Bayer CropScience

Document Title

Summary of the fate and behaviour in the environment

Isoxaflutole + Cyprosulfamide SC 480 (240+240) g/L

Data Requirements

EU Regulation 1107/2009 & EU Regulation 284/2013

Document MCP

Section 9: Fate and behaviour in the environment

According to the guidance document, SANCO 10181/2013, for preparing dossiers for the approval of a chemical active substance

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Version history

Date	Data points containing amendments or additions[1] and brief description	Document identifier and version number

[1] It is suggested that applicants adopt a similar approach to showing revisions and version history as outlined in SANCO/10180/2013 Chapter 4 How to revise an Assessment Report

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CP 9 FATE AND BEHAVIOUR IN THE ENVIRONMENT

Introduction

Isoxaflutole is an herbicidal active substance and was included into Annex I of Directive 91/414 by Directive 2002/68/EC (dated 11th of July 2003) on 1st of October 2003.

This dossier contains only summaries of studies, which were not available at the time of the Annex I inclusion of isoxaflutole and were therefore not evaluated during the first EU review of this compound. All other studies, which were already submitted by Bayer for the Annex I inclusion, are contained in the Monograph and in the baseline dossier (D-009256-01) provided by Bayer CropScience.

Intended application pattern

The formulation is intended for use as a herbicide against broad leaf weeds and grass weeds and maize. The critical use pattern for this formulation is summarised as follows.

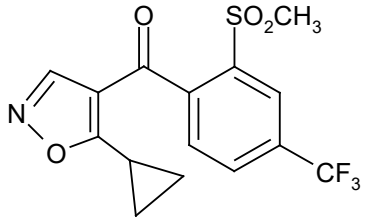
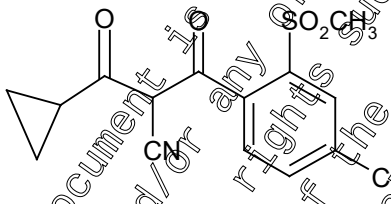
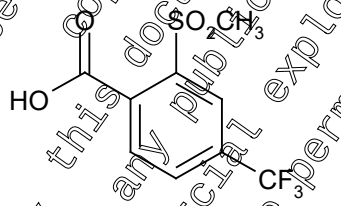
Table 9- 1: Intended application pattern

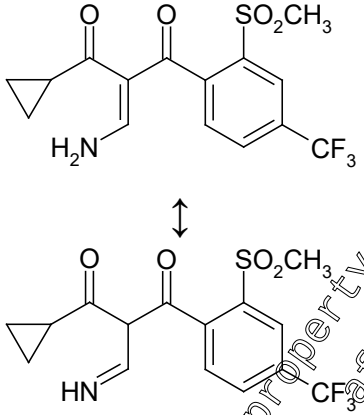
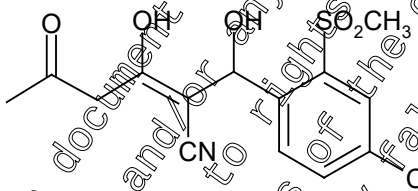
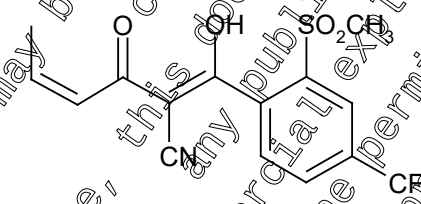
Crop	Timing of application	Number of appl.	Application interval [days]	Maximum label rate [L/ha]	Maximum application rate, individual treatment [g a.s./ha] isoxaflutole
Maize, Pre-emergence	BBCH 00 - 13	1	-	0.417	100

Compounds addressed in this document

In addition to the active substance(s), the following metabolites were addressed in this document.

Table 9- 2: Active substance and metabolites addressed in this document

Report name **Structure** **IUPAC name** **CAS name** **[CAS registry number]**	**Molecular formula** **molar mass** **Other names / codes**	**Occurrence**
Isoxaflutole (parent substance)  (5-cyclopropyl-1,2-oxazol-4-yl)-[2-methylsulfonyl-4-(trifluoromethyl)phenyl]methanone (IUPAC) Methanone,(5-cyclopropyl-4-isoxazolyl){2-(methylsulfonyl)-4-(trifluoromethyl)phenyl}- (9CI) (CAS) CAS no: 141112-29-0	$C_{15} H_{12} F_3 N O_4 S$ 359.32 g/mol **Isoxaflutole** (common name) RPA 201772 RPA 591428 AE B197278 BCS-AH21981	Parent substance used as test material in all reports
Diketonitrile  2-cyclopropylcarbonyl-3-(2-methylsulfonyl-4-trifluoromethylphenyl)-3-oxopropanenitrile (IUPAC) Benzenepropanenitrile, a-(cyclopropylcarbonyl)-2-(methylsulfonyl)-b-oxo-4-(trifluoromethyl)- (CAS) CAS no: 143701-75-1	$C_{15} H_{12} F_3 N O_4 S$ 359.32 g/mol RPA 202348 AE 0540092 BCS-AB59005 DKN	Soil, aerobic Soil, anaerobic Soil photolysis Abiotic hydrolysis
Benzoic acid  2-mesyl-4-trifluoromethylbenzoic acid (IUPAC) Benzoic acid, 2-(methylsulfonyl)-4-(trifluoromethyl)- (CAS) CAS no: 142994-06-7	$C_9 H_7 F_3 O_4 S$ 268.22 g/mol RPA 203328 AE B197555 Pyrasulfotole-benzoic acid BCS-AB49990 BA IFT acid	Soil, aerobic Soil, anaerobic Soil photolysis

Report name **Structure** **IUPAC name** **CAS name** **[CAS registry number]**	**Molecular formula** **molar mass** **Other names / codes**	**Occurrence**
RPA 205834 Enamine-amidine tautomeric forms:  2-(1-aminomethylidene)-1-cyclopropyl-3-(2-mesyl-4-trifluoromethylphenyl)propane-1,3-dione (IUPAC) CAS no: n.a.	$C_{15}H_{14}F_3NO_4S$ 361.34 g/mol RPA 205834 AE 0692291 BCS-BY16134	Soil, aerobic Soil, anaerobic Water/Sediment
Met 14  (2Z)-3-hydroxy-2-{hydroxy[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methyl}-5-oxohex-2-enenitrile (IUPAC) CAS no: n.a.	$C_{15}H_{14}F_3NO_5S$ 377 g/mol M14 Peak 14 AE Code: None BCS Code: None	Photolysis, buffer
Met 20  (2Z,4Z)-2-{hydroxy[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methylene}-3-oxohex-4-enenitrile (IUPAC) CAS no: n.a.	$C_{15}H_{12}F_3NO_4S$ 359 g/mol M20 Peak 20 AE Code: None BCS Code: None	Photolysis, buffer

CP 9.1 Fate and behaviour in soil

Information of this and the following sections (CP 9.1.1 and CP 9.1.2) are already given in the MCA. Please refer to the corresponding section in the MCA.

CP 9.1.1 Rate of degradation in soil

For further information on the fate and behaviour in soil please refer to MCA Section 7, points 7.1.1 and 7.1.2.

CP 9.1.1.1 Laboratory studies

For information on laboratory studies please refer to MCA Section 7, point 7.1.2.1.

CP 9.1.1.2 Field studies

For information on field studies please refer to MCA Section 7, point 7.1.2.2.

CP 9.1.1.2.1 Soil dissipation studies

For information on field dissipation studies please refer to MCA Section 7, point 7.1.2.2.1.

CP 9.1.1.2.2 Soil accumulation studies

For information on field accumulation studies please refer to MCA Section 7, point 7.1.2.2.2.

CP 9.1.2 Mobility in the soil

For information on mobility studies please refer to MCA Section 7, point 7.1.4.

CP 9.1.2.1 Laboratory studies

For information on laboratory studies please refer to MCA Section 7, point 7.1.4.1

CP 9.1.2.2 Lysimeter studies

For information on lysimeter studies please refer to MCA Section 7, point 7.1.4.2.

CP 9.1.2.3 Field leaching studies

For information on field leaching studies please refer to MCA Section 7, point 7.1.4.3.

CP 9.1.3 Estimation of concentrations in soil

New calculations were performed to reflect findings from new studies presented in the active substance dossier, section 7 "Fate and behavior in the environment". In addition these calculations considered the most recent guidance documents for exposure calculations.
Calculations of predicted environmental concentrations in soil (PEC_{soil}) are presented below.

Predicted environmental concentrations in soil (PEC_S)

Endpoints for PEC_{soil}

Table 9.1.3- 1: Modelling input parameters for isoxaflutole

Endpoint	Isoxaflutole and metabolites Value used for modelling
Isoxaflutole	
DT_{50} [days] (non-referenced field DT_{50})	2.8 [A]
RPA 202248	
DT_{50} [days]	53.4 [B]
Maximum occurrence [%]	100 [C]
Molecular mass correction	1 [D]
RPA 203328	
DT_{50} [days]	(maximum initial PEC_{soil} was calculated, therefore no DT_{50} is needed)
Maximum occurrence [%]	62.0
Molecular mass correction	268/359 [E]

[A] Non-normalized worst-case field DT_{50} from six sets of field trials ([redacted], 2001, M-200918-01-1)
[B] conservative approach using a pseudo-SFO DT_{50}
[C] conservative approach
[D] molar masses of isoxaflutole and RPA 202248 are identical
[E] molar mass of RPA 203328, divided by the molar mass of isoxaflutole

PEC_{soil} modelling approach

Calculations were based on a simple first tier approach (Excel sheet) assuming even distribution of the compound in upper 0-5 cm soil layer. A standard soil density of 1.5 g/cm³ was assumed.

Crop interception will reduce the amount of a compound reaching the soil and therefore this has been taken into account depending on the growth stage at application. The interception rates follow the recommendations of the FOCUS groundwater guidance paper (FOCUS 2002) for maize.

PEC_{soil} for isoxaflutole and its metabolites

For isoxaflutole, the metabolites RPA 202248 and RPA 203328 were considered.

Report:	[redacted]3;[redacted];2013;M-469725-01
Title:	Predicted Environmental Concentrations of Isoxaflutole and its Major Metabolites RPA 202248 and RPA 203328 in Soil (PEC_{soil}) Following Application at 100 g/ha to Maize in Europe
Document No:	M-469725-01-1 (VC/13/007M)
Guidelines:	EU Commission, 2000, Guidance Document on Persistence in Soil (Working Document), 9188/VI/97 rev.8 FOCUS 1997, Soil persistence models and EU registration FOCUS, 2002, Generic Guidance for FOCUS Groundwater Scenarios, Version 1.1
GLP:	No (calculation)

Methods and Materials: The predicted environmental concentrations in soil (PEC_{soil}) of isoxaflutole and its metabolites were estimated using a simple first tier approach (Excel sheet). Detailed application data used for simulation of PEC_{soil} were compiled in Table 9.1.3- 3.

Substance Specific Parameters: PEC_{soil} calculations were based on the DT_{50} of 2.8 days (worst case of field studies; non-normalized) for the parent compound isoxaflutole. Further compound specific input parameters are summarized below.

Table 9.1.3- 2: Input parameters for PEC_{soil} for isoxaflutole and its metabolites

Compound	DT_{50} [days]	Max. occurrence in soil [%]	Molar mass [g/mol]	Molar mass correction factor
Isoxaflutole	2.8	100	359	-
RPA 202248	53.4	100	359	1
RPA 203328	- [a]	62.0	268	268/359 [b]

[a] maximum initial PEC_{soil} calculated, therefore no DT_{50} needed
[b] molar mass of RPA 203328, divided by the molar mass of isoxaflutole

Table 9.1.3- 3: Application pattern used for PEC_{soil} calculations of isoxaflutole

Individual Crop	FOCUS Crop Used for Interception	Application				Amount Reaching the Soil per Season application
		Rate per Season	Interval	Plant Interception	BBCH Stage	
		[g a.s. /ha]	[days]	[%]		[g a.s./ha]
Maize – GAP and simulation	maize	1 × 100	-	0	00-13	1 × 100

Findings: The (annual) maximum PEC_{soil} values for isoxaflutole and its metabolites are summarised in the following table. The maximum, short-term and long-term PEC_{soil} values and the time weighted average values (TWA_{soil}) of isoxaflutole and its metabolites are provided thereafter exemplarily for 1 × 100 g a.s./ha. No PEC with time or time-weighted average concentrations have been calculated for the metabolite RPA 203328.

Table 9.1.3- 4: (Annual) Maximum PEC_{soil} of isoxaflutole and its metabolites for the uses assessed

Use pattern	Isoxaflutole [mg/kg]	RPA 202248 [mg/kg]	RPA 203328 [mg/kg]
Maize, 1 × 100 g a.s./ha	0.1333	0.1333	0.0617

Table 9.1.3- 5: PEC_{soil} (actual) and TWA_{soil} of isoxaflutole (1 × 100 g a.s./ha)

	Time [days]	Isoxaflutole	
		PEC_{soil} [mg/kg]	TWA_{soil} [mg/kg]
Initial	0	0.1333	
Short term	1	0.1041	0.1181
	2	0.0813	0.1052
	4	0.0495	0.0846
Long term	7	0.0236	0.0633
	14	0.0042	0.0373
	21	0.0007	0.0253
	28	0.0001	0.0192
	50	0.0000	0.0108
	100	0.0000	0.0054

Table 9.1.3- 6: PEC_{soil} (actual) and TWA_{soil} of RPA 202248 (1 × 100 g a.s./ha)

	Time [days]	RPA 202248	
		PEC_{soil} [mg/kg]	TWA_{soil} [mg/kg]
Initial	0	0.1333	
Short term	1	0.1316	0.1325
	2	0.1299	0.1316
	4	0.1266	0.1299
Long term	7	0.1218	0.1275
	14	0.1112	0.1219
	21	0.1015	0.1167
	28	0.0927	0.1118
	50	0.0693	0.0981
	100	0.0364	0.0747

Table 9.1.3- 7: PEC_{soil} (actual) of RPA 203328 (1 × 100 g a.s./ha)

	Time [days]	RPA 203328	
		PEC_{soil} [mg/kg]	TWA_{soil} [mg/kg]
Initial	0	0.047	---

CP 9.2 Fate and behaviour in water and sediment

CP 9.2.1 Aerobic mineralisation in surface water

For information on aerobic mineralisation in surface water studies please refer to MCA Section 7, point 7.2.2.2.

CP 9.2.2 Water/sediment study

For information on water/sediment studies please refer to MCA Section 7, point 7.2.2.3.

CP 9.2.3 Irradiated water/sediment study

For information on irradiated water/sediment studies please refer to MCA Section 7, point 7.2.2.4.

CP 9.2.4 Estimation of concentrations in groundwater

New calculations were performed, to reflect findings from new studies presented in the active substance dossier, section 7 "Fate and behavior in the environment". In addition these calculations consider the most recent guidance documents for exposure calculations.
Calculations of predicted environmental concentrations in groundwater (PEC_{gw}) are presented below.

Endpoints for PEC_{gw}

Table 9.2.4- 1: Modelling input parameters for isoxaflutole

Endpoint	isoxaflutole and metabolites Value used for modelling
Isoxaflutole	
Aqueous solubility [mg/L]	6.2 (20°C)
Vapour pressure [Pa]	3.22×10^{-7} (20°C)
DT_{50} soil [days]	0.9 (geomean) [A]
K_{oc} [L/kg]	79.8 (mean) [B]
1/n	0.935 [D]
RPA 202248	
Aqueous solubility [mg/L]	22660 (20°C)
Vapour pressure [Pa]	0 (20°C)
DT_{50} soil [days]	15.5 (geomean)
K_{oc} [L/kg]	34.9 (mean)
1/n	0.876 [D]
Formation fraction	1 [F]
RPA 203328	
Aqueous solubility [mg/L]	>110000 (20°C)
Vapour pressure [Pa]	0 (20°C)
DT_{50} soil [days]	11.4 (geomean)
K_{oc} [L/kg]	1.17 (mean)
1/n	0.649
Formation fraction	1 [E]

[A] Geometric mean of normalized field DT_{50} from laboratory trials ([redacted], 2013a & c, M-464596-01-1 & M-464899-01-1)
[B] Arithmetic mean K_{OC} from a range of 5 soils.
[C] Geometric mean laboratory DT_{50} from laboratory trials ([redacted], 2013a & b, M-464596-01-1 & M-464592-01-1)
[D] Excluding sediment
[E] Conservative worst-case

PEC_{gw} modelling approach

The predicted environmental concentrations in groundwater (PEC_{gw}) for the active substance were calculated using the simulation models PEARL and PELMO following the recommendations of the FOCUS working group on groundwater scenarios.

The leaching calculations were run over 26 years, as proposed for pesticides which may be applied every year. The simulation length increases to 46 and 66 years for pesticides which are applied only every second and third year, respectively.The first six years are a 'warm up' period; only the last 20 years were considered for the assessment of the leaching potential. The 80th percentile of the average annual groundwater concentrations in the percolate at 1 m depth under a treated plantation were evaluated and were taken as the relevant PEC_{GW} values. In respect to the assessment of a potential groundwater contamination this shallow depth reflects a worst case. The effective long-term groundwater concentrations will be even lower due to dilution in the groundwater layer.
According to FOCUS, the calculations were conducted based on mean soil half-lives, referenced to standard temperature and moisture conditions. Crop interception will reduce the amount of a compound reaching the soil and therefore this has been taken into account depending on the growth stage at application. The interception rates follow the FOCUS recommendations (Table 9.2.4- 2).

Table 9.2.4- 2: FOCUS groundwater crop interception values

	Crop stage Interception [%]				
Crop	**Bare – emergence**	**Leaf development**	**Stem elongation**	**Flowering**	**Senescence Ripening**
	BBCH stage				
	00 - 09	**10 - 19**	**20 - 39**	**40 - 89**	**90 - 99**
maize	0	25	50	75	90

CP 9.2.4.1 Calculation of concentrations in groundwater

Predicted environmental concentrations in groundwater (PEC_{gw})

For isoxaflutole, the metabolites RPA 202248 and RPA 203328 were assessed.

Report:	[redacted]3;[redacted];2013;M-469721-01
Title:	Predicted Environmental Concentrations of Isoxaflutole and its metabolites RPA 202248 and RPA 203328 in Groundwater (PEC_{gw}) Following Application to Maize in Europe at 100 g/ha
Document No:	M-469721-01-1 (VC/13/007L)
Guidelines:	FOCUS 2000, SANCO/321/2000 FOCUS 2011, Generic Guidance for FOCUS Groundwater Assessments, v. 2.0
GLP:	No (calculation)

Materials and Methods: The predicted environmental concentrations in groundwater (PEC_{gw}) for isoxaflutole and its metabolites were calculated using the simulation models FOCUS PEARL (version 4.4.4) and FOCUS PELMO (version 5.5.3). Detailed application data used for simulation of PEC_{gw} were compiled in Table 9.2.4.1- 1.

Table 9.2.4.1- 1: Comparison of simulated and actual use pattern

Individual Crop	FOCUS Crop Used for Interception	Application				Amount Reaching the Soil per Season application
		Rate per Season	Interval	Plant Interception	BBCH Stage	
		[g a.s./ha]	[days]	[%]		[g a.s./ha]
Maize – GAP and simulation	maize	1 × 100	-	0	00-13	1 × 100

Application dates for the simulation runs were defined following the crop event dates of the respective crop and scenario (**Table 9.2.4.1- 2**) as given by FOCUS (2000). Crop interception was taken into account according to the BBCH growth stage, as recommended by FOCUS (2011).

Table 9.2.4.1- 2: First application dates and related information for isoxaflutole as used for the simulation runs

Individual crop	Maize Single application
Repeat Interval for App. Events	Every year
Application Technique	Spray
Absolute / Relative to	Absolute
Scenario	1st App. Date
[redacted]	1st May 5th May 5th May 25th May 15th May 1st May 7th March 20th April

Further input parameters for PEC_{gw} modelling of isoxaflutole and its metabolites are summarised in **Table 9.2.4.1- 3**.

Table 9.2.4.1- 3: Substance specific and model related input parameter for PEC_{gw} calculation of isoxaflutole and its metabolites

Parameter	Unit	Isoxaflutole	RPA 202248	RPA 203328
Molar mass	[g/mol]	359	359	268
Water solubility (20°C)	[mg/L]	6.2	22660	110000
Vapour Pressure (20°C)	[Pa]	3.22E-07	0	0
Freundlich Exponent	[-]	0.935	0.876	0.649
Plant uptake factor	[-]	0.0	0.5	0.5
DT_{50} (20°C)	[days]	0.9	15.5	11.4
K_{oc}	[mL/g]	79.8	34.9	1.17
K_{om}	[mL/g]	46.3	20.2	0.68

Findings: PEC_{gw} were evaluated as the 80th percentile of the mean annual leachate concentration at 1 m soil depth. PEC_{gw} values for isoxaflutole and its metabolites RPA 202248 and RPA 203328 are given in the following tables.

Table 9.2.4.1- 4: Maize: PEC_{gw} (PEARL and PELMO) of isoxaflutole and its metabolites RPA 202248 and RPA 203328 (1 × 100 g a.s./ha)

FOCUS Scenario	Isoxaflutole		RPA 202248		RPA 203328	
	PEARL	PELMO	PEARL	PELMO	PEARL	PELMO
	PEC_{gw} [µg/L]	PEC_{gw} [µg/L]	PEC_{gw} [µg/L]	PEC_{gw} [µg/L]	PEC_{gw} [µg/L]	PEC_{gw} [µg/L]
[redacted]	<0.001	<0.001	0.004	<0.001	0.200	0.084
[redacted]	<0.001	<0.001	0.021	0.009	1.006	0.329
[redacted]	<0.001	<0.001	0.013	0.010	0.395	0.328
[redacted]	<0.001	<0.001	0.036	0.033	0.573	0.497
[redacted]	<0.001	<0.001	0.007	0.010	0.084	0.117
[redacted]	<0.001	<0.001	0.001	0.001	0.030	0.020
[redacted]	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
[redacted]	<0.001	<0.001	<0.001	<0.001	0.023	0.009

Conclusion: There are no concerns for groundwater from the active substance isoxaflutole and its metabolite RPA 202248 in accordance with the use pattern for the current formulation. For the non-relevant metabolite RPA 203328, the results of the simulations showed a maximum concentration of 1.0 $\mu g \cdot L^{-1}$.

The metabolite RPA 203328 is not biologically active and has been declared non-relevant during the European review process for Annex I inclusion. The non-relevance of RPA 203328 according to Sanco/221/2000-rev.10 is also described in Document M4 of this submission and supported by information given in the EFSA opinion[1] on the residue definition in plants.

CP 9.2.4.2 Additional field tests

No additional field testing was required.

[1] Reasoned opinion of EFSA prepared by the Pesticides Unit (PRAPeR) on the modification of the residue definition for isoxaflutole. EFSA Scientific Report (2009) 323, 1-26

CP 9.2.5 Estimation of concentrations in surface water and sediment

New calculations were performed, to reflect findings from new studies presented in the active substance dossier, section 7 "Fate and behavior in the environment". In addition these calculations consider the most recent guidance documents for exposure calculations.
Calculations of predicted environmental concentrations in surface water (PEC_{sw}) are presented below.

Endpoints for PEC_{sw}

Table 9.2.5- 1: Modelling input parameters for isoxaflutole and its metabolites

Isoxaflutole :	
Endpoint	**Value used for modelling**
isoxaflutole	
Aqueous solubility [mg/L]	6.2 (20°C)
Vapour pressure [Pa]	3.22×10^{-7} (20°C)
DT_{50} soil [days]	0.9 [A]
K_{oc} [L/kg]	79.8 [B]
1/n	0.935
DT_{50} total system [days]	0.36 [C]
DT_{50} water [days]	0.36 [C]
DT_{50} sediment [days]	0.36/1000 [C, D]
RPA 202248	
Aqueous solubility [mg/L]	22660 (20 °C)
DT_{50} soil [days] (geo-mean laboratory)	15.5
K_{oc} [L/kg]	34.9 [E]
1/n	0.876 [E]
Maximum in soil [%]	100
Formation fraction	n.a.
DT_{50} total system [days]	237
DT_{50} water [days]	237
DT_{50} sediment [days]	237/1000[D]
Maximum in water/sediment [%]	70.3
RPA 203328	
Aqueous solubility [mg/L]	110000
DT_{50} soil [days] (geo-mean laboratory)	11.4
K_{oc} [L/kg]	1.17 [F]
1/n	-
Maximum in soil [%]	62.0
Maximum in water/sediment [%]	10.8
Formation fraction	n.a.
DT_{50} total system [days]	1000
DT_{50} water [days]	1000
DT_{50} sediment [days]	1000
RPA 205834	
Aqueous solubility [mg/L]	29
DT_{50} soil [days]	1000 (worst-case)
K_{oc} [L/kg]	0 (default)
1/n	-
Maximum in soil [%]	2.3
Maximum in water [%]	-
Maximum in total system [%]	26.4
Formation fraction	n.a.

Isoxaflutole :	
Endpoint	**Value used for modelling**
DT_{50} water [days]	76.2 [C]
DT_{50} sediment [days]	76.2 [C]
DT_{50} total system [days]	76.2 [C]

[A] Geometric mean of normalized field DT_{50} from aerobic soils ([redacted]2013, M-464596-01-1)
[B] Arithmetic mean K_{OC} from a range of 4 soils and 1 sediment
[C] Geometric mean, degradation DT_{50}
[D] 1000 days used for Step 3 calculations
[E] Arithmetic mean K_{OC} and Freundlich exponent from a range of 13 soils (excluding sediment)
[F] Arithmetic mean K_{OC} from a range of 3 soils
n.a. not assessed

PEC_{sw} modelling approach

Calculation of PEC values for the active substances according to FOCUS

$FOCUS_{sw}$ is a four step tiered approach.

Step 1: In this, the most conservative step, all inputs are considered as a single loading to the water body and a worst-case PEC_{sw} and PEC_{sed} is calculated.

Step 2: A refinement is made whereby individual loadings into the water body from different entry routes are considered. Scenarios are also considered for Northern and Southern Europe separately but no specific crop scenarios are defined.

Step 3: An exposure assessment using realistic worst-case scenarios is made. The scenarios are representative of agricultural conditions in Europe and consider weather, soil, crop and different water-bodies. Simulations use the models PRZM, MACRO and TOXSWA.

Step 4: PEC values are refined by considering mitigation measures or specific scenario descriptions on a case-by-case basis.

Predicted environmental concentrations in surface water (PEC_{sw}) and sediment (PEC_{sed})

PEC_{sw} and PEC_{sed} for isoxaflutole and metabolites

For isoxaflutole, the metabolites RPA 202248, RPA 203328 and RPA 205834 were assessed.

Report:	[redacted]**4;**[redacted]**;2013;M-469717-01**
Title:	Predicted Environmental Concentrations in Surface Water (PEC_{sw}) and Sediment (PEC_{sed}) for Isoxaflutole and its metabolites RPA 202248, RPA 205834 and RPA 203328, Following Application to Maize at 100 g/ha
Document No:	M-469717-01-1 (VC/13/007K)
Guidelines:	FOCUS 2003, SANCO/4802/2001 rev 2 FOCUS 2007, SANCO/10422/2005 v. 2.0
GLP:	No (calculation)

Materials and Methods: Predicted environmental concentrations in surface water and sediment (PEC_{sw} and PEC_{sed}) of isoxaflutole and its metabolites RPA 202248, RPA 203328 and RPA 205834 have been calculated for the use in maize in Europe.

At FOCUS Step 2 the application period was set to March to May. Details of the parameters used in the calculations are summarised in Table 9.2.5- 2.

Table 9.2.5- 2: Comparison of actual and calculated use pattern (for FOCUS step 1&2)

Individual Crop	FOCUS Crop Used for Interception	Application				Amount Reaching the Soil per Season/ application
		Rate per Season	Interval	Plant Interception	Growth Stage	
		[g a.s./ha]	[days]	[%]	BBCH	[g a.s./ha]
Maize, GAP and simulation identical	maize	1× 100		0	00-13	100

At FOCUS step 3, actual application dates were determined by the PAT (pesticide application timer) included within SWASH. Details of the parameters used in the calculations are summarised below.

Table 9.2.5- 3: Application dates of isoxaflutole for the FOCUS Step 3 calculations

Parameter	Maize 1 x 100 g/ha	
PAT start date rel./absolute	Absolute	
Appl. method (appl. type)	ground spray (CAM 2)	
No of appl.	1	
PAT window range	30	
Appl. interval	1	
Application Details	Appl. Date	PAT Start Date
D3 [redacted]	21st April	20th April
D4 [redacted]	26th April	26th April
D5 [redacted]	26th April	26th April
D6 [redacted]	6th April	9th April
R1 [redacted]	19th April	26th April
R2 [redacted]	17th April	22nd April
R3 [redacted]	17th April	22nd April
R4 [redacted]	27th March	7th April

Compound specific input data are summarised below for (Table 9.2.5- 4).

Table 9.2.5- 4: Substance parameters used for isoxaflutole and its metabolites

Parameter	Unit	Isoxaflutole	RPA 202248	RPA 203328	RPA 205834
Molar Mass	g/mol	359	359	268	361
Water Solubility	mg/L	6.2	22660	110000	29
Vapour Pressure	Pa	3.22e-7	-	-	-
Q_{10}	-	2.58	-		
K_{oc}	mL/g	79.8	34.9	1.17	1.0
Degradation					
Soil	days	0.9	15.5	11.4	1000
Total System	days	0.36	237	1000	76.2
Water	days	0.36	237	1000	76.2
Sediment	days	0.36/1000*	237/1000*	1000	76.2
Max Occurrence					
Water / Sediment	%		70.3	10.8	25.4
Soil	%	-	100	62.0	2.3

* 1000 days used for Step 3 calculations

Findings:

Step 1 and 2: The maximum PEC values for Steps 1 and 2 are given in the tables below.

Table 9.2.5- 5: Maximum PEC_{sw} and PEC_{sed} values for isoxalutole and its metabolites at Step 1& 2

Use pattern	FOCUS scenario	Isoxaflutole		RPA 202248		RPA 203328		RPA 205834	
		PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]
Maize 1× 100 g a.s./ha	Step 1	31.05	24.04	32.50	11.30	15.48	0.18	1.02	0.00
	Step 2								
	N-EU Single	0.92	0.22	5.95	2.07	2.49	0.03	0.39	0.00
	S-EU Single	0.92	0.44	11.27	3.92	4.91	0.06	0.54	0.00

Step 3: The maximum PEC_{sw} and PEC_{sed} values for relevant FOCUS Step 3 scenarios are given in the tables below. Time dependent PEC values or time-weighted average concentrations are not included in this summary, because they were not used in the risk assessment.

Table 9.2.5- 6: Maximum PEC_{sw} and PEC_{sed} of isoxaflutole and RPA 202248 for all scenarios at Step 3 following application to maize (1 × 100 g a.s./ha)

Compound	Isoxaflutole		RPA 202248	
FOCUS scenario	**PEC_{sw} [µg/L]**	**PEC_{sed} [µg/kg]**	**PEC_{sw} [µg/L]**	**PEC_{sed} [µg/kg]**
D3 (ditch)	0.524	0.074	0.335	0.057
D4 (pond)	0.021	0.005	0.018	0.051
D4 (stream)	0.442	0.018	0.012	0.016
D5 (pond)	0.021	0.004	0.023	0.054
D5 (stream)	0.446	0.011	0.009	0.015
D6 (ditch)	0.524	0.064	0.363	0.129
R1 (pond)	0.021	0.004	0.022	0.039
R1 (stream)	0.363	0.029	1.688	0.216
R2 (stream)	0.482	0.022	1.568	0.216
R3 (stream)	0.513	0.054	0.061	0.008
R4 (stream)	0.362	0.043	4.208	0.690

Step 4: The maximum PEC_{sw} and PEC_{sed} values for isoxaflutole for relevant FOCUS Step 4 scenarios and different buffer zones are given in the tables below. Time-weighted average concentrations (7d-TWA_{sw}) are included in this summary, because they were used in the risk assessment (for 5 m buffer only).

Table 9.2.5- 7: Maximum PEC_{sw} and 7d-TWA_{sw} values and PEC_{sed} of isoxaflutole for all scenarios at Step 4 following application to maize (1 × 100 g a.s./ha) at different buffer zones

Compound	Isoxaflutole				
FOCUS scenario	**PEC_{sw} [µg/L]**	**PEC_{sed} [µg/kg]**	**7d-TWA_{sw}[a] [µg/L]**	**PEC_{sw} [µg/L]**	**PEC_{sed} [µg/kg]**
Buffer	**5m**			**10m**	
D3 (ditch)	0.172	0.025	0.0170	0.091	0.013
D4 (pond)	0.019	0.005	0.0056	0.014	0.003
D4 (stream)	0.186	0.008	0.00203	0.099	0.004
D5 (pond)	0.019	0.004	0.000077	0.014	0.003
D5 (stream)	0.188	0.005	0.00121	0.100	0.003
D6 (ditch)	0.172	0.022	0.000212	0.091	0.013
R1 (pond)	0.019	0.004	0.00210	0.014	0.003
R1 (stream)	0.153	0.012	0.00395	0.081	0.010
R2 (stream)	0.203	0.009	0.00259	0.107	0.005
R3 (stream)	0.216	0.023	0.00992	0.114	0.013
R4 (stream)	0.182	0.041	0.0194	0.182	0.040

[a] worst-case 7d-TWA values

CP 9.3 Fate and behaviour in air

For information on the fate and behaviour in air please refer to MCA Section 7, point 7.3.

CP 9.3.1 Route and rate of degradation in air and transport via air

For information on route and rate of degradation in air and transport via air please refer to MCA Section 7, points 7.3.1 and 7.3.2.

CP 9.4 Estimation of concentrations for other routes of exposure

There are no other routes of exposure if the product is used according to good agricultural practice.