Bayer CropScience

Document Title

Summary of the fate and behaviour in the environment

Thiacloprid OD 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

Date

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Author(s)

[redacted]

Bayer CropScience

M-497689-01-3

OWNERSHIP STATEMENT

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

Use pattern considered in the environmental exposure and risk assessment

Table CP 9- 1: Intended application pattern

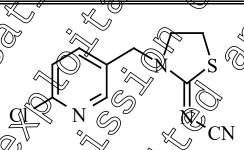
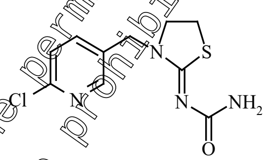
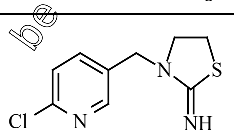
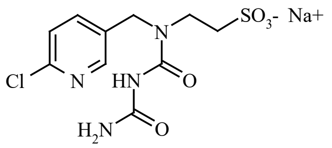
Crop	Timing of application (range)	Number of applications	Application interval [days]	Maximum label rate [L/ha]	Maximum application rate, individual treatment [g/ha] Thiacloprid
OSR*	BBCH 30-59	2	10	0.3	72
* oilseed rape					

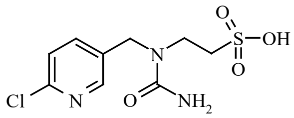
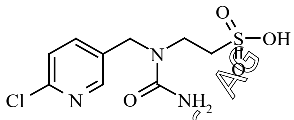
Crop	F G or I (b)	Application				Application rate per treatment			Remarks: (m)
		method kind (f-h)	growth stage & season (j)	number min max (k)	interval between applications (min)	g a.s./hL min max	water L/ha min max	g a.s./ha min max	
Oil Seed Rape	F	Foliar spray	BBCH 30-59	1-2	10	24-72	100-300	72	Product label rate: Max. 0.3 L/ha

Compounds addressed in this document

In addition to the active substance thiacloprid, the degradation products summarised in Table 9- 2 were addressed in this document as they have to be considered for exposure assessments.

Table CP 9- 1: Active substance and degradation products addressed in this document

Compound / Codes	Chemical Structure	Considered for
Thiacloprid (YRC 2894) Active Substance (a.s.)		PEC_{soil} PEC_{gw} PEC_{sw} & PEC_{sed}
YRC 2894-amide **(M02)**		PEC_{soil} PEC_{gw} PEC_{sw} & PEC_{sed}
YRC 2894-des-cyano **(M29)**		PEC_{soil} PEC_{gw} PEC_{sw} & PEC_{sed}
YRC 2894-sulfonic acid (sodium salt shown) **(M30)**		PEC_{soil} PEC_{gw} PEC_{sw} & PEC_{sed}

Compound / Codes	Chemical Structure	Considered for
YRC 2894-sulfonic acid amide (M34)		PEC_{gw}
YRC 2894-thiadiazine (M46)		PEC_{gw}

A list of metabolites, which contains the structures, the synonyms and code numbers attributed to the compound thiacloprid, is presented in Document N3 of this dossier.

Definition of the residue for risk assessment

Justification for the residue definition for risk assessment is provided by MCA Section 7.

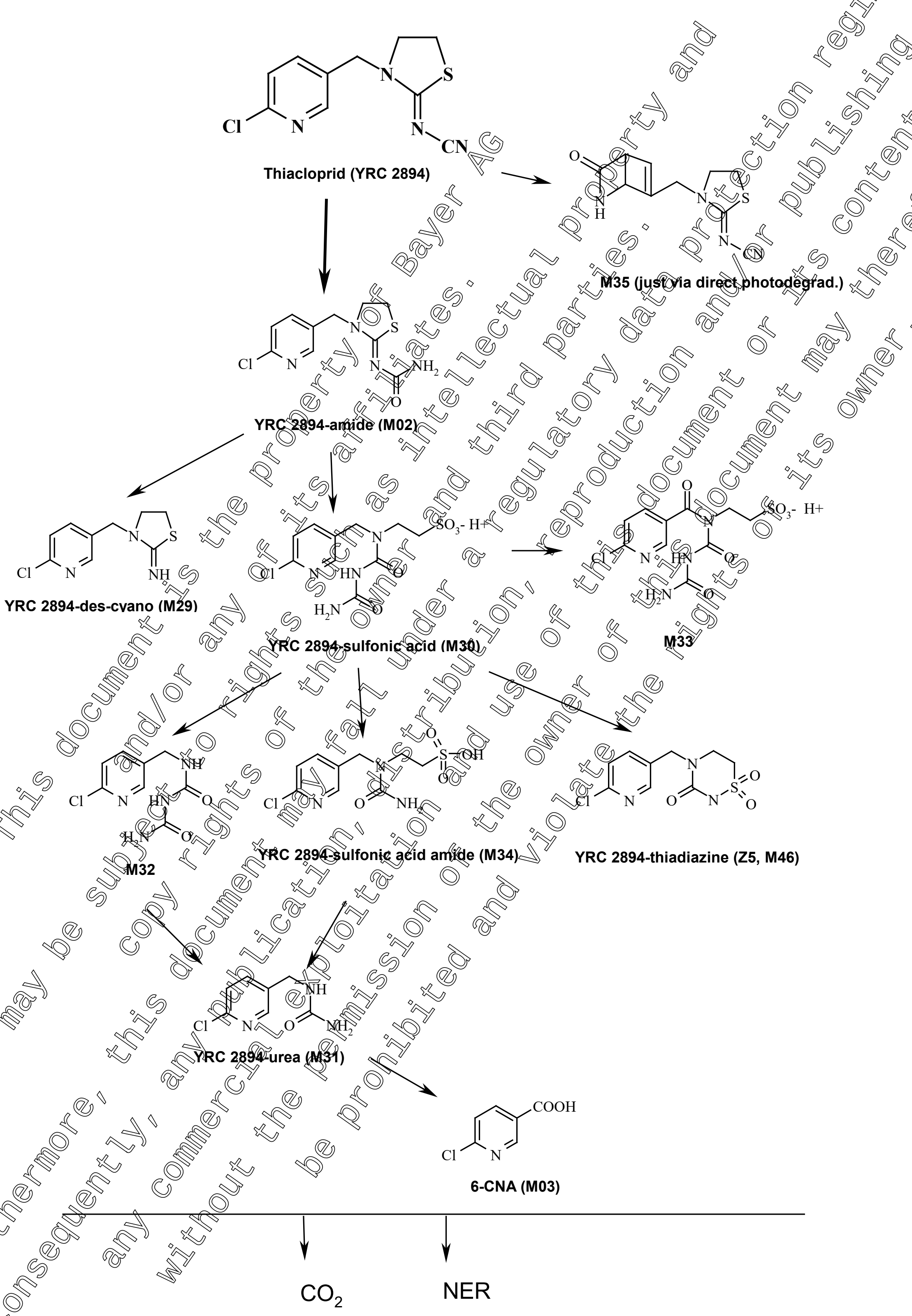
Table CP 9- 2: Definition of the residue for risk assessment

Compartment	Residue Definition for risk assessment
Soil	Thiacloprid (YRC 2894) YRC 2894-amide (M02) YRC 2894-des-cyano (M29) YRC 2894-sulfonic acid (M30)
Groundwater	Thiacloprid (YRC 2894) YRC 2894-amide (M02) YRC 2894-des-cyano (M29) YRC 2894-sulfonic acid (M30) YRC 2894-sulfonic acid amide (M34) YRC 2894-thiadiazine (M46)
Surface water	Thiacloprid (YRC 2894) YRC 2894-amide (M02) YRC 2894-des-cyano (M29) YRC 2894-sulfonic acid (M30)
Sediment	Thiacloprid (YRC 2894)
Air	Thiacloprid (YRC 2894)

CP 9.1 Fate and behaviour in soil

For information on the fate and behaviour in soil please refer to MCA Section 7, data point 7.1.
The proposed degradation pathway of thiacloprid in soil is shown in Figure CP 9.1- 1.

Figure CP 9.1- 1: Proposed degradation pathway of thiacloprid in soil under laboratory conditions considering all routes of soil degradation and lysimeter studies.



CP 9.1.1 Rate of degradation in soil

No specific studies with the formulation are required. For further information on the fate and behaviour in soil please refer to MCA Section 7, data 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, data point 7.1.2.1.

CP 9.1.1.2 Field studies

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

CP 9.1.2.1 Laboratory studies

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

CP 9.1.2.2 Lysimeter studies

For information on lysimeter studies please refer to MCA Section 7, data 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, data 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 behaviour 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}

For deriving the respective end points please refer to MCA Section 7, data point 7.1.

Table CP 9.1.3- 1: Key modelling input parameters for thiacloprid and its metabolites

Compound	Worst case DT_{50} non-normalised [days]	Maximum occurrence in soil [%]	Molar mass [g/mol]	Molar mass correction factor
Thiacloprid	13.7)*	100	252.7	1
YRC 2894-amide (M02)	321.1)*	86.7)1	270.7	1.0712
YRC 2894-sulfonic acid (M30)	97.6)*	19.7)2	336.8	1.3328
YRC 2894-des-cyano (M29)	789.3)#	33.2)1	227.7	0.9011

*: worst case non-normalized field DT_{50} value. #: worst case non-normalized laboratory DT_{50} value.

)1: [redacted], N.; 2011; M-404822-01-1)2: [redacted], R.; [redacted], W.; 1998; M-001076-02-1 (KCA 7.1.1.1 /02

Report: [redacted]; [redacted]; [redacted]; 2014; M-491012-01-1
Title: Thiacloprid (TCP) and metabolites: PECsoil EUR - Use in oil seed rape and maize in Europe
Report No.: EnSa-14-0806
Document No.: M-491012-01-1
Guidelines: **not applicable**
GLP/GEP: **no**

Methods and Materials: The predicted environmental concentrations in soil (PEC_{soil}) of thiacloprid and its metabolites were estimated based on a first tier approach using a Microsoft® Excel spreadsheet. A bulk density of 1.5 kg/L and a soil mixing depths of 5 cm were used as recommended by FOCUS (1997) and EU Commission (1995, 2000). The accumulation potential of thiacloprid and metabolites after long term use was also assessed, employing the mixing depth of 20 cm for the calculation of the background concentration.
Detailed application data used for simulation of PEC_{soil} were compiled in Table CP 9.1.3- 2.

Table CP 9.1.3- 2: Application pattern used for PEC_{soil} calculations of thiacloprid

Individual crop	FOCUS crop used for interception	Application				Amount reaching soil per season application [g a.s./ha]
		Rate per season [g a.s. /ha]	Interval [days]	Plant interception [%]	BBCH stage	
oilseed rape, GAP & simulation	oilseed rape	2 × 72	10	2 × 80	2 × 30-59	2 × 14.4

Substance Specific Parameters: The compound specific input parameters (end points for PEC_{soil} calculations) are summarized in Table CP 9.1.3- 1.

Findings: The maximum PEC_{soil} values for thiacloprid and its metabolites are summarised in Table CP 9.1.3- 3. The maximum, short-term and long-term PEC_{soil} values and the time weighted average values ($TWAC_{soil}$) are provided thereafter.

Table CP 9.1.3- 3: Maximum PEC_{soil} of thiacloprid and its metabolites for the uses assessed

	Thiacloprid	YRC 2894 -amide	YRC 2894 -sulfonic acid	YRC 2894 -des-cyano
Use Pattern	**PEC_{soil} [mg/kg]**	**PEC_{soil} [mg/kg]**	**PEC_{soil} [mg/kg]**	**PEC_{soil} [mg/kg]**
oilseed rape 2×72 g a.s./ha, 10 days, 2×80%	0.031	0.035	0.010	0.011

Table CP 9.1.3- 4: PEC_{soil} (actual) of thiacloprid and its metabolites

		Oilseed rape 2×72 g a.s./ha, 10 days, 2×80%			
		Thiacloprid	**YRC 2894 -amide**	**YRC 2894 -sulfonic acid**	**YRC 2894 -des-cyano**
	Time [days]	**PEC_{soil} [mg/kg]**	**PEC_{soil} [mg/kg]**	**PEC_{soil} [mg/kg]**	**PEC_{soil} [mg/kg]**
Initial	0	0.031	0.035	0.010	0.011
Short term	1	0.029	0.035	0.010	0.011
	2	0.028	0.035	0.010	0.011
	4	0.025	0.035	0.009	0.011
Long term	7	0.022	0.035	0.009	0.011
	14	0.015	0.034	0.009	0.011
	21	0.011	0.034	0.008	0.011
	28	0.007	0.033	0.008	0.011
	42	0.004	0.032	0.007	0.011
	50	0.002	0.032	0.007	0.011
	100	<0.001	0.028	0.005	0.010

Table CP 9.1.3- 5: TWAC$_{soil}$ of thiacloprid and its metabolites

		Oilseed rape 2×72 g a.s./ha, 10 days, 2×80%			
		Thiacloprid	YRC 2894 -amide	YRC 2894 -sulfonic acid	YRC 2894 -des-cyano
	Time [days]	TWAC$_{soil}$ [mg/kg]	TWAC$_{soil}$ [mg/kg]	TWAC$_{soil}$ [mg/kg]	TWAC$_{soil}$ [mg/kg]
Initial	0	---	---	---	---
Short term	1	0.030	0.035	0.010	0.011
	2	0.029	0.035	0.010	0.011
	4	0.028	0.035	0.010	0.011
Long term	7	0.026	0.035	0.009	0.011
	14	0.022	0.035	0.009	0.011
	21	0.019	0.034	0.009	0.011
	28	0.016	0.034	0.009	0.011
	42	0.013	0.034	0.008	0.011
	50	0.011	0.033	0.008	0.011
	100	0.006	0.032	0.007	0.011

Potential accumulation in soil:

The accumulation potential after long term use was also assessed. The results for a standard-mixing depth of 20 cm for an arable crop with tillage are presented in Table CP 9.1.3- 6.

Table CP 9.1.3- 6: PEC$_{soil}$ of thiacloprid and its metabolites taking the effect of accumulation into account (mixing depth of 20 cm)

Use Pattern	PEC$_{soil}$	Thiacloprid [mg/kg]	YRC 2894 -amide [mg/kg]	YRC 2894 -sulfonic acid [mg/kg]	YRC 2894 -des-cyano [mg/kg]
Oilseed rape 2×72 g a.s./ha, 10 days, 2×80%	plateau	<0.001	0.007	<0.001	0.008
	total*	0.031	0.043	0.010	0.019

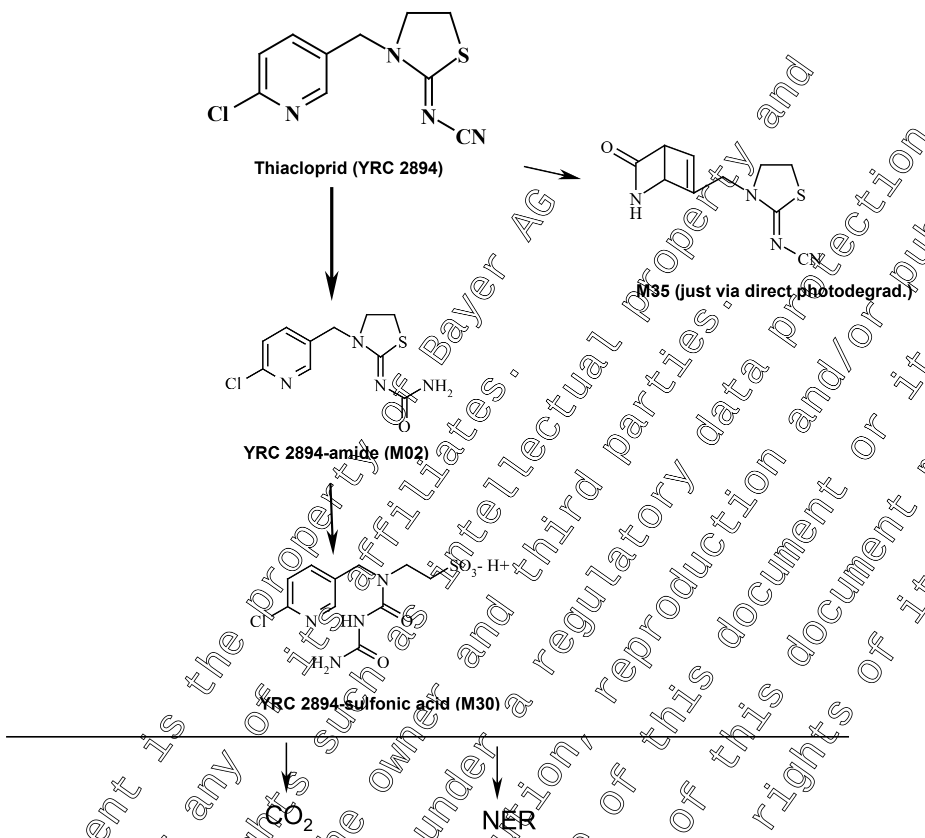
* total = plateau (background concentration after multi-year use) + max. PEC$_{soil}$ (see)

CP 9.2 Fate and behaviour in water and sediment

The proposed degradation pathway of thiacloprid in water and sediment is shown in Figure CP 9.2- 1.

For information on the fate and behaviour in water and sediment please refer to MCA Section 7, data point 7.2.

Figure CP 9.2- 1: Proposed bio-degradation pathway of Thiacloprid (YRC 2894) in the aquatics.



CP 9.2.1 Aerobic mineralisation in surface water

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

CP 9.2.2 Water/sediment study

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

CP 9.2.4 Estimation of concentrations in groundwater

Calculations were performed, to reflect findings from new studies presented in the active substance dossier, section 7 "Fate and behaviour 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}

For deriving the respective end points please refer to MCA Section 7, data point 7.1.

Table CP 9.2.4- 1: Key modelling input parameters for thiacloprid and its metabolites

Compound	Formation fraction	DT_{50} [days]	Koc)2 [mL/g]	Kom)2 [mL/g]	FREUNDLICH)2 exponent
Thiacloprid	1.0	5.4)1	615.0	357.0	0.880
YRC 2894-amide (M02)	0.61)2	41.3)1	293.0	170.0	0.830
YRC 2894- sulfonic acid (M30)	0.80)2	15.6)1	20.2	11.7	0.940
YRC 2894-thiadiazine (M46)	0.44)5	19.8)3	9.6	5.6	0.960
YRC 2894-des-cyano (M29)	0.23)2	140.7)3	371.0	215.0	0.840
YRC 2894-sulfonic acid amide (M34)	0.56)2	48.8)4	7.0	4.1	1.000

)1: Median of complete data set of normalized lab and field DT_{50} values.
)2: Arithmetic mean of data set.
)3: Geometric mean of lab data set.
)4: Worst case of lab data set.
)5: Worst case assumption that M30 can only degrade to M34 and M46.

CP 9.2.4.1 Calculation of concentrations in groundwater

Predicted environmental concentrations in groundwater (PEC_{GW})

Report: [redacted]; 2014; M-491013-01-1
Title: Thiacloprid (TCP) and metabolites: PECgw FOCUS PEARL, PELMO EUR - Use in oil seed rape and maize in Europe
Report No.: EnSa-14-0807
Document No.: M-491013-01-1
Guidelines: **not applicable**
GLP/GEP: **no**

Materials and Methods: The predicted environmental concentrations in groundwater (PEC_{gw}) for thiacloprid and its metabolites were calculated using the simulation model FOCUS PEARL (version 4.4.4) and FOCUS PELMO (version 5.5.3). Crop interception was taken into account according to the BBCH growth stage, as recommended by FOCUS (2012). Application dates for the simulation runs were defined following the crop event dates of the respective crop and scenario as given by FOCUS (2000, 2009).

Detailed application data used for simulation of PEC_{gw} were compiled in Table CP 9.2.4.1- 1.

Table CP 9.2.4.1- 1: Application pattern used for PEC_{gw} calculations

Individual crop	FOCUS crop used for interception	Application				Amount reaching soil per season application [g a.s./ha]
		Rate per season [g a.s. /ha]	Interval [days]	Plant interception [%]	BBCH stage	
Oilseed rape, GAP	-	2 × 72	10	-	2 × 30-59	-
Oilseed rape (summer) simulation 1	oil seed rape (summer)	2 × 72	10	2 × 80	2 × 30-59	2 × 14.4
Oilseed rape (winter) simulation 2	oil seed rape (winter)	2 × 72	10	2 × 80	2 × 30-59	2 × 14.4

For oilseed rape applications, absolute dates were derived for the simulation runs. All application dates are summarised in the table below.

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

Individual crop	Oilseed rape (summer)	Oilseed rape (winter)
Repeat Interval for App. Events	Every Year	Every Year
Application Technique	Spray	Spray
Absolute / Relative to	Absolute	Absolute
Scenario	1st App. Date/(Julian day)	1st App. Date/(Julian day)
[redacted]	-	19 Apr/(109)
		05 May/(125)
	18 Jun/(169)	-
	-	01 May/(121)
	08 May/(128)	20 Apr/(110)
	-	11 Apr/(101)
	04 May/(124)	19 Apr/(109)
	-	-
	-	-

Substance specific and model related input parameters for FOCUS PEARL & PELMO PEC_{gw} calculations are summarised in Table CP 9.2.4.1- 3. Degradation pathway related parameters are given in Table CP 9.2.4.1- 4.

Table CP 9.2.4.1- 3: Compound input parameters for thiacloprid and its metabolites

Parameter	Unit	TCP	YRC 2894-amide	YRC 2894-sulfonic acid	YRC 2894-thiadiazine	YRC 2894-des-cyano	YRC 2894-sulfonic acid amide
Common							
Molar Mass	[g/mol]	252.7	270.7	336.8	275.7	227.7	293.7
Solubility	[mg/L]	159	660	56000	130000	57000	135000
Vapour Pressure	[Pa]	3.00E-10	3.40E-10	3.80E-04	2.30E-05	1.10E-04	5.90E-07
Freundlich Exponent		0.880	0.830	0.940	0.960	0.840	1.000
Plant Uptake Factor		0.0A	0.0	0.0	0.0	0.0	0.0
Walker Exponent		0.7	0.7	0.7	0.7	0.7	0.7
PEARL Parameters							
Substance Code		TCP	M02	M30	MZ5	M29	M34
DT_{50}	[days]	5.4	41.3	15.6	19.8	140.7	48.8
Molar Activ. Energy	[kJ/mol]	65.4	65.4	65.4	65.4	65.4	65.4
K_{om}	[mL/g]	357.0	170.0	11.7	5.6	215.0	3.6
K_f	[mL/g]	-	-	-	-	-	-
PELMO Parameters							
Substance Code		AS	A1	B1	C1	A2	B2
Rate Constant	[1/day]	0.12860	0.01680	0.04450	0.03500	0.00490	0.01420
Q_{10}		2.58	2.58	2.58	2.58	2.58	2.58
K_{oc}	[mL/g]	615.0	293.0	20.2	9.6	371.0	6.3 #

* TCP = thiacloprid
A Since degradation data from field trials are considered here, the plant uptake factor was set to zero as a worst case assumption.

Table CP 9.2.4.1- 4: Degradation pathway related parameters for thiacloprid and its metabolites

Degradation fraction from → to (FOCUS PEARL)	0.61 TCP -> M02 0.23* M02 -> M29 0.8 M02 -> M30 0.56 M30 -> M34 0.44 M30 -> MZ5
Degradation rate from → to (FOCUS PELMO)	0.0787000 AS -> A1 0.0499000 AS -> <BR/CO_2 0.0134000 A1 -> B1 0.0034000* A1 -> A2 0.0196000 B1 -> C1 0.0249000 B1 -> B2 0.0350000 C1 -> <BR/CO_2 0.0049000 A2 -> <BR/CO_2 0.0142000 B2 -> <BR/CO_2
* The sum of formation fractions of YRC 2894-des-cyano (0.23) and YRC 2894-sulfonic acid (0.80) is slightly larger than 1. In FOCUS PELMO, this would lead to faster disappearance of YRC 2894-amide (by 3 %) due to the way the specification of degradation parameters is technically implemented (FOCUS PEARL is not affected). In order to overcome this issue, the formation of YRC 2894-des-cyano was limited to 0.20 in FOCUS PELMO runs. This change does not have any measurable effect on the PEC_{gw} of YRC 2894-des-cyano but is essential to keep internal consistency of the description of other metabolites.	

Findings: PEC_{GW} were evaluated as the 80th percentile of the mean annual leachate concentration at 1 m soil depth. FOCUS PEARL and PELMO PEC_{gw} results for thiacloprid and its metabolites after application to winter oilseed rape are given in Table CP 9.2.4.1- 5 and after application to summer oilseed rape in Table CP 9.2.4.1- 6.

Table CP 9.2.4.1- 5: Oilseed rape (winter): FOCUS PEARL & PELMO PEC_{gw} results of thiacloprid and its metabolites

Use Pattern	Oilseed rape (winter): 2 × 72 g a.s./ha, 2 × 80% interception, 10 d interval					
	TCP	YRC 2894-amide	YRC 2894-sulfonic acid	YRC 2894-thiadiazine	YRC 2894-des-cyano	YRC 2894-sulfonic acid amide
FOCUS PEARL	**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	0.020	0.119	<0.001	1.181
[redacted]	<0.001	<0.001	0.162	0.436	<0.001	2.068
[redacted]	<0.001	<0.001	0.066	0.212	<0.001	1.039
[redacted]	<0.001	<0.001	0.116	0.238	<0.001	1.028
[redacted]	<0.001	<0.001	0.039	0.097	<0.001	0.581
[redacted]	<0.001	<0.001	0.070	0.151	<0.001	0.928
FOCUS 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	0.020	0.120	<0.001	1.095
[redacted]	<0.001	<0.001	0.155	0.414	<0.001	1.849
[redacted]	<0.001	<0.001	0.076	0.242	<0.001	1.193
[redacted]	<0.001	<0.001	0.141	0.266	<0.001	1.077
[redacted]	<0.001	<0.001	0.067	0.149	<0.001	0.829
[redacted]	<0.001	<0.001	0.105	0.184	<0.001	0.937

* TCP = thiacloprid

Table CP 9.2.4.1- 6: Oilseed rape (summer): FOCUS PEARL & PELMO PEC_{gw} results of thiacloprid and its metabolites

Use Pattern	oilseed rape (summer), 2 × 72 g a.s./ha, 2 × 80% interception, 10 d interval					
	TCP	YRC 2894-amide	YRC 2894-sulfonic acid	YRC 2894-thiadiazine	YRC 2894-des-cyano	YRC 2894-sulfonic acid amide
FOCUS PEARL	**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	0.136	0.425	<0.001	2.409
	<0.001	<0.001	0.126	0.252	<0.001	1.058
	<0.001	<0.001	0.055	0.115	<0.001	0.689
FOCUS 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	0.149	0.455	<0.001	2.307
	<0.001	<0.001	0.134	0.263	<0.001	1.047
	<0.001	<0.001	0.075	0.144	<0.001	0.749

* TCP = thiacloprid

Conclusion: There are no concerns for groundwater from the use of thiacloprid in accordance with the use pattern for the representative formulation.

The concentration of the metabolites YRC 2894-sulfonic acid, YRC 2894-thiadiazine and YRC 2894-sulfonic acid amide may exceed 0.1 µg/L, however the relevance of these metabolites has been assessed and all metabolites are non-relevant in groundwater (see Document N4).

CP 9.2.4.2 Additional field tests

No additional field studies were performed or required due to low PEC_{gw} values calculated (see CP 9.2.4.1).

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 behaviour in the environment". In addition these calculations consider the most recent guidance documents for exposure calculations. Calculations of predicted environmental concentrations are presented below.

Predicted environmental concentrations in water (PEC_{SW}) and in sediment (PEC_{Sed})

Endpoints for PEC_{SW} and sediment (PEC_{SED})

For deriving the respective end points please refer to MCA Section 7, data point 7.2.

Table CP 9.2.5- 1: Key modelling input parameters for thiacloprid and its metabolites at Steps 1-2 level PEC calculations

Parameter	Unit	Thiacloprid	YRC 2894 -amide	YRC 2894 -des-cyano	YRC 2894 -sulfonic acid
Molar Mass	g/mol	252.7	270.7	227.7	336.8
Water Solubility	mg/L	159	660	57000	56000
Koc	mL/g	615	293	371	20.2
Degradation					
Soil	days	5.4	41.3	140.7	15.6
Total System	days	15.8	99.2	1000 *	1000 *
Water	days	15.8	99.2	1000 *	1000 *
Sediment	days	15.8	99.2	1000 *	1000 *
Max Occurrence					
Water / Sediment	%	100	69	0.0001	9.7
Soil	%	100	86.7	33.2	19.7

* Default value used

Table CP 9.2.5- 2: Additional modelling input parameters for thiacloprid and its metabolites at steps 3/4 level PEC calculations

Parameter	Unit	Thiacloprid	YRC 2894 -amide	YRC 2894 -des-cyano
Vapour Pressure	Pa	3.0E-10	3.4E-10	1.1E-04
Plant Uptake Factor		0.0	0.0	0.0
Wash-Off Factor PRZM	1/cm	0.5	0.5	0.5
Wash-Off Factor MACRO	1/mm	0.05	0.05	0.05
Degradation				
Soil	days	5.4	41.3	140.7
Form. Frac. PRZM	molar basis	-	0.610	0.230
Form. Frac. MACRO	molar basis	-	0.653	0.207
Aquatic Metabolite				
Molar Mass Corr. Factor		-	1.07123	-
Max Occ.	%	-	69	-
Tot. Corr. Factor		-	0.73915	-
Max Occ. at Day		-	35	-

Report:	[redacted]x;[redacted];[redacted]; 2014; M-491014-01-1
Title:	Thiacloprid (TCP) and metabolites: PECsw,sed FOCUS EUR - Use in maize and oil seed rape in Europe
Report No.:	EnSa-14-0808
Document No.:	M-491014-01-1
Guidelines:	**not applicable; not applicable**
GLP/GEP:	**no**

Report:	[redacted]$;[redacted];[redacted]; 2014; M-491773-01-1
Title:	Thiacloprid (TCP) and metabolite: PECsw,sed FOCUS EUR (M29 assessment) - Use in maize and oil seed rape in Europe
Report No.:	EnSa-14-0882
Document No.:	M-491773-01-1
Guidelines:	**not applicable; not applicable**
GLP/GEP:	**no**

Materials and Methods: Predicted environmental concentrations in surface water and sediment (PEC_{sw} and PEC_{sed}) of thiacloprid and its metabolites have been calculated for the use in spring and winter oilseed rape in Europe. All relevant entry routes of a compound into surface water (combination of spray drift and runoff/erosion or drain flow) were considered in these calculations.

At FOCUS Step 2 the application period was set to March to May and the use in Northern and Southern Europe was considered. Details of the application pattern used in the Step 2 calculations are summarised in Table CP 9.2.5-3.

Table CP 9.2.5-3: Application pattern used for $PEC_{sw,sed}$ calculations at FOCUS Steps 1&2

Crop	Rate [g a.s./ha]	Interval [days]	BBCH stage	FOCUS crop (crop group)	Season	Crop cover
Oilseed rape, GAP	2 × 72	10	30-59	-	-	-
Oilseed rape (spring), simulation 1	2 × 72	10	30-59	oilseed rape, spring (arable crops)	Mar. - May	average
Oilseed rape (winter), simulation 2	2 × 72	10	30-59	oilseed rape, winter (arable crops)	Mar. - May	average

In FOCUS Step 3, the application date for each scenario is determined by the Pesticide Application Timer (PAT), which is part of the FOCUS SW Scenarios. The user may only define an application time window. Absolute application dates for oilseed rape simulation runs were estimated using a German regulatory tool AppDate[1]. Details of the parameters used in the Step 3 calculations are summarised in Table CP 9.2.5- 4.

[1] Klein M., 2010: Computer programme: “AppDate: Estimation of application dates based on crop development.” (v.1.01c.).

Table CP 9.2.5- 4: Application dates of thiacloprid for the FOCUS Step 3 calculations

Parameter	Oilseed rape (spring)		Oilseed rape (winter)	
PAT start date rel./absolute	Absolute		Absolute	
Appl. method (appl. type)	ground spray (CAM 2)		ground spray (CAM 2)	
No of appl.	2		2	
PAT window range	40		40	
Appl. interval	10		10	
Application Details	PAT Start Date (Julian Day)	Appl. Date	PAT Start Date (Julian Day)	Appl. Date
D1	21-Jun (172)	24-Jun 04-Jul	- -	- -
D2	- -	- -	29-Apr (119)	07-May 23-May
D3	20-May (140)	22-May 23-Jun	29-Apr (119)	04-May 22-May
D4	06-Jun (157)	04-Jul 16-Jul	13-May (133)	30-May 09-Jun
D5	24-Apr (114)	24-Apr 11-May	23-Apr (113)	23-Apr 11-May
D6	- -	- -	- -	- -
R1	17-May (137)	31-May 12-Jun	22-Apr (112)	26-Apr 09-May
R2	- -	- -	- -	- -
R3	- -	- -	06-Apr (96)	11-Apr 22-Apr
R4	- -	- -	- -	- -

Compound input parameters for the Steps 1&2 simulation runs are summarised in Table CP 9.2.5-1and for the Steps 3&4 simulation runs in Table CP 9.2.5- 2.

Note, Step 3 assessment was calculated also for the metabolites YRC 2894–amide and YRC 2894-des-cyano. Due to technical limitations of the models used for the calculations a special treatment is needed for YRC 2894-des-cyano. The metabolite is considered here to be a direct degradation product of the parent substance even though the evaluation of the soil degradation studies indicates that YRC 2894-des-cyano is formed from the YRC 2894-amide (this set up cannot be directly reproduced in Step 3 of $FOCUS_{sw}$). The employed formation fraction of 23 % from the parent represents a worst case estimate of the degradation behaviour of YRC 2894-des-cyano in soil.

Findings: Steps 1&2: The maximum PEC_{sw} and PEC_{sed} values for thiacloprid and its metabolites at Steps 1&2 are summarised in Table CP 9.2.5- 5.

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

Use pattern	Scenario	Thiacloprid		YRC 2894 -amide		YRC 2894 -des-cyano		YRC 2894 -sulfonic acid	
		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]
Oilseed rape (spring) 2 × 72 g a.s./ha	Step 1	27.70	162.2	33.04	93.93	9.607	35.64	12.44	2.479
	Step 2								
	N-EU Multi	1.127	6.171	2.304	6.529	0.552	2.046	0.654	0.132
	S-EU Multi	1.732	9.730	3.964	11.36	1.103	4.093	1.159	0.234
	N-EU Single	0.833	4.584	1.277	3.612	0.283	1.048	0.392	0.079
	S-EU Single	1.306	7.371	2.176	6.229	0.565	2.097	0.700	0.141
Oilseed rape (winter) 2 × 72 g a.s./ha	Step 1	27.70	162.2	33.04	93.93	9.607	35.64	12.44	2.479
	Step 2								
	N-EU Multi	1.127	6.171	2.304	6.529	0.552	2.046	0.654	0.132
	S-EU Multi	1.732	9.730	3.964	11.36	1.103	4.093	1.159	0.234
	N-EU Single	0.833	4.584	1.277	3.612	0.283	1.048	0.392	0.079
	S-EU Single	1.306	7.371	2.176	6.229	0.565	2.097	0.700	0.141

Step 3: The maximum PEC_{sw} and PEC_{sed} values of thiacloprid, YRC 2894-amide and YRC 2894-des-cyano for relevant FOCUS Step 3 scenarios are given in the following tables.

Table CP 9.2.5- 6: Spring oilseed rape: Maximum PEC_{sw} and PEC_{sed} values for thiacloprid at Step 3

Use pattern	Thiacloprid					
	Oilseed rape (spring), 2 × 72 g a.s./ha					
	Single application			Multiple application		
FOCUS scenario	Entry route*	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	Entry route*	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]
D1 (ditch)	S	0.461	0.972	S	0.625	1.588
D1 (stream)	S	0.404	0.200	S	0.349	0.228
D3 (ditch)	S	0.457	0.266	S	0.400	0.333
D4 (pond)	S	0.016	0.046	S	0.020	0.073
D4 (stream)	S	0.394	0.076	S	0.341	0.084
D5 (pond)	S	0.016	0.054	S	0.020	0.083
D5 (stream)	S	0.388	0.018	S	0.344	0.025
R1 (pond)	R	0.034	0.120	R	0.049	0.179
R1 (stream)	S	0.301	0.510	R	0.426	0.639

* Entry route: letters S, D, and R correspond to the dominant entry path – spray drift, drainage, and runoff.

Table CP 9.2.5- 7: Spring oilseed rape: Maximum PEC_{sw} and PEC_{sed} values for YRC 2894-amide at Step 3

Use pattern	YRC 2894-amide			
	Oilseed rape (spring), 2 × 72 g a.s./ha			
	Single application		Multiple application	
FOCUS scenario	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]
D1 (ditch)	0.355	1.375	0.533	2.357
D1 (stream)	0.067	0.660	0.119	1.121
D3 (ditch)	<0.001	<0.001	<0.001	<0.001
D4 (pond)	0.012	0.119	0.036	0.322
D4 (stream)	0.016	0.028	0.055	0.100
D5 (pond)	0.014	0.092	0.021	0.159
D5 (stream)	0.008	0.012	0.017	0.026
R1 (pond)	0.032	0.232	0.064	0.436
R1 (stream)	0.220	0.125	0.409	0.288

Table CP 9.2.5- 8: Spring oilseed rape: Maximum PEC_{sw} and PEC_{sed} values for YRC 2894-des-cyano at Step 3

Use pattern	YRC 2894-des-cyano			
	Oilseed rape (spring), 2 × 72 g a.s./ha			
	Single application		Multiple application	
FOCUS scenario	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]
D1 (ditch)	0.077	0.904	0.144	1.651
D1 (stream)	0.048	0.538	0.090	0.974
D3 (ditch)	<0.001	<0.001	<0.001	<0.001
D4 (pond)	0.009	0.097	0.027	0.251
D4 (stream)	0.017	0.034	0.045	0.091
D5 (pond)	0.010	0.132	0.019	0.241
D5 (stream)	0.018	0.027	0.033	0.050
R1 (pond)	0.009	0.101	0.019	0.193
R1 (stream)	0.064	0.055	0.125	0.109

Table CP 9.2.5- 9: Winter oilseed rape: Maximum PEC_{sw} and PEC_{sed} values for thiacloprid at Step 3

Use pattern	Thiacloprid					
	Oilseed rape (winter), 2 × 72 g a.s./ha					
	Single application			Multiple application		
FOCUS scenario	Entry route*	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	Entry route*	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]
D2 (ditch)	S	0.462	0.814	S	0.411	1.166
D2 (stream)	S	0.411	0.726	S	0.357	0.994
D3 (ditch)	S	0.457	0.301	S	0.400	0.354
D4 (pond)	S	0.016	0.051	S	0.021	0.081
D4 (stream)	S	0.392	0.065	S	0.341	0.083
D5 (pond)	S	0.016	0.055	S	0.020	0.085
D5 (stream)	S	0.406	0.035	S	0.368	0.091
R1 (pond)	S	0.016	0.090	R	0.047	0.217
R1 (stream)	S	0.300	0.112	R	0.501	0.390
R3 (stream)	S	0.424	0.456	S	0.368	0.453

* Entry route: letters S, D, and R correspond to the dominant entry path – spray drift, drainage, and runoff.

Table CP 9.2.5- 10: Winter oilseed rape: Maximum PEC_{sw} and PEC_{sed} values for YRC 2894-amide at Step 3

Use pattern	YRC 2894-amide Oilseed rape (winter), 2 × 72 g a.s./ha			
	Single application		Multiple application	
FOCUS scenario	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]
D2 (ditch)	0.104	0.488	0.222	1.008
D2 (stream)	0.065	0.286	0.139	0.596
D3 (ditch)	<0.001	<0.001	<0.001	<0.001
D4 (pond)	0.012	0.097	0.023	0.234
D4 (stream)	0.013	0.021	0.043	0.071
D5 (pond)	0.012	0.075	0.019	0.128
D5 (stream)	0.004	0.005	0.009	0.013
R1 (pond)	0.031	0.184	0.092	0.528
R1 (stream)	0.162	0.106	0.352	0.256
R3 (stream)	0.265	0.131	0.552	0.239

Table CP 9.2.5- 11: Winter oilseed rape: Maximum PEC_{sw} and PEC_{sed} values for YRC 2894-des-cyano at Step 3

Use pattern	YRC 2894-des-cyano Oilseed rape (winter), 2 × 72 g a.s./ha			
	Single application		Multiple application	
FOCUS scenario	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]	PEC_{sw} [µg/L]	PEC_{sed} [µg/kg]
D2 (ditch)	0.125	0.885	0.251	1.744
D2 (stream)	0.079	0.518	0.157	1.027
D3 (ditch)	<0.001	<0.001	<0.001	<0.001
D4 (pond)	0.009	0.095	0.022	0.210
D4 (stream)	0.018	0.037	0.044	0.082
D5 (pond)	0.005	0.069	0.010	0.129
D5 (stream)	0.010	0.015	0.019	0.027
R1 (pond)	0.008	0.066	0.019	0.155
R1 (stream)	0.040	0.042	0.102	0.101
R3 (stream)	0.072	0.047	0.144	0.084

Step 4: The maximum PEC_{sw} and PEC_{sed} values of thiacloprid for relevant FOCUS Step 4 scenarios are given in the following tables.

Table CP 9.2.5- 12: Spring oilseed rape: Maximum PEC$_{sw}$ values for thiacloprid at Step 4 after single and multiple applications

		Thiacloprid							
		Oilseed rape (spring), 2 × 72 g a.s./ha							
		Single application				Multiple application			
Buffer Width & Type	Scenario	PEC$_{sw}$ [µg/L]) Drift Reduction				PEC$_{sw}$ [µg/L] Drift Reduction			
		0%	50%	75%	90%	0%	50%	75%	90%
5m SD	D1 (ditch)	0.125	0.063	0.031	0.013	0.161	0.080	0.040	0.016
	D1 (stream)	0.147	0.074	0.037	0.015	0.123	0.062	0.031	0.012
	D3 (ditch)	0.124	0.062	0.031	0.013	0.104	0.052	0.026	0.010
	D4 (pond)	0.014	0.007	0.003	0.001	0.017	0.009	0.004	0.002
	D4 (stream)	0.144	0.072	0.036	0.014	0.121	0.060	0.030	0.012
	D5 (pond)	0.014	0.007	0.003	0.001	0.017	0.009	0.004	0.002
	D5 (stream)	0.141	0.071	0.035	0.014	0.122	0.061	0.030	0.012
	R1 (pond)	0.033	0.028	0.026	0.025	0.048	0.042	0.039	0.037
	R1 (stream)	0.280	0.280	0.280	0.280	0.426	0.426	0.426	0.426

* SD and RO denote spray drift and runoff buffer

Table CP 9.2.5- 13: Spring oilseed rape: Maximum PEC$_{sed}$ values for thiacloprid at Step 4 after single and multiple applications

		Thiacloprid							
		Oilseed rape (spring), 2 × 72 g a.s./ha							
		Single application				Multiple application			
Buffer Width & Type	Scenario	PEC$_{sed}$ [µg/kg]) Drift Reduction				PEC$_{sed}$ [µg/kg] Drift Reduction			
		0%	50%	75%	90%	0%	50%	75%	90%
5m SD	D1 (ditch)	0.279	0.144	0.074	0.031	0.439	0.226	0.117	0.048
	D1 (stream)	0.075	0.038	0.019	0.008	0.084	0.043	0.022	0.009
	D3 (ditch)	0.075	0.038	0.020	0.008	0.091	0.047	0.024	0.010
	D4 (pond)	0.040	0.021	0.011	0.005	0.063	0.033	0.017	0.007
	D4 (stream)	0.028	0.014	0.007	0.003	0.031	0.016	0.008	0.003
	D5 (pond)	0.047	0.024	0.013	0.005	0.072	0.037	0.020	0.008
	D5 (stream)	0.007	0.003	0.002	<0.001	0.009	0.005	0.002	<0.001
	R1 (pond)	0.114	0.096	0.087	0.082	0.170	0.142	0.128	0.119
	R1 (stream)	0.501	0.499	0.498	0.497	0.629	0.626	0.624	0.624

* SD and RO denote spray drift and runoff buffer

Table CP 9.2.5- 14: Winter oilseed rape: Maximum PEC_{sw} values for thiacloprid at Step 4 after single and multiple applications

		Thiacloprid							
		Oilseed rape (winter), 2 × 72 g a.s./ha							
		Single application				Multiple application			
Buffer Width & Type	Scenario	PEC_{sw} [µg/L]) Drift Reduction				PEC_{sw} [µg/L] Drift Reduction			
		0%	50%	75%	90%	0%	50%	75%	90%
5m SD	D2 (ditch)	0.125	0.063	0.031	0.013	0.107	0.053	0.027	0.011
	D2 (stream)	0.150	0.075	0.038	0.015	0.126	0.063	0.031	0.013
	D3 (ditch)	0.124	0.062	0.031	0.013	0.104	0.052	0.026	0.010
	D4 (pond)	0.014	0.007	0.003	0.001	0.018	0.009	0.005	0.002
	D4 (stream)	0.143	0.072	0.036	0.014	0.121	0.060	0.030	0.012
	D5 (pond)	0.014	0.007	0.003	0.001	0.017	0.009	0.004	0.002
	D5 (stream)	0.148	0.074	0.037	0.015	0.130	0.065	0.032	0.013
	R1 (pond)	0.014	0.012	0.011	0.010	0.045	0.040	0.038	0.037
	R1 (stream)	0.138	0.138	0.138	0.138	0.501	0.501	0.501	0.501
	R3 (stream)	0.362	0.362	0.362	0.362	0.362	0.362	0.362	0.362

* SD and RO denote spray drift and runoff buffer

Table CP 9.2.5- 15: Winter oilseed rape: Maximum PEC_{sed} values for thiacloprid at Step 4 after single and multiple applications

		Thiacloprid							
		Oilseed rape (winter), 2 × 72 g a.s./ha							
		Single application				Multiple application			
Buffer Width & Type	Scenario	PEC_{sed} [µg/kg]) Drift Reduction				PEC_{sed} [µg/kg] Drift Reduction			
		0%	50%	75%	90%	0%	50%	75%	90%
5m SD	D2 (ditch)	0.234	0.121	0.062	0.026	0.323	0.166	0.087	0.036
	D2 (stream)	0.277	0.143	0.074	0.031	0.369	0.191	0.098	0.041
	D3 (ditch)	0.085	0.044	0.022	0.009	0.097	0.050	0.026	0.011
	D4 (pond)	0.045	0.023	0.012	0.005	0.070	0.036	0.019	0.008
	D4 (stream)	0.024	0.012	0.006	0.002	0.030	0.015	0.008	0.003
	D5 (pond)	0.048	0.025	0.013	0.006	0.074	0.038	0.020	0.008
	D5 (stream)	0.013	0.006	0.003	0.001	0.033	0.017	0.008	0.003
	R1 (pond)	0.083	0.063	0.053	0.047	0.206	0.175	0.160	0.151
	R1 (stream)	0.108	0.107	0.106	0.106	0.382	0.380	0.379	0.378
	R3 (stream)	0.440	0.434	0.432	0.430	0.438	0.434	0.431	0.430

* SD and RO denote spray drift and runoff buffer

CP 9.3 Fate and behaviour in air

For information on the fate and behaviour in air please refer to MCA Section 7, data 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, data points 7.3.1 and 7.3.2.

Due to the low volatility and short half-life in air no PEC calculations are required.

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. Therefore no further estimations are considered necessary.