g. from "edge of field" to "landscape" scale.

To facilitate the implementation of Step 4 mitigation procedures, the software tool SWAN v1.1 has been developed by ECPA to amend drift and run-off inputs to the TOXSWA model. Guidance on how to implement these mitigation measures is given in the FOCUS Landscape and Mitigation report[(3)].

2.6 Model Assumptions and Scenarios

The physico-chemical and environmental fate properties of trifluralin and its metabolites that are required for input to the models are shown in Tables 1 to 3. Where possible, data were taken from the End Points section of the Draft Assessment Report (DAR) with the associated Addendum[(4)]. No new environmental fate data have been generated since these documents were issued that would influence the selection of the model input data. In

cases where metabolite model input data are not available, EPI Suite[(5)] has been used to estimate parameters for water solubility and Koc sorption values (see Appendix I). For metabolite DT_{50} in soil, water and sediment a conservative approach has been adopted and a value of 1000 days has been used. The key environmental fate inputs are described as follows.

2.6.1 Steps 1 and 2

The following GAP and input parameters were considered for Steps 1 and 2.

Spring appn. to cotton: 1.2 kg as/ha (1 Mar), soil incorporation to 20 cm
Autumn appn. to winter oilseed rape: 1.2 kg as/ha (30 Sep), soil incorporation to 20 cm
Spring appn. to sunflowers: 1.2 kg as/ha (1 Mar), soil incorporation to 20 cm

All simulations were carried out using the scenario appropriate for the particular crop as recommended by FOCUS. The key chemical input parameters used for trifluralin and its metabolites in the simulations are shown in Tables 1 and 2. A 100% conversion from parent to each metabolite was assumed as a worst case estimation for these metabolites. Since the use modelled is for pre-emergence, then no crop interception was applied.

Table 1: Chemical Specific Input Parameters for Steps 1 and 2 for Trifluralin

Property	Value
Solubility in water	0.194 mg/L (20ºC)
Koc	8765 mL/g
Half-life soil	212 d (20ºC)*
$DegT_{50}$ water	1000 d (20ºC)**
$DegT_{50}$ sediment	106 d (20ºC)***

* *From 181 d at 22°C using a Q_{10} of 2.2*
** *Default for non-degrading compartment (see also GHE-P-12080; Ref. 6)*
*** *See GHE-P-12080; Ref. 6*

Table 2: Chemical Specific Input Parameters for Steps 1 and 2 for Metabolites

TR-4	Value
Solubility in water	1.41 mg/L (20ºC)**
Koc	13600 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*
TR-6	**Value**
Solubility in water	586 mg/L (20ºC)**
Koc	622 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*
TR-7	**Value**
Solubility in water	27.8 mg/L (20ºC)**
Koc	19100 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*
TR-14	**Value**

Solubility in water	1.93 mg/L (20ºC)**
Koc	24000 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*
TR-15	**Value**
Solubility in water	21.1 mg/L (20ºC)**
Koc	2839 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*

** Conservative estimate of 1000 days used ** Calculated using EPI Suite*

2.6.2 Step 3

At Step 3, SWASH was used to set up input files to model the foliar application of TREFLAN to winter oilseed rape, cotton and sunflowers according to the GAP shown below.

Spring appn. to cotton: 1.2 kg as/ha (1 Mar), soil incorporation to 20 cm
Autumn appn. to winter oilseed rape: 1.2 kg as/ha (30 Sep), soil incorporation to 20 cm
Spring appn. to sunflowers: 1.2 kg as/ha (1 Mar), soil incorporation to 20 cm

All simulations were carried out using the scenario appropriate for the particular crop as recommended by FOCUS. The key chemical input parameters used for trifluralin in the simulations are shown in Table 3. Default FOCUS buffer zones were modelled for Step 3.

Table 3: Chemical Specific Input Parameters for Steps 3 and 4

Property	Value
Molar Mass	335 g/mol
Saturated vapour pressure	9.5 x 10^{-3} Pa (20ºC)
Molar enthalpy of vaporisation	95000 J/mol*
Solubility in water	0.194 mg/L (20ºC)
Molar enthalpy of dissolution	27000 J/mol*
Diffusion co-efficient in water	4.3 x 10^{-5} m^2/d*
Diffusion co-efficient in air	0.43 m^2/d*
Koc	8765 mL/g
Freundlich exponent	0.972
Ref. concentration in liquid phase	1 g/m^3*
Factor for uptake by plant roots in soil	0.50 *
Wash-off factor from crop	0.05 mm^{-1} (MACRO)* 0.50 cm^{-1} (PRZM)*
$DegT_{50}$ water	1000 d (20ºC)**
Half-life soil	181 d (22ºC)
$DegT_{50}$ sediment	106 d (20ºC)***
Half-life crop	10 d *
Activation energy (TOXSWA)	54000 J/mol*
Exponent (MACRO)	0.079 K^{-1}*

** FOCUS default*

*** Default for non-degrading compartment (see also GHE-P-12080; Ref. 6)*

*** *See GHE-P-12080; Ref. 6*

The data shown in Table 3 were then input into SWASH, and the relevant drainage (D) and runoff (R) scenarios, both with inclusive spray-drift, were run. For the runoff scenarios, the foliar linear application option and incorporation to 20 cm depth were chosen for the PRZM model. Default FOCUS buffer zones were used at Step 3.

2.6.3 Step 4

At Step 4, the effect of introducing vegetated buffer zones between the crop and surface water was evaluated. Such buffers will reduce the drift input and it is generally accepted that the runoff of both dissolved and particle-bound pesticide will also be reduced due to interception of water and eroded soil by the vegetated strip, although drainage will not be affected. In accordance with FOCUS Landscape and Mitigation guidance[4], a reduction in the volume of runoff and pesticide loading into water of 60% for a 14 m buffer and a reduction into sediment 85% for a 14 m buffer was implemented. For a 20m buffer, a reduction in the volume of runoff and pesticide loading into water of 80% for a 20 m buffer and a reduction into sediment 95% was implemented.

The SWAN interface was used to implement both drift and runoff reductions to TOXSWA. The appropriate buffer width was selected for the drift mitigation, firstly without runoff mitigation, and then inclusive with runoff mitigation. Using the Step 3 simulations as a starting point, the TOXSWA model was re-run using SWAN after applying the drift and runoff mitigations described above.

3. Results and conclusions

Following each model run, the TOXSWA summary file (*.sum) of the surface water and sediment concentrations versus time were collated. In summary, the global maximum PEC_{SW} and PEC_{SED} values (expressed as µg/L or µg/kg sediment dry weight, respectively), together with the time-weighted average (TWA) concentrations are given in Tables 4-8, and in detail at Steps 3 and 4 in Appendix II. Appendix II shows the actual and TWA concentrations and a graph of the exposure in the water. A summary is shown in Table 9.

Table 4: Summary PECsw for Trifluralin and Metabolites

Trifluralin	**Global Max. PEC_{SW} (µg/L)**				
Crop	**Step 1**	**Step 2**	**Step 3**	**Step 4, 20m buffer**	
				Drift mitigation only	**Drift + runoff mitigation (if applicable)**
wOSR	42.57	13.77	7.65 (D2d)	0.708 (D5s)	0.708 (D5s)
Cotton	42.57	13.77	6.23 (D6d)	0.796 (D6d)	0.796 (D6d)
Sunflowers	42.57	13.77	6.07 (R3s)	1.747 (R3s)	0.704 (R3s)

D or R = FOCUS drainage or runoff scenario, d = ditch, s = stream

All Crops	Global Max. PEC_{SW} (µg/L)	
	Step 1	Step 2
TR-4	10.1	10
TR-6	7.42	7.27
TR-7	9.06	9.05
TR-14	8.93	8.92
TR-15	8.59	8.52

Table 5: Trifluralin Step 1 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

Concentration	Max. PECSW *(µg/L)*	TWA PECSW 7 day	TWA PECSW 21 day	Max. PECSED *(µg/kg dw)*	TWA PECSED 7 day	TWA PECSED 21 day
ALL CROPS, NZ AND SZ	42.57	32.39	30.51	2820	2770	2650
	42.57	32.39	30.51	2820	2770	2650
	42.57	32.39	30.51	2820	2770	2650

Table 6: Trifluralin Step 2 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

Concentration	Max. PECSW *(µg/L)*	TWA PECSW 7 day	TWA PECSW 21 day	Max. PECSED *(µg/kg)*	TWA PECSED7 day	TWA PECSED 21 day
wOSR NZ	11.04	5.52	6.30	617	607	582
SZ	13.77	13.12	12.56	1160	1140	1090
Cotton SZ	13.77	13.12	12.56	1160	1140	1090
Sunflowers NZ	11.04	5.52	6.30	617	607	582
SZ	13.77	13.12	12.56	1160	1140	1090

Table 7: Metabolites Step 1 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

Concentration	TR-4 Max. PECSW *(µg/L)*	TR-6 Max. PECSW *(µg/L)*	TR-7 Max. PECSW *(µg/L)*	TR-14 Max. PECSW *(µg/L)*	TR-15 Max. PECSW *(µg/L)*
wOSR NZ/SZ	10.1	7.42	9.06	8.93	8.59
Cotton NZ/SZ	10.1	7.42	9.06	8.93	8.59
SUNFLOWERS NZ/SZ	10.1	7.42	9.06	8.93	8.59
Concentration	**TR-4 PECSED *(µg/kg)***	**TR-6 PECSED *(µg/kg)***	**TR-7 PECSED *(µg/kg)***	**TR-14 PECSED *(µg/kg)***	**TR-15 PECSED *(µg/kg)***
wOSR NZ/SZ	73.9	25.6	67.6	67.2	52.4
Cotton NZ/SZ	73.9	25.6	67.6	67.2	52.4
SUNFLOWERS NZ/SZ	73.9	25.6	67.6	67.2	52.4

Table 8: Metabolites Step 2 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

Concentration	**TR-4 Max. PECSW *(µg/L)***	**TR-6 Max. PECSW *(µg/L)***	**TR-7 Max. PECSW *(µg/L)***	**TR-14 Max. PECSW *(µg/L))***	**TR-15 Max. PECSW *(µg/L)***
wOSR NZ	10.0	7.27	9.05	8.92	8.52
SZ	10.0	7.27	9.05	8.92	8.52
Cotton SZ	10.0	7.27	9.05	8.92	8.52
Sunflowers NZ	10.0	7.27	9.05	8.92	8.52
SZ	10.0	7.27	9.05	8.92	8.52
Concentration	**TR-4 PECSED *(µg/kg)***	**TR-6 PECSED *(µg/kg)***	**TR-7 PECSED *(µg/kg)***	**TR-14 PECSED *(µg/kg)***	**TR-15 PECSED *(µg/kg)***
wOSR NZ	71.6	24.8	65.6	65.1	50.8
SZ	71.9	24.9	65.8	65.3	50.9
Cotton SZ	71.9	25.0	66.0	65.6	51.1
Sunflowers NZ	71.6	24.8	65.6	65.1	50.8
SZ	72.1	25.0	66.0	65.6	51.1

Table 9: Comparison of Trifluralin PECsw (µg/L) at Steps 3 and 4, With and Without Runoff Mitigation

Cotton	**D6d**	**Note:**
Step 3	6.227	*default*
Step 4, 14 m	0.796	*drift mitigation only (runoff N/A for D6)*
Step 4, 20 m	**0.796**	*drift mitigation only (runoff N/A for D6)*

Sunflowers	**D5p**	**D5s**	**R1p**	**R1s**	**R3s**	**R4s**	**Note:**
Step 3	0.252	5.058	0.252	4.329	6.070	4.307	*default*
Step 4, 14 m	0.134	0.823	0.143	1.613	1.747	2.380	*drift mitigation only*
Step 4, 20 m	0.108	0.586	0.142	1.613	1.747	2.380	*drift mitigation only*
Step 4, 14 m	0.134	0.823	0.134	0.735	0.988	1.075	*drift & (where applicable) runoff mitigation together*
Step 4, 20 m	0.108	0.586	0.108	0.502	**0.704**	0.562	*drift & (where applicable) runoff mitigation together*

wOSR	**D2d**	**D2s**	**D3d**	**D4p**	**D4s**	**D5p**	**D5s**	**R1p**	**R1s**	**R3s**	**Note:**
Step 3	7.646	6.803	7.575	0.260	6.529	0.260	7.044	0.260	4.933	6.835	*default*
Step 4, 14 m	0.801	0.960	0.793	0.134	0.922	0.134	0.994	0.221	1.495	1.350	*drift mitigation only*
Step 4, 20 m	0.638	0.684	0.566	0.108	0.657	0.108	0.708	0.221	1.495	1.350	*drift mitigation only*
Step 4, 14 m	0.801	0.960	0.793	0.134	0.922	0.134	0.994	0.134	0.696	0.965	*drift & (where applicable) runoff mitigation together*
Step 4, 20 m	0.638	0.684	0.566	0.108	0.657	0.108	**0.708**	0.108	0.496	0.687	*drift & (where applicable) runoff mitigation together*

Values highlighted in shade and emboldened are the maximum PECsw concentrations with drift, and where applicable, runoff mitigation applied with a 20 m buffer zone

References

Ref 1:
Knowles, S. (2008): The predicted environmental concentrations of trifluralin and metabolites using the FOCUS surface water tools and scenarios for critical good agricultural practice. Dow AgroSciences report no. GHE-P-11836. 9 July 2008.

Ref 2:
FOCUS (2001): "FOCUS Surface Water Scenarios in the EU Evaluation Process under 91/414/EEC". Report of the FOCUS Working Group on Surface Water Scenarios, EC Document Reference SANCO/4802/2001-rev.2 final (May 2003). 245 pp.

Ref 3:
FOCUS (2005): "Landscape and Mitigation Factors in Aquatic Risk Assessment, Volume 1, Extended Summary and Recommendations", Report of the FOCUS Working Group on Landscape and Mitigation Factors in Ecological Risk Assessment, EC Document Reference SANCO/10422/2005

Ref 4:
Draft Assessment Report for Trifluralin (2003)

Ref 5:
EPI (Estimation Program Interface) Suite v3.11 developed by the US EPA Office of Pollution Prevention & the Syracuse Research Corporation (SRC). Copywright US EPA, 2003.

Ref. 6:
Yon, D. (2009): Modelling the kinetics of the degradation of trifluralin in laboratory sediment-water test systems. Dow AgroSciences report no. GHE-P-12080. 20 April 2009.

B.8.6.2 Predicted Environmental Concentrations in Ground Water

Reeves, G. "PREDICTED ENVIRONMENTAL CONCENTRATIONS IN GROUNDWATER FOR TR 4 (AN ANAEROBIC SOIL METABOLITE OF TRIFLURALIN) ACCORDING TO THE FOCUS SCENARIOS – SUPPLEMENTARY ANALYSIS, report number GHE-P-12081, 2009. Not published.
Objective: To estimate the PEC_{GW} values for trifluralin and TR-4.
Guidelines: FOCUS Groundwater Scenarios Workgroup, 2000.
GLP: No (modelling study)

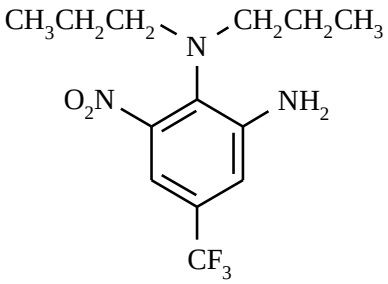
1. Introduction

This report provides supplementary data to modelling work previously carried out as described in GHE-P-10694 (Ref. 1), with the intention of addressing open points in the Evaluation Table (April 2009) for trifluralin metabolite, TR-4, in support of the Annex I resubmission of the parent compound. This report as well as GHE-P-10694 should be read as companion reports.

Trifluralin is the active substance in TREFLAN herbicides which are registered for the control of grass and broad-leaved weeds in a wide range of field crops. In support of Annex I inclusion under Directive 91/414/EEC, the Predicted Environmental Concentration in groundwater (PEC_{GW}) of parent compound and any major soil metabolites has to be derived to determine if they are relevant to groundwater, according to current guidance (Ref. 4). This has already been carried out for trifluralin (Ref. 2) for the supported uses and all associated FOCUS groundwater scenarios. In addition, this has also been carried out for the soil metabolite, TR-4, based on two of the four supported uses and two FOCUS scenarios in a screening exercise (Ref. 3). However, it has been requested at EU level that the screening modelling be expanded to include all the supported uses and relevant FOCUS scenarios.

The results of this modelling are the subject of this current report.

TR-4 (α,α,α-trifluoro-5-nitro-N^4,N^4-dipropyl-toluene-3,4-diamine) is a uniquely anaerobic metabolite of trifluralin that reaches a maximum of 11.6-13.2% AR during a 60-day anaerobic flooded soil study (Ref. 5). The structure is as follows.



TR-4 (MW 305.3)

2. LEACHING POTENTIAL

The key properties that determine leaching potential are the sorption Koc and the soil (aerobic) half-life, and these form the key inputs into the FOCUS models, together with the GAP. FOCUSPELMO modelling already carried out for trifluralin (Ref. 2) has shown that the PEC_{GW} for the parent is <0.001 µg/L for all FOCUS scenarios relevant to the supported uses. The key input parameters for trifluralin were a mean Koc of 8765 mL/g (Ref. 6), and a mean lab soil half-life of 181 days (Ref. 6).

Trifluralin has a high Koc value which indicates strong adsorption to soil. Based upon an assessment of the structural similarity of TR-4 to trifluralin, where one NO_2 group on the parent is replaced by an NH_2 group, it is also likely that the Koc for the metabolite would be equally high.

More scientifically, this can be demonstrated using software available from the US EPA, called EPI Suite v3.10 (Ref. 7). This suite of programs derives simple environmentally-relevant properties based upon input of the chemical structure (as a SMILES code). One of these programs i.e. "pckocwin v1.66" predicts Koc values. It should be noted the guidance document on relevant metabolites in groundwater (Ref. 3) references the use of extrapolated or estimated data for metabolites in cases where experimental data are not available. This has to be based upon expert judgement. In this case, the use of the "pckocwin v1.66" program to predict the Koc for TR-4 was validated by reference to trifluralin. As already mentioned, trifluralin has a mean Koc of 8765 mL/g. When the structure of trifluralin is converted to its SMILES code, i.e. O=[N+](c1cc(cc(c1N(CCC)CCC)[N+](=O)[O-])C(F)(F)F)[O-], and entered into "pckocwin v1.66", the program predicts a Koc of 9682 mL/g, which is in good agreement with the measured value. The model output is given in Figure 1.

When the structure of the metabolite TR-4 is entered into the same program as its SMILES code, i.e. N(c1cc(cc(c1N(CCC)CCC)[N+](=O)[O-])C(F)(F)F), it is predicted that the Koc will be 13600 mL/g. The model output is given in Figure 2. This estimate of Koc using the model suggests that TR-4 should have very low leaching potential, based upon the results already derived using FOCUSPELMO for trifluralin where the Koc was equally high. The estimated value for TR-4 should be considered reliable based upon the similarity of its structure to parent, where good agreement between predicted and the measured Koc was seen.

Although a half-life is not available for TR-4, an assumption could be made in an extreme case that it is ten times more persistent than trifluralin. This would give a half-life of 1810 days for input into the model. It should also be remembered in any case that TR-4 will only form at up to *ca* 13% AR, which will limit leaching potential still further when compared to parent.

3. ESTIMATION OF PEC_{GW} FOR TR-4

For estimation of the PEC_{GW} for TR-4, a predicted Koc value of 13600 mL/g was used for model input, using a Freundlich exponent of 1 as a default value. For the half-life of TR-4, an assumed value of 1810 days was used. A worst case formation fraction of 1 was assumed by application of the following degradation scheme into the model:

Trifluralin to TR-4 to sink

FOCUSPELMO 3.3.2 was used to model the PEC_{GW} for TR-4. The earlier work carried out using parent was used as a guide (Ref. 1), except that in this new work the degradation route was assumed to be trifluralin to TR-4 to CO_2/bound residue. This quantitative conversion of parent to metabolite is worst-case since in reality other minor metabolites will also be formed that will reduce the amount of TR-4 available for leaching. The uses modelled were:

Spring appn. to cotton: 1.2 kg as/ha (1 Mar), with soil incorporation to 20 cm.

Autumn appn. to oilseed rape: 1.2 kg as/ha (30 Sep), with soil incorporation to 20 cm.

Spring appn. to sunflowers: 1.2 kg as/ha (1 Mar), with soil incorporation to 20 cm.

The input parameters to the model are summarised in Tables 1 and 2, whilst the results are given in Table 3.

Table 1: Specific Input Parameters

Parameter	Value	
	Trifluralin	**TR-4**
Molecular weight	335.3 g/mol	305.3 g/mol
$DT_{50(lab)}$	181 days *mean of five soils at 22°C (not corrected for moisture)*	1810 days *estimated worst-case (10x parent) at 22°C*
Koc	8765 mL/g *mean of four soils*	13600 mL/g *estimated using "pckocwin v1.66"*
Freundlich exponent (1/n)	0.972 *mean of four soils*	1 *default*
Water solubility	0.194 mg/L at 20°C *distilled water*	N/A
Vapour pressure	9.5×10^{-3} Pa at 25°C	N/A

N/A = not applicable

Table 2: Model Inputs to PELMO

Scenario No.	**1**	**2**	**3**
Crop	Cotton	Oilseed rape	Sunflowers
Application mode	Bare soil		
Application depth	20 cm		
Plant uptake factor	0.5 *(default)*		
Air diffusion co-efficient	0.046 cm^2/s *(calculated using diffu.exe)*		
Volatilisation depth	0.1 cm *(default)*		
pH during sorption test	7 *(default)*		
pKa	20 *(default)*		
Limit for Freundlich equation	0.01 µg/L *(default)*		
Sorption annual increase	0% *(default)*		
Individual rate correction in soil	temperature = 22ºC, Q_{10} = 2.2 *(default)*, 100% relative moisture, moisture exponent 0.7 *(default)*		
FOCUS scenario	Sevilla, Thiva	Châteaudun, Hamburg, Kremsmünster, Okehampton, Piacenza, Porto	Piacenza, Sevilla

Table 3: 80th 'ile Annual Average Leachate Concentrations at 1 m Depth (µg/L)

Scenario/Use	Châteaudun	Hamburg	Jokioinen	Kremsmünst	Okehampton	Piacenza	Porto	Sevilla	Thiva
Cotton (spring appn.)									
Trifluralin	-	-	-	-	-	-	-	<0.001	<0.001
TR-4	-	-	-	-	-	-	-	<0.001	<0.001
Oilseed rape (autumn appn.)									
Trifluralin	<0.001	<0.001	-	<0.001	<0.001	<0.001	<0.001	-	-
TR-4	<0.001	<0.001	-	<0.001	<0.001	<0.001	<0.001	-	-
Sunflowers (spring appn.)									
Trifluralin	-	-	-	-	-	<0.001	-	<0.001	-
TR-4	-	-	-	-	-	<0.001	-	<0.001	-

"-" = no FOCUS location for this crop

The FOCUSPELMO results showed, even when using an extreme soil half-life of 1810 days for TR-4, that the PEC_{GW} was <0.001 µg/L. This was the same as seen for trifluralin. An example output file from FOCUSPELMO (oilseed rape, Piacenza) is shown in Appendix I.

4. CONCLUSIONS

The PEC_{GW} for the major anaerobic metabolite of trifluralin, i.e. TR-4, is estimated to be <0.001 µg/L for all FOCUS scenarios relevant to the supported uses. This is the same as for parent compound and is indicative of their high Koc values. Therefore, this metabolite would not be considered relevant to groundwater, as prescribed under current guidance (Ref. 4).

References

1. Reeves, G. (2004): Predicted environmental concentrations in groundwater for TR-4 (an anaerobic soil metabolite of trifluralin) according to the FOCUS scenarios. *Dow AgroSciences, unpublished report no. GHE-P-10694*

2. Reeves, G. (2001): Modelling the leaching of trifluralin to groundwater in the EU using PELMO in the FOCUS scenarios. *Dow AgroSciences, unpublished report no. GHE-P-9392*

3. Reeves, G. (2003): Predicted environmental concentration in groundwater for TR-4 (an anaerobic soil metabolite of trifluralin). *Dow AgroSciences, unpublished report no. GHE-P-10273*

4. Guidance document on the assessment of the relevance of metabolites in groundwater of substances regulated under Council Directive 91/414/EEC. *Sanco/221/2000 – rev.10 -final, 25 February 2003*

5. Graper, L.K. and Rainey, D.P. (1989): Anaerobic metabolism of ^{14}C trifluralin in sandy loam, loam and clay loam soils. *Dow AgroSciences, unpublished report no. 152 ESMETB AM 47-72*

6. Document N submitted in support of Annex I inclusion for trifluralin (April 2002).

7. EPI (Estimation Program Interface) Suite v3.10 developed by the US EPA Office of Pollution Prevention and the Syracuse Research Corporation (SRC). *Copywright US EPA, 2000*

Figure 1. pckocwin v1.66 output for trifluralin

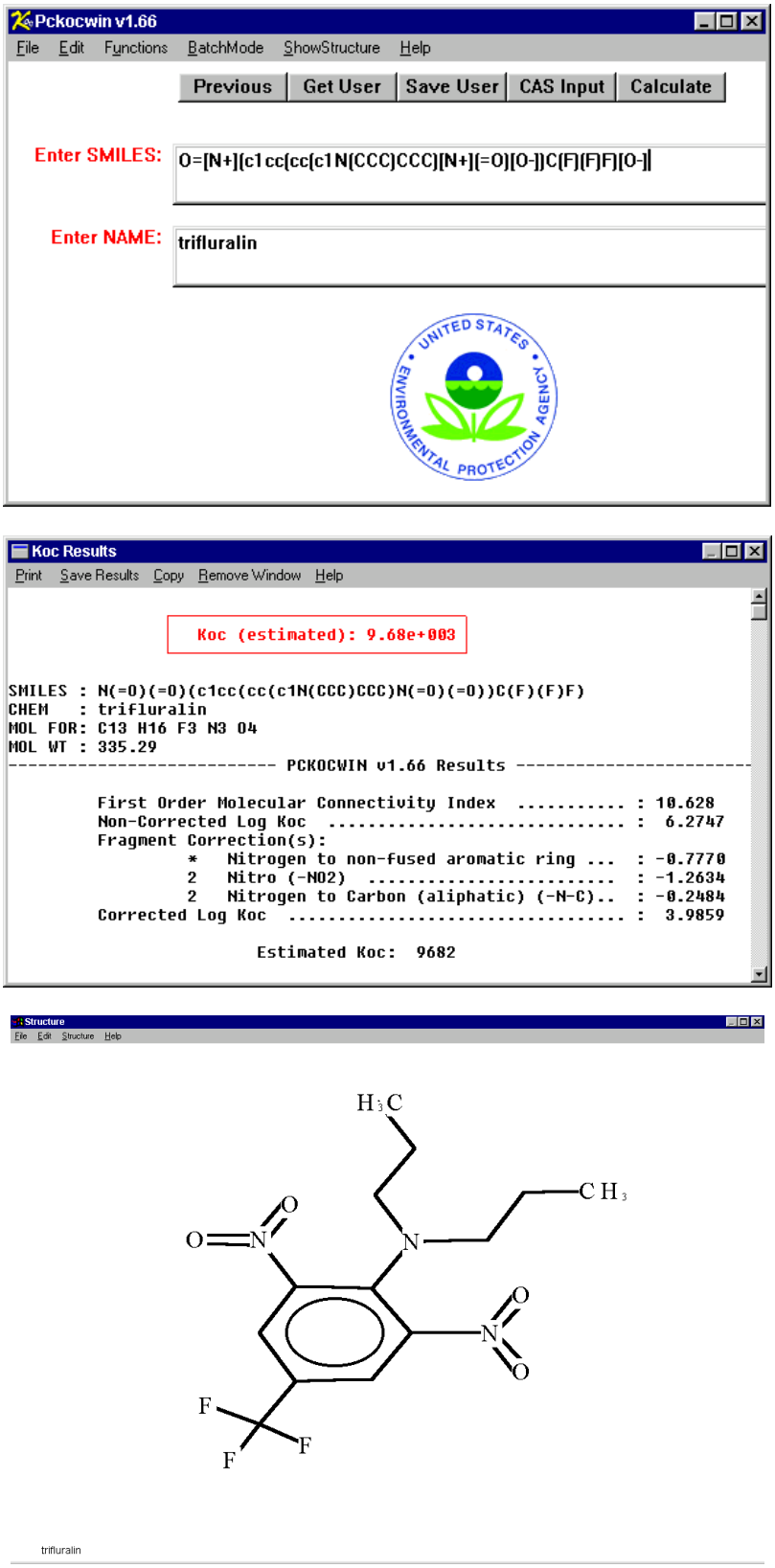
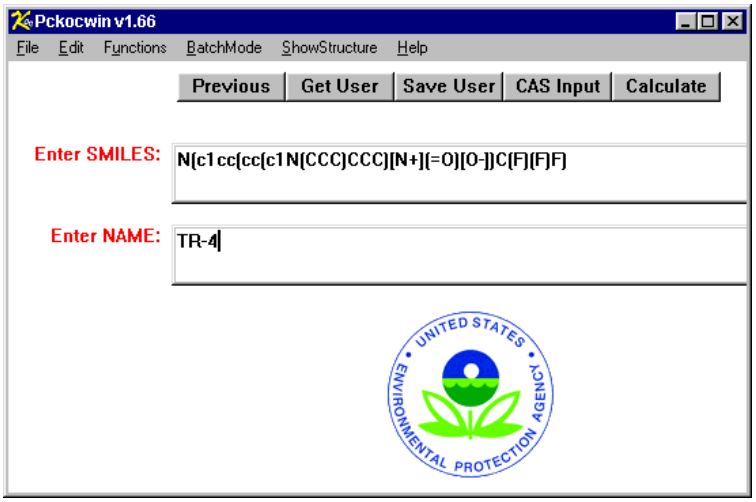
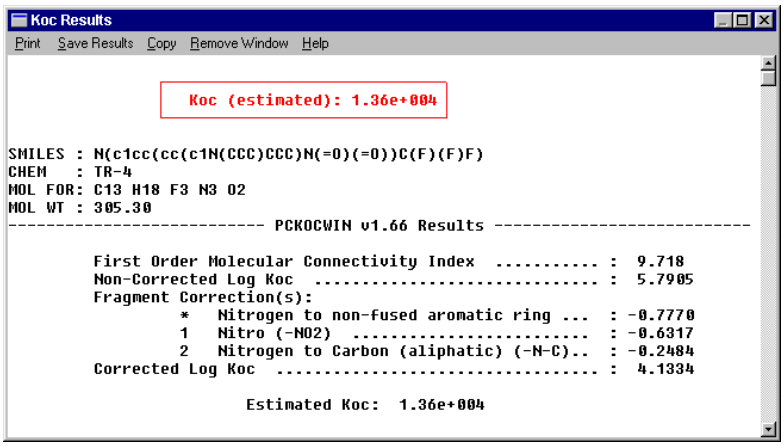
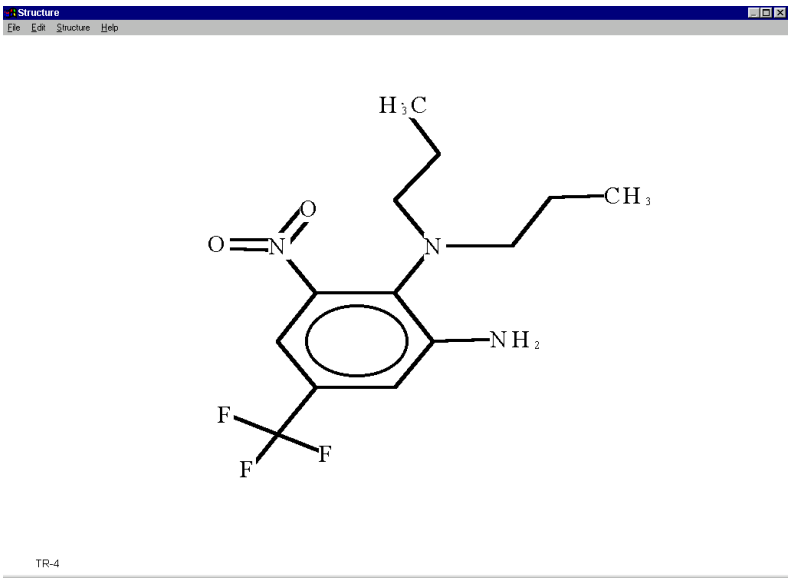


Figure 2. pckocwin v1.66 output for TR-4


Pckocwin v1.66
File Edit Functions BatchMode ShowStructure Help
Previous
Get User
Save User
CAS Input
Calculate
Enter SMILES:
N(c1cc(cc(c1N(CCC)CCC)[N+](=O)[O-])C(F)(F)F)
Enter NAME:
TR-4
UNITED STATES ENVIRONMENTAL PROTECTION AGENCY


Koc Results
Print Save Results Copy Remove Window Help
Koc (estimated): 1.36e+004
SMILES : N(c1cc(cc(c1N(CCC)CCC)N(=O)(=O))C(F)(F)F)
CHEM : TR-4
MOL FOR: C13 H18 F3 N3 O2
MOL WT : 305.30
PCKOCWIN v1.66 Results
First Order Molecular Connectivity Index ..... : 9.718
Non-Corrected Log Koc ..... : 5.7905
Fragment Correction(s):
* Nitrogen to non-fused aromatic ring ... : -0.7770
1 Nitro (-NO2) ..... : -0.6317
2 Nitrogen to Carbon (aliphatic) (-N-C).. : -0.2484
Corrected Log Koc ..... : 4.1334
Estimated Koc: 1.36e+004


Structure
File Edit Structure Help
H3C
CH3
O
O=N
N
NH2
F
F
F
TR-4

Reeves, G. "MODELLING THE LEACHING OF TRIFLURALIN AND A POTENTIALLY-RELEVANT METABOLITE (TR-4) TO GROUNDWATER IN THE EU USING PEARL AND THE FOCUS SCENARIOS – SUPPLEMENTARY ANALYSIS, report number GHE-P-12082, 2009. Not published.
Objective: To estimate the PEC_{GW} values for trifluralin and TR-4.
Guidelines: FOCUS Groundwater Scenarios Workgroup, 2000.
GLP: No (modelling study)

1. Introduction

This report provides supplementary data to modelling work previously carried out as described in GHE-P-11131 (Reeves, 2005), with the intention of addressing open points in the Evaluation Table (April 2009) for trifluralin metabolite, TR-4, in support of the Annex I resubmission of the parent compound. This report as well as GHE-P-11131 should be read as companion reports.

Trifluralin is the active substance in TREFLAN herbicides which are registered for the control of grass and broad-leaved weeds in a wide range of field crops. To support Annex I inclusion under Directive 91/414/EEC, a study has been carried out to model the leaching of trifluralin, and a potentially-relevant metabolite (α,α,α-trifluoro-5-nitro-N^4,N^4-dipropyl-toluene-3,4-diamine, designated TR-4) to groundwater in the EU. This was following the pre-emergence use of TREFLAN herbicides in cotton, oilseed rape, and sunflowers according to GAP.

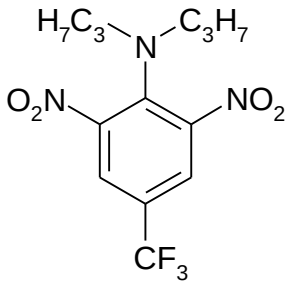
The modelling was carried out using the FOCUS groundwater scenarios and the FOCUSPEARL model. Modelling carried out using FOCUSPELMO for trifluralin and TR-4 is reported elsewhere (Reeves, 2009).

The modelling was conducted within the Regulatory Laboratories group of Dow AgroSciences, European Development Centre, 2nd Floor, 3 Milton Park, Abingdon, Oxon., OX14 4RN, UK.

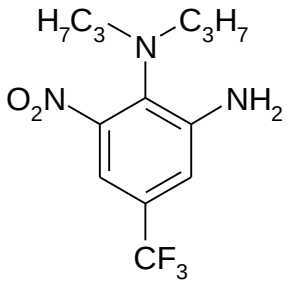
2. MODELLING INFORMATION

2.1 Test Items

The structures of the test items modelled are shown below:



trifluralin



TR-4

TR-4 was modelled, in addition to parent compound, because this metabolite reached up to 13.4% AR in flooded soil under anaerobic conditions, and according to current guidance (Sanco, 2003) must be assessed as to its relevance to groundwater.

2.2 Model Background

The modelling was carried out using FOCUSPEARL (ver. 3.3.3), which is derived from PEARL ver. 3.0. A full description of the model is given in the report of the FOCUS Groundwater Scenarios Workgroup (FOCUS, 2000) and so is not repeated here. The model calculates the annual average pore water concentration at 1 m

depth over a 20 year period, and the 80th percentile value is then normally selected for regulatory decision making.

2.3 Model Assumptions and Scenarios

FOCUSPEARL was used to model the bare soil application of TREFLAN to cotton, oilseed rape and sunflowers. Following soil application, the modelling assumed incorporation to a maximum depth of 20 cm, according to GAP (Table 1).

Table 1: Description of GAP Modelled

GAP
Spring application to cotton: 1.2 kg as/ha (1 March), with soil incorporation to 20 cm.
Autumn application to winter oilseed rape: 1.2 kg as/ha (30 September), with soil incorporation to 20 cm.
Spring application to sunflowers: 1.2 kg as/ha (1 March), with soil incorporation to 20 cm.

2.4 Model Inputs

For each GAP (Table 1), a project was created within FOCUSPEARL using the model input and application parameters for trifluralin and TR-4 shown in Tables 2 and 3.

For trifluralin, the source of the model input data was the dossier submitted in support of Annex I inclusion (Document N, 2002). Individual $DT_{50(lab)}$ values for trifluralin leading to the overall geometric mean $DT_{50(lab)}$ of 161 days at 22ºC (or arithmetic mean of 181 days) were corrected for soil moisture content at field capacity (10 kPa) using the procedure recommended in the FOCUS guidance (FOCUS, 2000). This gave a geometric mean standardised $DT_{50(lab)}$ value of 115 days at 22ºC for input into the model (Appendix II).

For the metabolite TR-4, a number of parameters from direct measurement were not available for model input. However, estimates were made using the US EPA's EPI program suite (Appendix I) for vapour pressure, water solubility and Koc (from which Kom was derived). Furthermore, in order to arrive at a half-life value for input into FOCUSPEARL in the absence of data, a value of 10x parent, i.e. 1150 days at 22ºC was used. This is deemed to be sufficiently conservative for a worst case approach.

The transformation scheme (first-order kinetics) assumed within FOCUSPEARL was trifluralin → TR-4, and the transformation factor used in the model was set at a worst case value of 1.

2.5 Model Runs

All simulations were carried out using the scenario appropriate for the particular crop as recommended by FOCUS. Each use was investigated as consecutive annual applications for a period of 20 years.

Table 2: Model Inputs to FOCUSPEARL

Parameter	Trifluralin	TR-4	Comments
General:			
Molar mass (g/mol)	335	245	-
Saturated vapour pressure (Pa)	9.5×10^{-3}	4.3×10^{-4}*	25ºC
Molar enthalpy of vaporisation (kJ/mol)	95	95	FOCUS default
Solubility in water (mg/L)	0.194	1.4*	20ºC & 25ºC, respectively
Molar enthalpy of dissolution (kJ/mol)	27	27	FOCUS default
Freundlich Sorption:			
Option	Kom	Kom	pH independent
Kom (L/kg)	5096	7907*	Mean Koc ÷ 1.72
Molar enthalpy of sorption (kJ/mol)	0	0	FOCUS default
Reference conc. in liquid phase (mg/L)	1	1	FOCUS default
Freundlich sorption exponent	0.972	1	Mean measured value & default, respectively
Desorption rate coefficient (1/d)	0	0	FOCUS default
Factor relating CofFreNeq & CofFreEql	0	0	FOCUS default
Transformation:			
Half-life (d)	115	1150**	22ºC, geomean
Optimum moisture conditions (pF2/wetter)	Yes	Yes	FOCUS default
Exponent for the effect of liquid	0.7	0.7	FOCUS default
Molar activation energy (kJ/mol)	54	54	FOCUS default
Diffusion:			
Reference temperature for diffusion (ºC)	20	20	FOCUS default
Reference diffusion coeff. water (m^2/d)	4.3×10^{-5}	4.3×10^{-5}	FOCUS default
Reference diffusion coeff. air (m^2/d)	0.43	0.43	FOCUS default
Crop data:			
Wash-off factor (1/m)	0.0001	0.0001	FOCUS default
Canopy process option	Lumped	Lumped	FOCUS default
Half-life at crop surface (d)	1000000	1000000	FOCUS default
Coefficient for uptake by plant	0.5	0.5	FOCUS default

* *See Appendix I*

** *Conservative estimate based on 10x parent value*

Table 3: Application Parameters

Application:	**Value**	**Comments**
Option	Absolute	-
Application type	Incorporation	Cotton, winter oilseed rape and sunflowers
Depth (m)	0.2	According to GAP, equivalent to 20 cm

3. RESULTS AND CONCLUSIONS

The 80th percentile results for each crop and FOCUS-scenario combination for the annual average trifluralin and TR-4 concentrations in the leachate at 1 m soil depth (µg/L) are summarised in Table 4.

Table 4: 80th Percentile Annual Average Leachate Concentrations at 1 m Depth (µg/L)

Use	CHA	HAM	JOK	KRE	OKE	PIA	POR	SEV	THI
Cotton									
Trifluralin	-	-	-	-	-	-	-	<0.001	<0.001
TR-4								<0.001	<0.001
Oilseed rape									
Trifluralin	<0.001	<0.001	-	<0.001	<0.001	<0.001	<0.001	-	-
TR-4	<0.001	<0.001		<0.001	<0.001	0.001	<0.001		
Sunflowers									
Trifluralin	-	-	-	-	-	<0.001	-	<0.001	-
TR-4						0.018		<0.001	

- no FOCUS location for this crop

In all the runs modelled, the 80th percentile annual average leachate concentrations for trifluralin at 1 m depth (PEC_{GW}) were estimated to be <0.1 µg/L. This was also true for the metabolite, and as such TR-4 would be considered non-relevant to groundwater according to current guidance (Sanco, 2003).

These findings are supported by the modelling carried out using FOCUSPELMO (Reeves, 2009).

REFERENCES

3. Reeves, G. (2005): Modelling the leaching of trifluralin and a potentially-relevant metabolite (TR-4) to groundwater in the EU using PEARL and the FOCUS scenarios. Dow AgroSciences unpublished report no. GHE-P-11131. 1 July 2005.

4. Reeves, G. (2009): Predicted environmental concentrations in groundwater for TR-4 (an anaerobic soil metabolite of trifluralin) according to the FOCUS scenarios – Amended report. Dow AgroSciences unpublished report no. GHE-P-10694R. 16 April 2009.

5. Sanco (2003): Guidance Document on the Assessment of the Relevance of Metabolites in Groundwater of Substances Regulated Under Council Directive 91/414/EEC, Sanco/221/2000 – rev.10 –final. February 2003.

6. FOCUS (2000): "FOCUS groundwater scenarios in the EU pesticide registration process" Report of the FOCUS Groundwater Scenarios Workgroup, EC Document Reference Sanco/321/2000 rev.2, 202pp.

7. Document N (2002): EU Dossier in support of Annex I inclusion under 91/414/EEC. April 2002.

8. EPI (Estimation Program Interface) Suite v3.11 developed by the US EPA Office of Pollution Prevention & the Syracuse Research Corporation (SRC). Copywright US EPA, 2003.

APPENDIX I

Estimation of Vapour Pressure, Water Solubility and Koc for TR-4

Software is available, called EPI Suite v3.11 (US EPA, 2003), which is a suite of programs which can derive simple environmentally-relevant properties based upon input of the chemical structure (as a SMILES code). Three programs are available within this suite, i.e. "mpbpwin v1.41", "wskowwin v1.41", and "pckocwin v1.66" which can estimate vapour pressure, water solubility and Koc values, respectively. It should be noted the guidance document on relevant metabolites in groundwater (Sanco, 2003) references the use of extrapolated or estimated data for metabolites in cases where experimental data are not available.

The use of the "pckocwin v1.66" program to predict the important Koc parameter for TR-4 was validated by reference to trifluralin, which has a measured mean Koc of 8765 mL/g. When the structure of trifluralin is converted to its SMILES code, i.e. O=[N+](c1cc(cc(c1N(CCC)CCC)[N+](=O)[O-])C(F)(F)F)[O-], and entered into "pckocwin v1.66", the program predicts a Koc of 9682 mL/g, which is in good agreement with the measured value. Therefore, the estimated value for TR-4 should be considered reliable based upon the similarity of its structure to parent, where good agreement between predicted and the measured Koc was seen.

When the structure of the metabolite TR-4 was entered into the programs as its SMILES code, i.e. N(c1cc(cc(c1N(CCC)CCC)[N+](=O)[O-])C(F)(F)F), it was predicted that the vapour pressure, water solubility and Koc would be 3.24×10^{-6} mm Hg (25ºC), 1.4 mg/L (25ºC), and 13600 mL/g. Using a unit converter for vapour pressure gives a value of 4.3×10^{-4} Pa (25ºC) for input into FOCUSPEARL.

The various model outputs from EPI Suite v3.11 are given in Figures AI.1 to AI.4.

Figure AI.1: Verification of Molecular Structure of TR-4 Based Upon SMILES Code

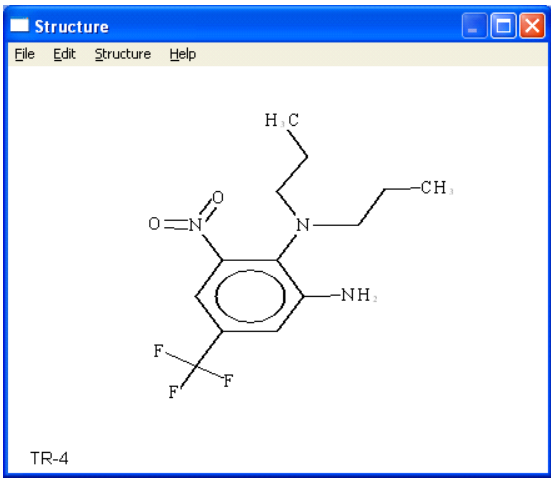


Figure AI.2: Vapour Pressure Estimation for TR-4

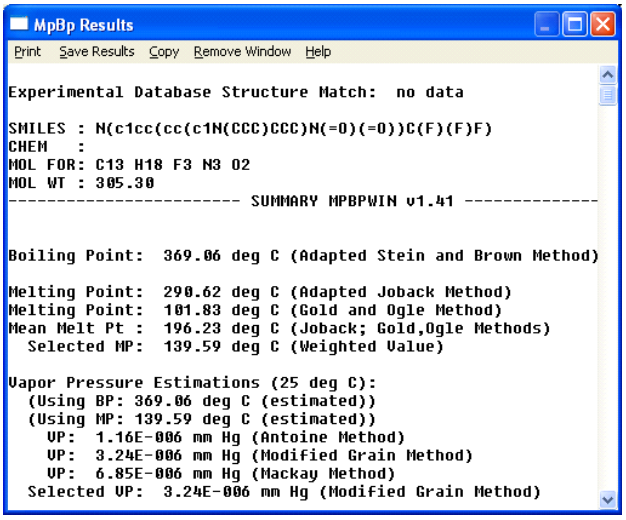


Figure AI.3: Water Solubility Estimation for TR-4

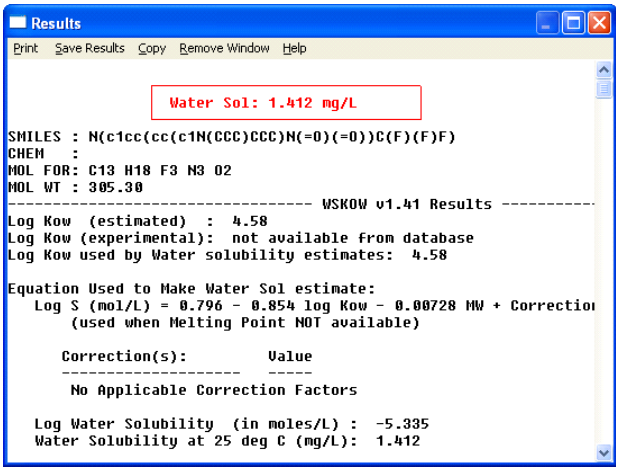
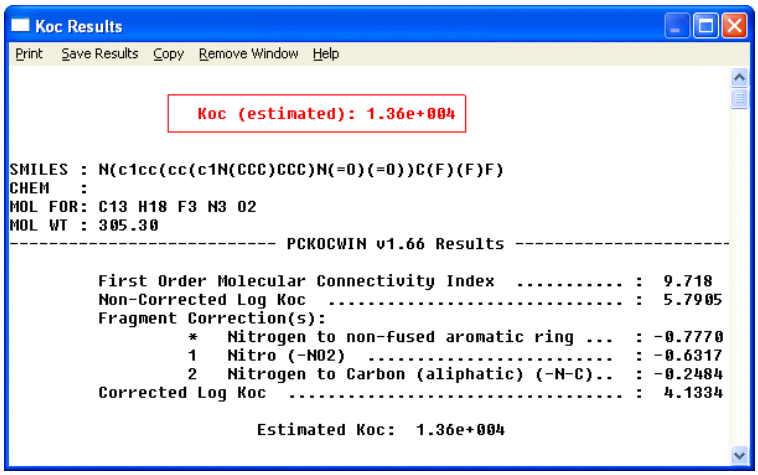


Figure AI.4: Koc Estimation for TR-4



APPENDIX II
Calculation of Trifluralin $DT_{50(lab)}$ Corrected for Soil Moisture Content at Field Capacity

Individual $DT_{50(lab)}$ values for trifluralin leading to the overall geometric mean $DT_{50(lab)}$ of 161 days at 22ºC (or arithmetic mean of 181 days) were corrected for soil moisture content at field capacity (10 kPa) using the procedure recommended in the FOCUS guidance (FOCUS, 2000). This gave a geometric mean standardised $DT_{50(lab)}$ value of 115 days at 22ºC for input into the model.

The calculation to determine the soil water content at field capacity and its impact upon the $DT_{50(lab)}$ values are shown below:

soil (USDA)	DT50 at 22C (days)	actual moisture (% w/w)	comments	gravimetric w/c at 10kPa (% w/w)	correction factor	corrected DT50 at 10 kPa (days)
sandy loam	154	8.9	actual moisture as stated in report	19	0.59	91
loam	81	15.3	actual moisture as stated in report	25	0.71	57
clay loam	179	19.5	actual moisture as stated in report	28	0.78	139
sand	136	9.6	actual moisture as stated in report	12	0.86	116
sandy loam	356	10.8	actual moisture as stated in report	19	0.67	240
arithmetic mean (d)	**181**				**arithmetic mean (d)**	**129**
geo mean (d)	**161**				**geo mean (d)**	**115**
					CV (%)	**53.8**

B.8.11 REFERENCES RELIED ON

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
IIA 7.2.1	Yon, D.A.,	2009	MODELING THE KINETICS OF THE DEGRADATION OF TRIFLURALIN IN LABORATORY SEDIMENT-WATER TEST SYSTEMS GLP: Not required Report No.: GHE-P-12080, 2009. Not published	Y	DOW
IIIA 9.2.3	Reeves, G.,	2009	THE PREDICTED ENVIRONMENTAL CONCENTRATIONS OF TRIFLURALIN AND METABOLITES USING THE FOCUS SURFACE WATER TOOLS AND SCENARIOS FOR CRITICAL GOOD AGRICULTURAL PRACTICE – SUPPLEMENTARY ANALYSIS, GLP: Not required Report No: GHE-P-12083, 2009 Not published	Y	DOW
IIIA 9.2.1	Reeves, G.	2009	PREDICTED ENVIRONMENTAL CONCENTRATIONS IN GROUNDWATER FOR TR 4 (AN ANAEROBIC SOIL METABOLITE OF TRIFLURALIN) ACCORDING TO THE FOCUS SCENARIOS – SUPPLEMENTARY ANALYSIS, GLP: Not required Report No: GHE-P-12081, 2009 Not published	Y	DOW
IIIA 9.2.1	Reeves, G.	2009	MODELLING THE LEACHING OF TRIFLURALIN AND A POTENTIALLY RELEVANT METABOLITE (TR 4) TO GROUNDWATER IN THE EU USING PEARL AND THE FOCUS SCENARIOS – SUPPLEMENTARY ANALYSIS GLP: Not required Report No:GHE-P-12082, 2009 Not published	Y	DOW

Council Directive 91/414/EEC

TRIFLURALIN

Addendum 2 to Additional Report to the DAR

Summary, Scientific Evaluation and Assessment

May 2009

Report and Proposed Decision of Hellas
made to the European Commission under Article 8 of 91/414/EEC

HELLENIC MINISTRY OF RURAL DEVELOPMENT AND FOOD
GENERAL DIRECTORATE OF PLANT PRODUCTION
DIRECTORATE OF PLANT PROTECTION
DEPARTMENT OF PESTICIDES
Hippokratous 3-5,
10164 Athens
Hellas

VOLUME 3
ANNEX B

RAPPORTEUR MEMBER STATES SUMMARY, EVALUATION AND ASSESSMENT OF THE DATA AND INFORMATION SUBMITTED

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VOLUME 3

B.8 ENVIRONMENTAL FATE AND BEHAVIOUR

B.8.1.2 RATE OF DEGRADATION

In response to Open point 4.5

"RMS to calculate the normalised DT50 for the temperature to 20°C as well as moisture to -10kPa and to update the LoEP to include the individual normalised values."

of the Evaluation Table of Trifluralin following PRAPeR Expert Meeting TC 10 (19 May 2009), the RMS has calculated the temperature-normalized soil DT50's for trifluralin using a Walker coefficient of 0.7 and a Q10 factor of 2.2, based on the data from studies Washbrooke, 1976 and Graper, L.K., 1989 of the DAR.

Soil type	Moisture (MWHC)	Temperature, °C	DT_{50} (days)	DT_{50} (days) @ pF 2	DT_{50} (days) @ pF 2 & @ 20 °C
Speyer 2.1	40%	22	136	116	134.9
Speyer 2.2	40%	22	356	240	279
Sandy loam	75%	22	154	91	105.8
Loam	75%	22	81	57	66.3
Clay loam	75%	22	179	139	161.6
		Geomean	**161**	**115**	**134**

B.8.6.2 PREDICTED ENVIRONMENTAL CONCENTRATIONS IN GROUND WATER

In response to Open point 4.9

"RMS to carry out new groundwater simulations for the active substance trifluralin using an incorporation depth of 5cm to confirm the groundwater exposure assessment. Substance properties to be used: soil DT50 geometric mean of normalised to FOCUS reference condition laboratory values (ca. 135 days see open point 4.5), KFoc 8765 mL / g; 1/n=0.972"

of the Evaluation Table of Trifluralin following PRAPeR Expert Meeting TC 10 (19 May 2009), the RMS has conducted new groundwater simulations for the active substance trifluralin using FOCUS PELMO v.3.2.2.
Objective: To estimate the PEC_{GW} values for trifluralin.
Guidelines: FOCUS Groundwater Scenarios Workgroup, 2000.
GLP: No (modelling study)

Results:

The uses modelled were:

Spring appn. to cotton: 1.2 kg as/ha (1 Mar), with soil incorporation to 5 cm.

Autumn appn. to oilseed rape: 1.2 kg as/ha (30 Sep), with soil incorporation to 5 cm.

Spring appn. to sunflowers: 1.2 kg as/ha (1 Mar), with soil incorporation to 5 cm.

The input parameters to the model are summarized in Tables 1 and 2, whilst the results are given in Table 3.

Table 1: Specific Input Parameters

Parameter	Trifluralin
Molecular weight	5. 335.3 g/mol
$DT_{50(lab)}$	6. 134 days 7. *geomean of five soils at 20°C and pF 2*
Koc	8765 mL/g *mean of four soils*
Freundlich exponent (1/n)	0.972 *mean of four soils*
Water solubility	0.194 mg/L at 20°C *distilled water*
Vapour pressure	9.5 x 10^{-3} Pa at 25°C

Table 2: Model Inputs to PELMO

Scenario No.	1	2	3
Crop	Cotton	Oilseed rape	Sunflowers
Application mode	Bare soil		
Application depth	5 cm		
Plant uptake factor	0.5 *(default)*		
Air diffusion co-efficient	0.046 cm^2/s *(calculated using diffu.exe)*		
Volatilisation depth	0.1 cm *(default)*		
pH during sorption test	7 *(default)*		
pKa	20 *(default)*		
Limit for Freundlich equation	0.01 µg/L *(default)*		
Sorption annual increase	0% *(default)*		
FOCUS scenario	Sevilla, Thiva	Châteaudun, Hamburg, Kremsmünster, Okehampton, Piacenza, Porto	Piacenza, Sevilla

Table 3: 80th %ile Annual Average Leachate Concentrations at 1 m Depth (µg/L)

Scenario/Use	Châteaudun	Hamburg	Jokioinen	Kremsmünst	Okehampton	Piacenza	Porto	Sevilla	Thiva
Cotton (spring appn.)	-	-	-	-	-	-	-	<0.001	<0.001
Oilseed rape (autumn appn.)	<0.001	<0.001	-	<0.001	<0.001	<0.001	<0.001	-	-
Sunflowers (spring appn.)	-	-	-	-	-	<0.001	-	<0.001	-

"-" = no FOCUS location for this crop

Conclusion:

The FOCUSPELMO results showed that the PEC_{GW} was <0.001 µg/L in all scenarios relevant to the supported uses. Example output files from FOCUSPELMO are shown below.

*** FOCUSPELMO 3. 3. 2 *** (PELMO 3.22)

Ver 2 Thiva, cotton

(T) Pesticide A, Cotton <TRIFLURALIN>

Ver 2 THIVA scenario (38.32 N, 23.32 E) maize IRR Year:01

Pesticide in the percolate at 1 m soil depth

Year	Pesticide Flux (g/ha)	Percolate (L/m²)	Pesticide Conc. (µg/L)
1	0.0E+00	7.53500	0.000
2	0.0E+00	0.0E+00	0.000
3	0.0E+00	61.9900	0.000
4	0.0E+00	0.0E+00	0.000
5	0.0E+00	0.0E+00	0.000
6	0.0E+00	0.0E+00	0.000
7	0.0E+00	91.4300	0.000
8	0.0E+00	131.600	0.000
9	0.0E+00	24.8300	0.000
10	0.0E+00	101.600	0.000
11	0.0E+00	149.000	0.000
12	0.0E+00	119.900	0.000
13	0.0E+00	153.900	0.000
14	0.0E+00	87.3700	0.000
15	0.0E+00	97.0400	0.000
16	0.0E+00	103.500	0.000
17	0.0E+00	97.7000	0.000
18	0.0E+00	89.2900	0.000
19	0.0E+00	72.5500	0.000

20	0.0E+00	172.200	0.000
21	0.0E+00	0.0E+00	0.000
22	0.0E+00	0.0E+00	0.000
23	0.0E+00	61.9900	0.000
24	0.0E+00	0.0E+00	0.000
25	0.0E+00	0.0E+00	0.000
26	0.0E+00	0.0E+00	0.000
Total	0.0E+00	1553.90	0.000
80 Perc.(10)	0.0E+00	101.600	0.000

*** FOCUSPELMO 3. 3. 2 *** (PELMO 3.22)

Ver 2 Porto, oil seed rape (winter)

(O) Pesticide A, Oil seed rape <TRIFLURALIN>

Ver 2 Porto scenario (41.23 N, 8.68 W) Year:01

Pesticide in the percolate at 1 m soil depth

Year	Pesticide Flux (g/ha)	Percolate (L/m²)	Pesticide Conc. (µg/L)
1	0.0E+00	527.500	0.000
2	0.0E+00	429.700	0.000
3	0.0E+00	508.200	0.000
4	0.0E+00	111.100	0.000
5	0.0E+00	329.600	0.000
6	0.0E+00	370.800	0.000
7	0.0E+00	474.800	0.000
8	0.0E+00	671.900	0.000
9	0.0E+00	915.200	0.000
10	0.0E+00	842.700	0.000
11	0.0E+00	849.100	0.000
12	0.0E+00	411.700	0.000
13	0.0E+00	543.900	0.000
14	0.0E+00	543.800	0.000
15	0.0E+00	512.700	0.000
16	0.0E+00	816.700	0.000
17	0.0E+00	689.200	0.000
18	0.0E+00	653.300	0.000
19	0.0E+00	808.000	0.000

20	0.0E+00	476.400	0.000
21	0.0E+00	472.100	0.000
22	0.0E+00	429.700	0.000
23	0.0E+00	508.200	0.000
24	0.0E+00	111.100	0.000
25	0.0E+00	329.600	0.000
26	0.0E+00	370.800	0.000
Total	0.0E+00	11430.9	0.000
Perc.(10)	0.0E+00	842.700	0.000

*** FOCUSPELMO 3. 3. 2 *** (PELMO 3.22)

Ver 2 Sevilla. sunflower

(S) Pesticide A, Sunflowers <TRIFLURALIN>

Ver 2 SEVILLA scenario (37.42 N, 5.88 W) maize IRR Year:01

Pesticide in the percolate at 1 m soil depth

Year	Pesticide Flux (g/ha)	Percolate (L/m²)	Pesticide Conc. (µg/L)
1	0.0E+00	137.200	0.000
2	0.0E+00	21.5800	0.000
3	0.0E+00	0.0E+00	0.000
4	0.0E+00	0.0E+00	0.000
5	0.0E+00	0.0E+00	0.000
6	0.0E+00	0.0E+00	0.000
7	0.0E+00	0.0E+00	0.000
8	0.0E+00	30.4100	0.000
9	0.0E+00	106.200	0.000
10	0.0E+00	61.5600	0.000
11	0.0E+00	106.800	0.000
12	0.0E+00	0.0E+00	0.000
13	0.0E+00	0.0E+00	0.000
14	0.0E+00	0.0E+00	0.000
15	0.0E+00	4.42100	0.000
16	0.0E+00	0.0E+00	0.000
17	0.0E+00	38.8600	0.000
18	0.0E+00	4.35600	0.000
19	0.0E+00	0.0E+00	0.000
20	0.0E+00	0.0E+00	0.000

21	0.0E+00	103.100	0.000
22	0.0E+00	21.5800	0.000
23	0.0E+00	0.0E+00	0.000
24	0.0E+00	0.0E+00	0.000
25	0.0E+00	0.0E+00	0.000
26	0.0E+00	0.0E+00	0.000

Total	0.0E+00	477.287	0.000
Perc.(10)	0.0E+00	61.5600	0.000

Council Directive 91/414/EEC

TRIFLURALIN

Corrigendum 1 to Additional Report to the DAR

Summary, Scientific Evaluation and Assessment

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HELLENIC MINISTRY OF RURAL DEVELOPMENT AND FOOD
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DEPARTMENT OF PESTICIDES
Hippokratous 3-5,
10164 Athens
Hellas

VOLUME 3
ANNEX B

RAPPORTEUR MEMBER STATES SUMMARY, EVALUATION AND ASSESSMENT OF THE DATA AND INFORMATION SUBMITTED

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B.8 ENVIRONMENTAL FATE AND BEHAVIOUR

The notifier has generated two new studies in the context of the resubmission dossier, although relevant data requirements are not stipulated either in the EFSA Scientific Report (2005) 28, or the Evaluation Table [SANCO 16395/EPCO/BVL/04 rev. 3-1 (04.03.05)]. These new studies provide with PECgw values for trifluralin and metabolite TR-4 using FOCUS PEARL and PECsw/sed values trifluralin and metabolites TR-4, TR-6, TR-7, TR-14 and TR-15 using FOCUS Steps 1-4. Those studies were evaluated by the RMS and are summarized below.

B.8.6 PREDICTED ENVIRONMENTAL CONCENTRATIONS IN SURFACE WATER AND IN GROUND WATER (PECsw, PECgw) (Annex IIIA 9.2.3, 9.2.1)

B.8.6.1 Predicted Environmental Concentrations in Surface Water and Sediment

Knowles, S.J. "Predicted environmental concentrations of trifluralin and metabolites using the FOCUS models focus surface water tools and scenarios for critical Good Agricultural Practice", 2008. Not published.
Objective: To estimate the PECsw and PECsed values for trifluralin and metabolites TR-4, TR-6, TR-7, TR-14 and TR-15.
Guidelines: According to guidance given in "FOCUS surface water scenarios in the EU evaluation process under 91/414/EEC". Report of the FOCUS Working Group on Surface Water Scenarios, EC Document Reference SANCO/4802/2001-rev.2 final (May 2003). 245 pp.
GLP: No (modelling study)

Materials and methods - Methodology:

The physico-chemical and environmental fate properties of trifluralin and its metabolites that are required for input to the models are shown in Tables 8.6.1.1 to 8.6.1.3. Where possible, data were taken from the End Points section of the Draft Assessment Report (DAR) with the associated Addenda. No new environmental fate data have been generated since these documents were issued that would influence the selection of the model input data. In cases where metabolite model input data are not available, EPI Suite has been used to estimate parameters for water solubility and Koc sorption values. For metabolite DT_{50} in soil, water and sediment a conservative approach has been adopted and a value of 1000 days has been used. The key environmental fate inputs are described in the following sections

Steps 1 and 2

The following GAP and input parameters were considered for Steps 1and 2.

Application of TREFLAN to oilseed rape (winter) 1 x 1.2 kg/ha for Northern zone (NZ) and Southern zone (SZ) default buffer
Application of TREFLAN to cotton 1 x 1.2 kg/ha for Northern zone (NZ) and Southern zone (SZ) default buffer
Application of TREFLAN to sunflowers 1 x 1.2 kg/ha for Northern zone (NZ) and Southern zone (SZ) default buffer

All simulations were carried out using the scenario appropriate for the particular crop as recommended by FOCUS. The key chemical input parameters used for trifluralin parent and its metabolites in the simulations are shown in Tables 8.6.1.1 and 8.6.1.2. 100 % conversion from parent to metabolite was assumed as a worst case estimation for these metabolites.

Table 8.6.1.1: Chemical Specific Input Parameters for Steps 1 and 2 for trifluralin

Property	Value
Solubility in water	0.194 mg/L (20ºC)**
Koc	8765 mL/g **
Half-life soil	181 d (20ºC)
Half-life water	13 d (20ºC)
Half-life sediment	17 d (20ºC)

Table 8.6.1.2: Chemical Specific Input Parameters for Steps 1 and 2 for trifluralin metabolites

Property	Value
TR-4	
Solubility in water	1.41 mg/L (20ºC)**
Koc	1.36 x 10^4 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*

Half-life sediment	1000 d (20ºC)*
TR-6	
Solubility in water	586 mg/L (20ºC)**
Koc	622 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*
TR-7	
Solubility in water	27.8 mg/L (20ºC)**
Koc	1.91×10^4 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*
TR-14	
Solubility in water	1.93 mg/L (20ºC)**
Koc	2.40×10^4 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*
TR-15	
Solubility in water	21.1 mg/L (20ºC)**
Koc	2.84×10^3 mL/g **
Half-life soil	1000 d (20ºC)*
Half-life water	1000 d (20ºC)*
Half-life sediment	1000 d (20ºC)*

* conservative estimate of 1000 days used

** Calculated using EPI Suite

Step 3

SWASH was used to set up input files to model the foliar application of TREFLAN to winter oilseed rape, cotton and sunflowers according to the GAP shown below.

Description of GAP Modelled for Step 3

Application of TREFLAN to oilseed rape (winter) 1 x 1.2 kg/ha application 30th September, default buffer zone
Application of TREFLAN to cotton 1 x 1.2 kg/ha application 1st March, default buffer zone
Application of TREFLAN to sunflowers 1 x 1.2 kg/ha application 1st March, default buffer zone

All simulations were carried out using the scenario appropriate for the particular crop as recommended by FOCUS. The key chemical input parameters used for trifluralin in the simulations are shown in Table 3. Default FOCUS buffer zones were modelled for Step 8.6.1.3.

Table 8.6.1.3: Chemical Specific Input Parameters for Step 3 and 4

Property	Value
Molar Mass	335 g/mol
Saturated vapour pressure	9.5 x 10^{-3} Pa (25ºC)
Molar enthalpy of vaporisation	95000 J/mol
Solubility in water	0.194 mg/L (20ºC)
Molar enthalpy of dissolution	27000 J/mol
Diffusion co-efficient in water	4.3 x 10^{-5} m^2/d
Diffusion co-efficient in air	0.43 m^2/d
Koc	8765 mL/g
Freundlich exponent	0.972
Ref. concentration in liquid phase	1 g/m^3
Factor for uptake by plant roots in soil	0.50
Wash-off factor from crop	0.05 mm^{-1} (MACRO) 0.50 cm^{-1} (PRZM)
Half-life water	13 d (20ºC)

Half-life soil	181 d (20ºC)
Half-life sediment	17 d (20ºC)
Half-life crop	10 d
Activation energy (TOXSWA)	54000 J/mol
Exponent (MACRO)	0.079 K^{-1}

The data shown in Table 8.6.1.3 were then input into SWASH, and the relevant drainage (D) and run-off (R) scenarios, both with inclusive spray-drift, were run. For the run-off scenarios, the foliar linear application option and incorporation to 5 cm depth were chosen for the PRZM model. Default FOCUS buffer zones were used at Step 3.

Step 4

At Step 4, the effect of introducing vegetated buffer zones between the crop and surface water was evaluated. Such buffers will reduce the drift input and it is generally accepted that the runoff of both dissolved and particle-bound pesticide will also be reduced due to interception of water and eroded soil by the vegetated strip. In accordance with FOCUS Landscape and Mitigation guidance, a reduction in the volume of runoff and pesticide loading into water of 60% for a 14 m buffer and a reduction into sediment 85% for a 14 m buffer was implemented. For a 20m buffer, a reduction in the volume of runoff and pesticide loading into water of 80% for a 20 m buffer and a reduction into sediment 95% was implemented.

The SWAN interface was used to implement both drift and runoff reductions to TOXSWA. The appropriate buffer width was selected for the drift mitigation. For the runoff reduction into streams, it is necessary to account for the fact that only 20% of the upstream catchment is treated with pesticide (and therefore has runoff reduction applied to it). Therefore, for a 14 m buffer, the reduction in pesticide flux is 60% but the reduction in runoff water volume is 12% (i.e. 60% of 20%). For a 20 m buffer, the reduction in pesticide flux is 80% but the reduction in runoff water volume is 16% (i.e. 80% of 20%).

Using the Step 3 simulations as a starting point, the TOXSWA model was re-run using SWAN after applying the drift and runoff mitigations described above

Description of GAP Modelled for Step 4

Application of TREFLAN to oilseed rape (winter) 1 x 1.2 kg/ha application 30th September, 14m and 20m buffer zone
Application of TREFLAN to cotton 1 x 1.2 kg/ha application 1st March, 14m and 20m buffer zone
Application of TREFLAN to sunflowers 1 x 1.2 kg/ha application 1st March, 14m and 20m buffer zone

Results

The global maximum PEC_{SW} and PEC_{SED} values (expressed in concentration units of µg/L or µg/kg sediment dry weight, respectively), together with the time-weighted average (TWA) concentrations are given in Tables 8.6.14-8.6.1.17.

Table 8.6.1.4. Summary PECsw for trifluralin and metabolites

	Global Max PEC_{SW} (µg/L)			
Crop	**Trifluralin Step 1**	**Trifluralin Step 2**	**Trifluralin Step 3**	**Trifluralin Step 4 20m buffer**
Winter Oilseed Rape	42.6	11.0	7.65	0.708
Cotton	42.6	13.5	6.23	0.572
Sunflowers	42.6	13.5	6.07	0.704
	TR-4 Step 1	**TR-4 Step 2**		
Winter Oilseed Rape, Cotton and Sunflowers	10.1	10		
	TR-6 Step 1	**TR-6 Step 2**		
Winter Oilseed Rape, Cotton and Sunflowers	7.42	7.27		
	TR-7 Step 1	**TR-7 Step 2**		
Winter Oilseed Rape, Cotton and Sunflowers	9.06	9.05		
	TR-14 Step 1	**TR-14 Step 2**		
Winter Oilseed Rape, Cotton and Sunflowers	8.93	8.92		
	TR-15 Step 1	**TR-15 Step 2**		
Winter Oilseed Rape, Cotton and Sunflowers	8.59	8.52		

Table 8.6.1.5: Trifluralin STEP 1 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

Concentration	Max. PEC_{SW} *(µg/L)*	TWA PEC_{SW} 7 day	TWA PEC_{SW} 21 day	Max. PEC_{SED} *(µg/kg dw)*	TWA PEC_{SED} 7 day	TWA PEC_{SED} 21 day
wOSR NZ/SZ	42.6	28.9	22.0	2760	2470	1910
Cotton NZ/SZ	42.6	28.9	22.0	2760	2470	1910
SUNFLOWERS NZ/SZ	42.6	28.9	22.0	2760	2470	1910

Table 8.6.1.6: Trifluralin STEP 2 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

Concentration	Max. PEC_{SW} *(µg/L)*	TWA PEC_{SW} 7 day	TWA PEC_{SW} 21 day	Max. PEC_{SED} *(µg/kg dw)*	TWA PEC_{SED} 7 day	TWA PEC_{SED} 21 day
wOSR NZ	11.0	5.15	4.77	606	528	406
SZ	11.0	6.62	6.63	878	764	587
Cotton SZ	13.5	11.3	8.67	1150	1000	768
Sunflowers NZ	11.0	5.15	4.77	606	428	406
SZ	13.5	11.3	8.67	1150	1000	768

Table 8.6.1.7: Metabolites STEP 1 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

PECsw

Concentration	TR-4 Max. PECSW *(µg/L)*	TR-6 Max. PECSW *(µg/L)*	TR-7 Max. PECSW *(µg/L)*	TR-14 Max. PECSW *(µg/L))*	TR-15 Max. PECSW *(µg/L)*
wOSR NZ/SZ	10.1	7.42	9.06	8.93	8.59
Cotton NZ/SZ	10.1	7.42	9.06	8.93	8.59
SUNFLOWERS NZ/SZ	10.1	7.42	9.06	8.93	8.59

PECsed

Concentration	TR-4 PECSED *(µg/kg dw)*	TR-6 PECSED *(µg/kg dw)*	TR-7 PECSED *(µg/kg dw)*	TR-14 PECSED *(µg/kg dw)*	TR-15 PECSED *(µg/kg dw)*
wOSR NZ/SZ	73.9	25.6	67.6	67.2	52.4
Cotton NZ/SZ	73.9	25.6	67.6	67.2	52.4
SUNFLOWERS NZ/SZ	73.9	25.6	67.6	67.2	52.4

Table 8.6.1.8: Metabolites STEP 2 PEC_{SW} and PEC_{SED} Values Following Use of TREFLAN

PECsw

Concentration	TR-4 Max. PECSW *(µg/L)*	TR-6 Max. PECSW *(µg/L)*	TR-7 Max. PECSW *(µg/L)*	TR-14 Max. PECSW *(µg/L))*	TR-15 Max. PECSW *(µg/L)*
wOSR NZ	10.0	7.27	9.05	8.92	8.52
SZ	10.0	7.27	9.05	8.92	8.52
Cotton SZ	10.0	7.27	9.05	8.92	8.52
Sunflowers NZ	10.0	7.27	9.05	8.92	8.52
SZ	10.0	7.27	9.05	8.92	8.52

PECsed

Concentration	TR-4 PECSED *(µg/kg dw)*	TR-6 PECSED *(µg/kg dw)*	TR-7 PECSED *(µg/kg dw)*	TR-14 PECSED *(µg/kg dw)*	TR-15 PECSED *(µg/kg dw)*
wOSR NZ	71.6	24.8	65.6	65.1	50.8
SZ	71.9	24.9	65.8	65.3	50.9
Cotton SZ	71.9	25.0	66.0	65.6	51.1
Sunflowers NZ	71.6	24.8	65.6	65.1	50.8
SZ	72.1	25.0	66.0	65.6	51.1

Table 8.6.1.9: STEP 3 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in winter oilseed rape - default buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D2	ditch	7.646	4.147	2.615	1.401	0.811	0.434	0.295	0.230	0.177	0.161	0.0998
D2	stream	6.803	3.692	2.329	1.247	0.722	0.378	0.258	0.200	0.149	0.133	0.0821
D3	ditch	7.575	3.249	1.806	0.912	0.524	0.265	0.178	0.134	0.0893	0.0750	0.0376
D4	pond	0.260	0.205	0.166	0.116	0.0774	0.0414	0.0279	0.0211	0.0141	0.0119	0.00722
D4	stream	6.529	1.528	0.765	0.383	0.219	0.110	0.0733	0.0550	0.0367	0.0308	0.0181
D5	pond	0.260	0.194	0.151	0.0984	0.0620	0.0322	0.0216	0.0163	0.0109	0.00916	0.00459
D5	stream	7.044	1.848	0.925	0.463	0.265	0.133	0.0888	0.0667	0.0445	0.0374	0.0187
R1	pond	0.260	0.215	0.180	0.144	0.110	0.0686	0.0484	0.0370	0.0310	0.0281	0.0180
R1	stream	4.933	0.888	0.683	0.459	0.263	0.132	0.0891	0.0681	0.0600	0.0556	0.0370
R3	stream	7.013	1.477	1.136	0.821	0.485	0.305	0.274	0.206	0.142	0.133	0.0838

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D2	ditch	3.666	3.650	3.606	3.465	3.210	2.725	2.365	2.104	1.793	1.713	1.346
D2	stream	3.249	3.235	3.196	3.070	2.845	2.398	2.066	1.828	1.533	1.441	1.100
D3	ditch	2.475	2.452	2.395	2.251	2.050	1.692	1.439	1.252	0.994	0.890	0.536
D4	pond	0.300	0.300	0.299	0.295	0.286	0.255	0.224	0.198	0.160	0.144	0.101
D4	stream	1.126	1.098	1.060	0.986	0.891	0.725	0.610	0.526	0.413	0.369	0.250
D5	pond	0.242	0.241	0.240	0.236	0.226	0.197	0.169	0.148	0.116	0.104	0.0615
D5	stream	1.347	1.315	1.267	1.172	1.052	0.845	0.704	0.602	0.466	0.413	0.241
R1	pond	0.522	0.522	0.521	0.518	0.509	0.477	0.439	0.402	0.370	0.360	0.262
R1	stream	1.570	1.532	1.490	1.412	1.308	1.124	0.991	0.889	0.800	0.798	0.616
R3	stream	3.132	3.060	2.975	2.814	2.618	2.206	1.891	1.672	1.464	1.398	1.117

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.10: STEP 4 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in winter oilseed rape – 14m buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D2	ditch	0.801	0.435	0.274	0.147	0.102	0.0921	0.0763	0.0651	0.0606	0.0581	0.0479
D2	stream	0.960	0.521	0.329	0.176	0.102	0.0656	0.0501	0.0437	0.0444	0.0455	0.0383
D3	ditch	0.793	0.340	0.189	0.0955	0.0549	0.0277	0.0186	0.0140	0.00935	0.00786	0.00393
D4	pond	0.134	0.106	0.0858	0.0600	0.0399	0.0214	0.0144	0.0109	0.00728	0.00613	0.00434
D4	stream	0.922	0.216	0.108	0.0540	0.0309	0.0166	0.0124	0.00943	0.00631	0.00569	0.00482
D5	pond	0.134	0.1000	0.0778	0.0508	0.0320	0.0166	0.0112	0.00840	0.00562	0.00473	0.00237
D5	stream	0.994	0.261	0.131	0.0654	0.0375	0.0188	0.0125	0.00941	0.00628	0.00527	0.00264
R1	pond	0.134	0.111	0.0930	0.0683	0.0466	0.0275	0.0194	0.0148	0.0124	0.0112	0.00801
R1	stream	0.696	0.364	0.279	0.188	0.107	0.0538	0.0364	0.0278	0.0245	0.0227	0.0141

R3	stream	0.990	0.484	0.466	0.337	0.199	0.125	0.0932	0.0700	0.0486	0.0468	0.0303

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D2	ditch	0.877	0.874	0.867	0.858	0.847	0.794	0.776	0.774	0.757	0.762	0.661
D2	stream	0.641	0.640	0.639	0.634	0.621	0.594	0.580	0.579	0.560	0.563	0.512
D3	ditch	0.260	0.258	0.252	0.238	0.217	0.181	0.154	0.134	0.107	0.0958	0.0578
D4	pond	0.156	0.155	0.155	0.153	0.148	0.132	0.117	0.103	0.0830	0.0748	0.0580
D4	stream	0.159	0.155	0.150	0.140	0.127	0.106	0.104	0.0982	0.0848	0.0791	0.0586
D5	pond	0.125	0.125	0.124	0.122	0.117	0.102	0.0880	0.0767	0.0604	0.0539	0.0320
D5	stream	0.190	0.186	0.180	0.167	0.150	0.121	0.101	0.0868	0.0673	0.0597	0.0349
R1	pond	0.213	0.213	0.213	0.212	0.208	0.195	0.180	0.165	0.152	0.148	0.108
R1	stream	0.610	0.595	0.578	0.547	0.506	0.433	0.380	0.340	0.305	0.304	0.234
R3	stream	1.138	1.111	1.079	1.017	0.944	0.791	0.674	0.594	0.524	0.500	0.397

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.11: STEP 4 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in winter oilseed rape – 20m buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D2	ditch	0.571	0.310	0.195	0.126	0.102	0.0921	0.0763	0.0651	0.0606	0.0581	0.0461
D2	stream	0.684	0.371	0.234	0.126	0.0727	0.0582	0.0501	0.0437	0.0423	0.0416	0.0362
D3	ditch	0.566	0.243	0.135	0.0681	0.0391	0.0198	0.0133	0.00997	0.00666	0.00560	0.00280
D4	pond	0.108	0.0852	0.0691	0.0483	0.0321	0.0172	0.0116	0.00874	0.00586	0.00493	0.00374
D4	stream	0.657	0.154	0.0769	0.0405	0.0241	0.0166	0.0124	0.00943	0.00631	0.00569	0.00420
D5	pond	0.108	0.0805	0.0626	0.0409	0.0258	0.0134	0.00898	0.00676	0.00452	0.00380	0.00191
D5	stream	0.708	0.186	0.0931	0.0466	0.0267	0.0134	0.00893	0.00671	0.00447	0.00376	0.00188
R1	pond	0.108	0.0891	0.0748	0.0550	0.0375	0.0203	0.0138	0.0105	0.00706	0.00596	0.00512
R1	stream	0.496	0.183	0.141	0.0945	0.0541	0.0271	0.0183	0.0140	0.0123	0.0114	0.00712
R3	stream	0.705	0.244	0.235	0.170	0.100	0.0630	0.0491	0.0369	0.0255	0.0244	0.0157

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D2	ditch	0.862	0.859	0.852	0.843	0.832	0.779	0.768	0.766	0.746	0.752	0.653
D2	stream	0.640	0.639	0.637	0.632	0.620	0.593	0.571	0.570	0.551	0.551	0.502
D3	ditch	0.186	0.184	0.180	0.170	0.155	0.129	0.110	0.0962	0.0766	0.0686	0.0414
D4	pond	0.125	0.125	0.125	0.123	0.119	0.107	0.0940	0.0831	0.0670	0.0604	0.0491
D4	stream	0.121	0.121	0.120	0.116	0.111	0.103	0.102	0.0956	0.0825	0.0769	0.0535
D5	pond	0.101	0.101	0.100	0.0985	0.0944	0.0822	0.0710	0.0618	0.0488	0.0435	0.0258
D5	stream	0.136	0.133	0.128	0.119	0.107	0.0866	0.0724	0.0621	0.0481	0.0427	0.0250
R1	pond	0.148	0.148	0.147	0.146	0.141	0.127	0.113	0.101	0.0827	0.0781	0.0616
R1	stream	0.306	0.299	0.291	0.275	0.255	0.218	0.192	0.171	0.153	0.153	0.118
R3	stream	0.580	0.566	0.550	0.519	0.482	0.404	0.345	0.304	0.267	0.255	0.203

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.12: STEP 3 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in cotton - default buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D6	ditch	6.227	2.776	1.480	0.744	0.427	0.215	0.145	0.119	0.0801	0.0676	0.0345

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D6	ditch	2.151	2.127	2.075	1.952	1.777	1.452	1.221	1.051	0.816	0.720	0.421

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.13: STEP 4 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in cotton – 14m buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D6	ditch	0.789	0.352	0.188	0.0944	0.0543	0.0285	0.0226	0.0259	0.0178	0.0151	0.0102

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D6	ditch	0.342	0.339	0.331	0.314	0.289	0.240	0.205	0.179	0.169	0.159	0.125

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.14: STEP 4 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in cotton – 20m buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D6	ditch	0.572	0.251	0.144	0.0790	0.0473	0.0259	0.0176	0.0221	0.0153	0.0129	0.0102

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
D6	ditch	0.269	0.268	0.266	0.260	0.246	0.213	0.184	0.162	0.152	0.145	0.125

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.15: STEP 3 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in sunflowers - default buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
R1	pond	0.252	0.219	0.193	0.152	0.112	0.0652	0.0624	0.0526	0.0375	0.0316	0.0207
R1	stream	4.329	0.849	0.425	0.213	0.156	0.120	0.0908	0.0765	0.0641	0.0585	0.0549
R3	stream	6.070	1.520	0.761	0.381	0.301	0.205	0.196	0.182	0.142	0.128	0.0906
R4	stream	4.307	1.402	1.159	0.588	0.454	0.307	0.259	0.204	0.163	0.137	0.116

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
R1	pond	0.548	0.547	0.546	0.541	0.528	0.506	0.479	0.465	0.428	0.400	0.292

R1	stream	2.319	2.291	2.252	2.175	2.090	2.042	2.039	1.949	1.739	1.640	1.387
R3	stream	5.637	5.592	5.508	5.338	5.112	4.984	4.917	4.720	4.234	4.070	2.893
R4	stream	3.007	2.938	2.853	2.695	2.671	2.451	2.158	1.913	1.658	1.593	1.270

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.16: STEP 4 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in sunflowers - 14m buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
R1	pond	0.134	0.117	0.103	0.0811	0.0596	0.0348	0.0309	0.0255	0.0180	0.0152	0.00954
R1	stream	0.704	0.318	0.159	0.0798	0.0637	0.0490	0.0371	0.0312	0.0262	0.0239	0.0203
R3	stream	0.988	0.495	0.258	0.155	0.0889	0.0773	0.0695	0.0610	0.0489	0.0466	0.0333
R4	stream	0.972	0.575	0.475	0.241	0.186	0.126	0.106	0.0835	0.0669	0.0562	0.0475

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Trifluralin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
R1	pond	0.249	0.249	0.248	0.246	0.240	0.228	0.228	0.222	0.201	0.186	0.131
R1	stream	0.551	0.541	0.530	0.509	0.479	0.468	0.453	0.434	0.387	0.367	0.349
R3	stream	1.200	1.186	1.164	1.130	1.098	1.048	1.015	0.991	0.911	0.895	0.672
R4	stream	1.149	1.122	1.089	1.027	1.020	0.936	0.822	0.726	0.625	0.596	0.482

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

Table 8.6.1.17: STEP 4 PEC_{SW} and PEC_{SED} Values Following Application Use of TREFLAN in sunflowers - 20m buffer

Trifluralin maximum and TWA water concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
R1	pond	0.108	0.0940	0.0826	0.0653	0.0480	0.0280	0.0227	0.0183	0.0127	0.0107	0.00632
R1	stream	0.502	0.160	0.0803	0.0402	0.0321	0.0247	0.0187	0.0157	0.0132	0.0120	0.0105
R3	stream	0.704	0.250	0.130	0.0781	0.0448	0.0389	0.0350	0.0326	0.0259	0.0237	0.0173
R4	stream	0.499	0.290	0.240	0.121	0.0937	0.0633	0.0534	0.0421	0.0337	0.0283	0.0240

* Maximum Time Weighted Averaged Exposure Concentrations in water layer in µg.L-1

Triflualin maximum and TWA sediment concentrations.

Location	Water body	Global Max	TWA 1d	TWA 2d	TWA 4d	TWA 7d	TWA 14d	TWA 21d	TWA 28d	TWA 42d	TWA 50d	TWA 100d
R1	pond	0.193	0.193	0.192	0.191	0.187	0.178	0.172	0.164	0.144	0.132	0.0889
R1	stream	0.264	0.258	0.251	0.238	0.228	0.209	0.201	0.192	0.171	0.164	0.159
R3	stream	0.538	0.531	0.520	0.503	0.487	0.459	0.445	0.430	0.397	0.392	0.299
R4	stream	0.574	0.560	0.544	0.513	0.510	0.469	0.411	0.363	0.313	0.298	0.241

* Maximum Time Weighted Averaged Exposure Concentrations in sediment in µg.kg-1 DW

B.8.6.2 Predicted Environmental Concentrations in Ground Water

Reeves, G. "Modelling the leaching of trifluralin and a potentially- relevant metabolite (TR 4) to groundwater in the EU using PEARL and the FOCUS scenarios", 2005. Not published.
Objective: To estimate the PEC_{GW} values for trifluralin and TR-4.
Guidelines: FOCUS Groundwater Scenarios Workgroup, 2000.
GLP: No (modelling study)

Materials and methods - Methodology:
FOCUSPEARL (ver. 2.2.2) was used to model the bare soil application of TREFLAN to cotton, oilseed rape, sunflowers and winter cereals. Following soil application, the modelling assumed incorporation to a maximum depth of 5 cm, according to GAP (Table 8.6.2.1), except for the winter cereals use which was to bare soil without subsequent incorporation.

Table 8.6.2.1: Description of GAP Modelled

GAP
Spring application to cotton: 1.2 kg as/ha (1 March), with soil incorporation to 5 cm.
Autumn application to winter oilseed rape: 1.2 kg as/ha (30 September), with soil incorporation to 5 cm.
Spring application to sunflowers: 1.2 kg as/ha (1 March), with soil incorporation to 5 cm.
Autumn application to winter cereals: 1.2 kg as/ha (30 November), without soil incorporation.

Model Inputs

For each GAP (Table 8.6.2.1), a project was created within FOCUSPEARL using the model input and application parameters for trifluralin and TR-4 shown in Tables 8.6.2.2 and 8.6.2.3.

For trifluralin, the source of the model input data was the dossier submitted in support of Annex I inclusion (Document N, 2002). Individual $DT_{50(lab)}$ values for trifluralin leading to the overall geometric mean $DT_{50(lab)}$ of 161 days at 22ºC (or arithmetic mean of 181 days) were corrected for soil moisture content at field capacity (10 kPa) using the procedure recommended in the FOCUS guidance (FOCUS, 2000). This gave a geometric mean standardised $DT_{50(lab)}$ value of 115 days at 22ºC for input into the model.

For the metabolite TR-4, a number of parameters from direct measurement were not available for model input. However, estimates were made using the US EPA's EPI program suite for vapour pressure, water solubility and Koc (from which Kom was derived). Furthermore, in order to arrive at a half-life value for input into FOCUSPEARL in the absence of data, a value of 10x parent, i.e. 1150 days at 22ºC was used. This is deemed to be sufficiently conservative for a worst case approach.

The transformation scheme (first-order kinetics) assumed within FOCUSPEARL was trifluralin → TR-4, and the transformation factor used in the model was set at a conservative 0.5, based upon only up to 13.4% AR of TR-4 being detected in the flooded anaerobic soil degradation study.

All simulations were carried out using the scenario appropriate for the particular crop as recommended by FOCUS. Each use was investigated as consecutive annual applications for a period of 20 years.

Table 8. 6.2.2: Model Inputs to FOCUSPEARL

Parameter	Trifluralin	TR-4	Comments
General:			
Molar mass (g/mol)	335	245	-
Saturated vapour pressure (Pa)	9.5×10^{-3}	4.3×10^{-4}	25ºC
Molar enthalpy of vaporisation (kJ/mol)	95	95	FOCUS default

Solubility in water (mg/L)	0.194	1.4	20ºC & 25ºC, respectively
Molar enthalpy of dissolution (kJ/mol)	27	27	FOCUS default
Freundlich Sorption:			
Option	Kom	Kom	pH independent
Kom (L/kg)	5096	7907	Mean Koc ÷ 1.72
Molar enthalpy of sorption (kJ/mol)	0	0	FOCUS default
Reference conc. in liquid phase (mg/L)	1	1	FOCUS default
Freundlich sorption exponent	0.972	0.9	Mean measured value & FOCUS default, respectively
Desorption rate coefficient (1/d)	0	0	FOCUS default
Factor relating CofFreNeq & CofFreEql	0	0	FOCUS default
Transformation:			
Half-life (d)	115	1150*	22ºC, geomean
Optimum moisture conditions (pF2/wetter)	Yes	Yes	FOCUS default
Exponent for the effect of liquid	0.7	0.7	FOCUS default
Molar activation energy (kJ/mol)	54	54	FOCUS default
Diffusion:			
Reference temperature for diffusion (ºC)	20	20	FOCUS default
Reference diffusion coeff. water (m^2/d)	4.3×10^{-5}	4.3×10^{-5}	FOCUS default
Reference diffusion coeff. air (m^2/d)	0.43	0.43	FOCUS default
Crop data:			
Wash-off factor (1/m)	0.0001	0.0001	FOCUS default
Canopy process option	Lumped	Lumped	FOCUS default
Half-life at crop surface (d)	1000000	1000000	FOCUS default
Coefficient for uptake by plant	0.5	0.5	FOCUS default

** Conservative estimate based on 10x parent value*

Table 8.6.2.3: Application Parameters

Application:		
Option	Absolute	-

Application type	Incorporation	Cotton, winter oilseed rape and sunflowers
Depth (m)	0.005	According to GAP
Application type	Soil application	Winter cereals only
Depth (m)	0	According to GAP

Results:

The 80th percentile results for each crop and FOCUS-scenario combination for the annual average trifluralin and TR-4 concentrations in the leachate at 1 m soil depth (µg/L) are summarised in Table 8.6.2.4.

Table 8.6.2.4: 80th Percentile Annual Average Leachate Concentrations at 1 m Depth (µg/L)

Use	Châteaudun	Hamburg	Jokioinen	Kremsmünste	Okehampton	Piacenza	Porto	Sevilla	Thiva
Cotton Trifluralin TR-4	-	-	-	-	-	-	-	<0.000001<0.000001	<0.000001<0.000001
Oilseed rape Trifluralin TR-4	<0.000001<0.000001	<0.000001<0.000001	-	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	-	-
Sunflowers Trifluralin TR-4	-	-	-	-	-	<0.000001<0.000001	-	<0.000001<0.000001	-
Winter cereals Trifluralin TR-4	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001	<0.000001<0.000001

- *no FOCUS location for this crop*

In all the runs modeled, the 80th percentile annual average leachate concentrations for trifluralin at 1 m depth (PEC_{GW}) were estimated to be <0.000001 µg/L. This was also true for the metabolite TR-4.

Conclusions:

These findings are in agreement with the results of the modeling carried out previously using FOCUSPELMO (Reeves 2001 and 2004, *see DAR*).

B.8.11 REFERENCES RELIED ON

Annex Point/ Reference Number	Author(s)	Year	Title Source (where different from the Company), Company, Report Number, GLP or GEP status (where relevant), Published or not	Data Protection claimed (Y/N)	Owner
IIIA 9.2.1	Reeves, G.	2005	Modelling the leaching of trifluralin and a potentially- relevant metabolite (TR-4) to groundwater in the EU using PEARL and the FOCUS scenarios. Dow AgroSciences DAS Report No.: GHE-P-11131 (Masterfile Number): K68 GLP/GEP (Y/N): N	Y	DAS
IIIA 9.2.3	Knowles, S.J.	2008	Predicted environmental concentrations of trifluralin and metabolites using the FOCUS models focus surface water tools and scenarios for critical Good Agricultural Practice Dow AgroSciences DAS Report No.: GHE-P-111836 (Masterfile Number): K67 GLP/GEP (Y/N): N	Y	DAS