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Document Title

Summary of the fate and behaviour in the environment Diflufenican+Flufenacet SC600 (200+400)G

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

2014-03-17

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Version history

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

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Table of Contents

Section 9 - Fate and behaviour in the environment

Introduction

The representative formulation FFA WG 60 submitted in the first Annex I listing process is no longer considered to be the representative formulation. The new representative formulation used for the submission of the renewal of the Annex I listing of flufenacet is a mixture formulation of flufenacet and diflufenican, Flufenacet + Diflufenican SC 600 (DFF+FFA SC600, Herold SC 600).

For the second active substance in the representative formulation, diflufenican, please refer to the EFSA Scientific Report (2007) 122. This evaluation was done under the Council Directive 91/414/EEC addressing the respective data requirements. With the present dossier only flufenacet is under evaluation and not the mixing partner diflufenican. Hence calucaltion of the predicted environmental concentrations (PEC) in soil, surface and groundwater presented in this dossier are only performed for flufenacet and not for the mixing partner diflufenican.

Intended application pattern

The formulation is intended for use as a herbicide in winter cereals. The critical use pattern for this formulation is summarised as follows.

Table 9- 1: Intended application pattern

Crop	Timing of application (range)	Number of applications	Application interval [days]	Maximum label rate (range) [L/ha]	Maximum application rate, individual treatment (ranges) [g/ha]	
					Diflufenican	Flufenacet
Cereals	10-13	1	-	0.6	120	240
Cereals	11-13	1	-	0.4	80	160
Cereals	00-22	1	-	0.3	60	120

Product density according to Section 1, point 2, MCP 2.6.1: 1.251g/mL at 20°C

Definition of the residue for risk assessment for flufenacet

Due to changes in triggers for metabolites to be further assessed as well as due to new studies on the route of degradation in various environmental compartments, additional metabolites are proposed to be included in the residue definition for the risk assessment (see Table 9-1). Accordingly, predicted environmental concentrations (PEC) of these metabolites for the relevant environmental compartment were prepared.

Justification for the residue definition for risk assessment is provided in MCA Sec.7, Point 7.4.1 and MCA Sec. 6, Point 6.7.1.

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

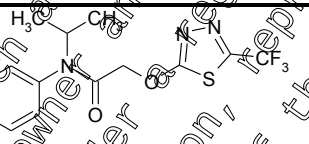
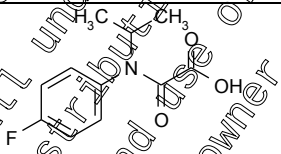
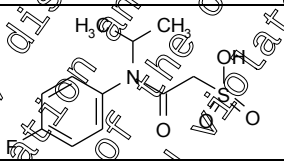
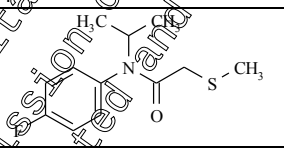
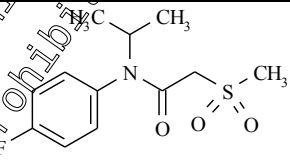
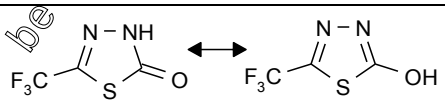
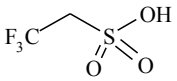
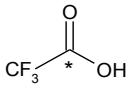
Compartment	Residue Definition for Risk Assessment
Soil	flufenacet, FOE oxalate, FOE sulfonic acid, FOE methylsulfone, FOE-thiadone, FOE 5043-trifluoroethanesulfonic acid and trifluoroacic acid
Groundwater	Same as for soil
Surface water	Same as for soil plus FOE methylsulone
Sediment	flufenacet
Air	flufenacet

In addition, a list of metabolites, which contains the structures, the synonyms and code numbers attributed to the compound flufenacet is presented in Document N3 of this dossier.

Compounds addressed in this document

In addition to the active substance flufenacet, the following metabolites summarised in the table below were addressed in this document as they were considered major in environmental fate studies.

Table 9- 3: Active substance and metabolites addressed in this document

Compound / Codes	Chemical Structure	Considered for
flufenacet (FOE 5043) a.s.		PEC_{soil} PEC_{gw} PEC_{sw} & PEC_{sed}
FOE oxalate M01		PEC_{soil} PEC_{gw} PEC_{sw}
FOE sulfonic acid M02		PEC_{soil} PEC_{gw} PEC_{sw}
FOE methylsulfide M05		PEC_{sw}
FOE methylsulfone M07		PEC_{soil} PEC_{gw} PEC_{sw}
FOE-thiadone M09		PEC_{soil} PEC_{gw} PEC_{sw}
FOE-5043-trifluoroethanesulfonic acid M44		PEC_{soil} PEC_{gw} PEC_{sw}
trifluoroacetic acid M45		PEC_{soil} PEC_{gw} PEC_{sw}

9.1 - Fate and behaviour in soil

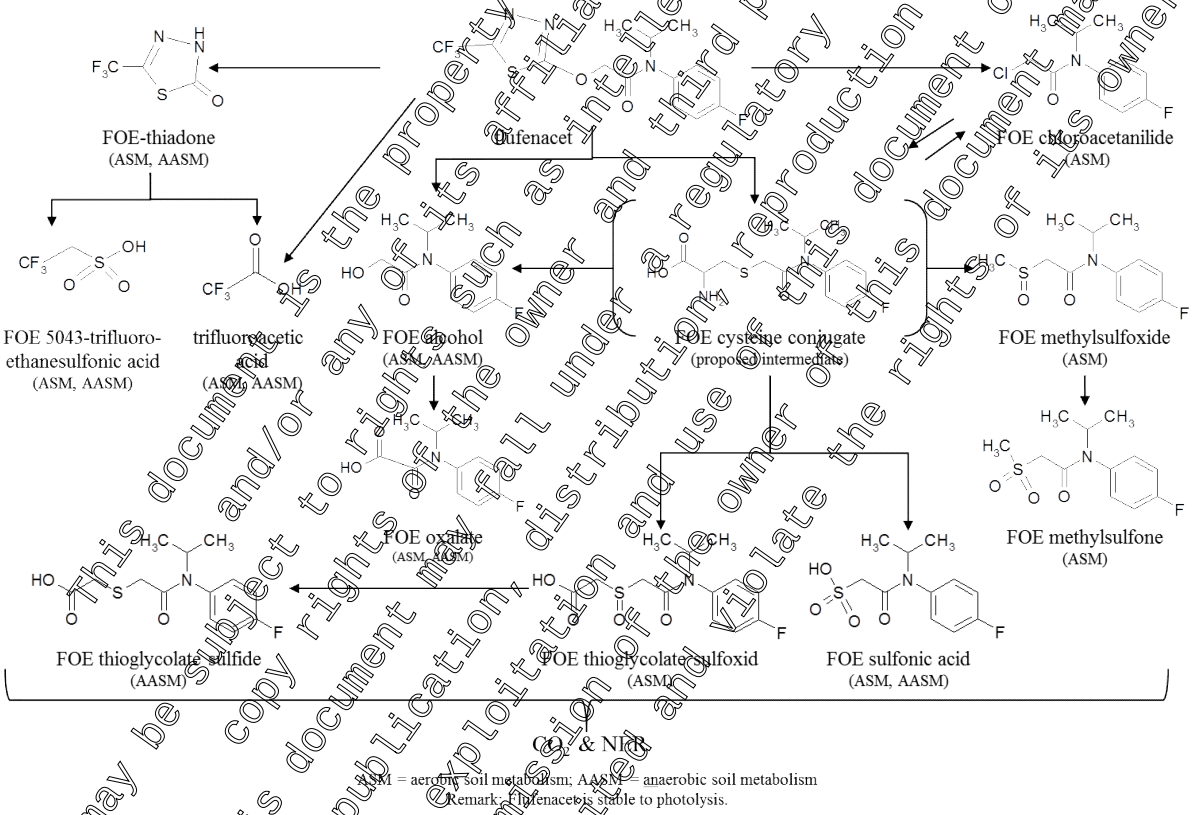
Information of this and the following sections (CP 9.1.1 and CP 9.1.2) are already given in the MCA. Please refer to the corresponding section in the MCA.

9.1.1 - Rate of degradation in soil

The proposed degradation pathway of flufenacet in soil is shown in below.

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

Proposed degradation pathway of flufeancet



9.1.1.1 - Laboratory studies

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

9.1.1.2 - Field studies

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

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.

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.

9.1.2 - Mobility in the soil

For information on mobility studies please refer to MCA Section 7, points 7.1.3 and 7.1.4.

9.1.2.1 - Laboratory studies

For information on laboratory studies please refer to MCA Section 7, points 7.1.3 and 7.1.4.1.

9.1.2.2 - Lysimeter studies

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

9.1.2.3 - Field leaching studies

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

9.1.3 - Estimation of concentrations in soil

PEC_{soil} modelling approach

The predicted environmental concentration in soil (PEC_{soil}) for the active substance flufenacet and its metabolites were calculated based on simple first tier approach (Microsoft® Excel spreadsheet) an assuming even distribution in the upper 0-5 cm soil layer. A standard soil density of 1.5 g/cm^3 was assumed. Crop interception will reduce the amound of the 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 papter (FOCUS 2002) for cereals (see 8.2.4 for details).

Derivation of kinetic modelling input values for flufenacet and its major degradation products is presented in the MCA Section 7.

Endpoints for PEC_{soil}

Table 9.1.3- 1: Modelling input parameters for flufenacet

End-Point	Flufenacet and metabolites
	Values used for modelling
Flufenacet	
Molecular mass [g/mol]	363.3
DT_{50} soil [days]	32.2
FOE sulfonic acid	
Molecular mass [g/mol]	275.3
DT_{50} soil [days]	258.4
Maximum occurrence in soil [%]	26.3
FOE oxalate	
Molecular mass [g/mol]	225.2
DT_{50} soil [days]	20.7
Maximum occurrence in soil [%]	26.5
FOE methylsulfone	
Molecular mass [g/mol]	273.3
DT_{50} soil [days]	163.0
Maximum occurrence in soil [%]	6.6
FOE-thiadone	
Molecular mass [g/mol]	170.1
DT_{50} soil [days]	2.9
Maximum occurrence in soil [%]	5.9
FOE 5043-trifluoroethanesulfonic acid	
Molecular mass [g/mol]	164.1
DT_{50} soil [days]	22.5
Maximum occurrence in soil [%]	6.0
trifluoroacetic acid	
Molecular mass [g/mol]	114.0
DT_{50} soil [days]	1000
Maximum occurrence in soil [%]	81.5

[a] All DT_{50} values represent a worst-case value based on laboratory studies, non-normalised
[b] All max. occurrence values are based on laboratory studies, aerobic soil

PEC_{soil} for flufenacet and its metabolites

Flufenacet and its metabolites FOE sulfonic acid, FOE oxalate, FOE methylsulfone, FOE-thiadone, FOE 5043-trifluoroethanesulfonic acid and trifluoroacetic acid were considered in this assessment.

Report:	**KCP 9.1.3 / 01, [redacted], G., [redacted], A.; 2014**
Title:	Flufenacet (FOE 5043) and metabolites: PEC_{soil} EUR - Autumn use in winter cereals in Europe
Document No:	M-478933-01-1
Guidelines:	EU Commission, 1995: Directive 95/36/EC, amending 91/414/EEC EU Commission, 2000: Guidance Document on Persistence in Soil (Working Document) 9188/VI/97 rev 8. FOCUS, 1997: Soil persistence models and EU registration. Final report of the work off the Soil Modelling Work group of FOCUS FOCUS, 2002: Generic Guidance for FOCUS Groundwater Scenarios, Ver 1.1
GLP:	No (calculation)

Methods and Materials:

The predicted environmental concentrations in soil (PEC_{soil}) of flufenacet and its metabolites were estimated using a simple first tier approach (Excel sheet). A bulk density of 1.5 kg/L and a soil mixing depth of 5 cm were used. Crop interception data which correspond to the intended growth stages were taken from the FOCUS groundwater guidance paper (FOCUS 2002). Detailed application data used for simulation of PEC_{soil} were compiled in Table 9.1.3- 2.

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

Individual Crop	FOCUS Crop Used for Interception	Application				Amount Reaching the Soil
		Rate per Season	Interval	Plant Interception	BBCH Stage	
		[g a.s. /ha]	[days]	[%]		[g a.s./ha]
Winter cereals, GAP	-	1 × 240	-	-	10-13	-
Winter cereals, Simulation	Winter cereals	1 × 240	-	25	10-13	1 × 180
Winter cereals, GAP	-	1 × 160	-	-	11-13	-
Winter cereals, Simulation	Winter cereals	1 × 160	-	25	11-13	1 × 120
Winter cereals, GAP	-	1 × 120	-	-	0-22	-
Winter cereals, Simulation	Winter cereals	1 × 120	-	0	0-22	1 × 120

Substance Specific Parameters:

PEC_{soil} calculations were based on the maximum DT_{50} of laboratory studies; normalized to 20 °C and 100 % field capacity according to FOCUS (2000). Further compound specific input parameters are summarized below.

Table 9.1.3- 3: Input parameters of flufenacet and its metabolites for PEC_{soil}

Compound	DT_{50} [1)] [days]	Max. occur. in soil [%]	Molar mass [g/mol]	Molar mass correction factor
Flufenacet	42.1	100	363.3	1
FOE sulfonic acid	258.4	26.3	275.3	0.7578
FOE oxalate	21.1	26.5	225.2	0.6199
FOE methylsulfone	163	6.6	273.3	0.7523
FOE-thiadone	2.9	5.9	170.1	0.4682
FOE 5043-trifluoroethanesulfonic acid	22.5	6	164.1	0.4517
trifluoroacetic acid	1000	81.5	114	0.3138

1) Maximum DT_{50} of laboratory studies; normalized to 20°C and 100 % field capacity, for details please refer to CA 7.1.2.1

Findings:

The maximum PEC_{soil} values for flufenacet and its metabolites are summarised in the following tables. The maximum, short-term and long-term PEC_{soil} values and the time weighted average values ($TWAC_{soil}$) are provided thereafter. Since the PEC values for winter cereals at rates 1 × 160 g a.s./ha and 1 × 120 g a.s./ha with 25 % and 0 % interception respectively are identical, these two uses are presented together.

Table 9.1.3- 4: Maximum PEC_{soil} of flufenacet and its metabolites for the uses assessed

	Winter cereals	
Use pattern	1 × 240 g a.s./ha, 25 % interception [mg/kg]	1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception [mg/kg]
Flufenacet	0.240	0.160
FOE sulfonic acid	0.048	0.032
FOE oxalate	0.039	0.026
FOE methylsulfone	0.012	0.008
FOE-thiadone	0.007	0.004
FOE 5043-trifluoroethanesulfonic acid	0.007	0.004
trifluoroacetic acid	0.061	0.041

Table 9.1.3- 5: Winter cereals: PEC_{soil} (actual) and $TWAC_{soil}$ of flufenacet

		Flufenacet			
		Winter cereals			
		1 × 240 g a.s./ha, 25 % interception		1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception	
	Time [days]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]
Initial	0	0.240	---	0.160	---
Short term	1	0.236	0.238	0.157	0.159
	2	0.236	0.238	0.157	0.159
	4	0.225	0.232	0.150	0.155
Long term	7	0.214	0.227	0.143	0.151
	14	0.191	0.214	0.127	0.143
	21	0.170	0.203	0.113	0.135
	28	0.151	0.192	0.101	0.128
	42	0.120	0.173	0.080	0.115
	50	0.105	0.164	0.070	0.109
	100	0.046	0.118	0.031	0.078

Table 9.1.3- 6: Winter cereals: PEC_{soil} (actual) and $TWAC_{soil}$ of FOE sulfonic acid

	Time [days]	FOE sulfonic acid			
		Winter cereals			
		1 × 240 g a.s./ha, 25 % interception		1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception	
		PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]
Initial	0	0.048	---	0.032	---
Short term	1	0.048	0.048	0.032	0.032
	2	0.048	0.048	0.032	0.032
	4	0.047	0.048	0.032	0.032
Long term	7	0.047	0.047	0.031	0.032
	14	0.046	0.047	0.031	0.031
	21	0.045	0.047	0.030	0.031
	28	0.044	0.046	0.030	0.031
	42	0.043	0.045	0.028	0.030
	50	0.042	0.045	0.028	0.030
	100	0.037	0.042	0.024	0.028

Table 9.1.3- 7: Winter cereals: PEC_{soil} (actual) and $TWAC_{soil}$ of FOE oxalate

	Time [days]	FOE oxalate			
		Winter cereals			
		1 × 240 g a.s./ha, 25 % interception		1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception	
		PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]
Initial	0	0.039	---	0.026	---
Short term	1	0.038	0.039	0.025	0.026
	2	0.037	0.038	0.025	0.025
	4	0.035	0.037	0.023	0.025
Long term	7	0.031	0.035	0.021	0.023
	14	0.025	0.032	0.017	0.021
	21	0.020	0.028	0.013	0.019
	28	0.016	0.026	0.010	0.017
	42	0.010	0.021	0.007	0.014
	50	0.008	0.019	0.005	0.013
	100	0.001	0.012	<0.001	0.008

Table 9.1.3- 8: Winter cereals: PEC_{soil} (actual) and $TWAC_{soil}$ of FOE methylsulfone

	Time [days]	FOE methylsulfone			
		Winter cereals			
		1 × 240 g a.s./ha, 25 % interception		1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception	
		PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]
Initial	0	0.012	---	0.008	---
Short term	1	0.012	0.012	0.008	0.008
	2	0.012	0.012	0.008	0.008
	4	0.012	0.012	0.008	0.008
Long term	7	0.012	0.012	0.008	0.008
	14	0.011	0.012	0.007	0.008
	21	0.011	0.011	0.007	0.008
	28	0.011	0.011	0.007	0.007
	42	0.010	0.011	0.007	0.007
	50	0.010	0.011	0.006	0.007
	100	0.008	0.010	0.005	0.006

Table 9.1.3- 9: Winter cereals: PEC_{soil} (actual) and $TWAC_{soil}$ of FOE-thiadone

	Time [days]	FOE-thiadone			
		Winter cereals			
		1 × 240 g a.s./ha, 25 % interception		1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception	
		PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]
Initial	0	0.007	---	0.004	---
Short term	1	0.005	0.006	0.003	0.004
	2	0.004	0.005	0.003	0.004
	4	0.003	0.004	0.002	0.003
Long term	7	0.001	0.003	<0.001	0.002
	14	<0.001	0.002	<0.001	0.001
	21	<0.001	0.001	<0.001	<0.001
	28	<0.001	<0.001	<0.001	<0.001
	42	<0.001	<0.001	<0.001	<0.001
	50	<0.001	<0.001	<0.001	<0.001
	100	<0.001	<0.001	<0.001	<0.001

Table 9.1.3- 10: Winter cereals: PEC_{soil} (actual) and $TWAC_{soil}$ of FOE 5043-trifluoroethanesulfonic acid

	Time [days]	FOE 5043-trifluoroethanesulfonic acid			
		Winter cereals			
		1 × 240 g a.s./ha, 25 % interception		1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception	
		PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]
Initial	0	0.007	---	0.004	---
Short term	1	0.006	0.006	0.004	0.004
	2	0.006	0.006	0.004	0.004
	4	0.006	0.006	0.004	0.004
Long term	7	0.005	0.006	0.003	0.004
	14	0.004	0.005	0.003	0.004
	21	0.003	0.005	0.002	0.003
	28	0.003	0.004	0.002	0.003
	42	0.002	0.004	0.001	0.002
	50	0.001	0.003	<0.001	0.002
	100	<0.001	0.002	<0.001	0.001

Table 9.1.3- 11: Winter cereals: PEC_{soil} (actual) and $TWAC_{soil}$ of trifluoroacetic acid

	Time [days]	trifluoroacetic acid			
		Winter cereals			
		1 × 240 g a.s./ha, 25 % interception		1 × 160 g a.s./ha, 25 % interception 1 × 120 g a.s./ha, 0 % interception	
		PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]	PEC_{soil} [mg/kg]	$TWAC_{soil}$ [mg/kg]
Initial	0	0.061	---	0.041	---
Short term	1	0.061	0.061	0.041	0.041
	2	0.061	0.061	0.041	0.041
	4	0.061	0.061	0.041	0.041
Long term	7	0.061	0.061	0.041	0.041
	14	0.061	0.061	0.041	0.041
	21	0.060	0.061	0.040	0.041
	28	0.060	0.061	0.040	0.041
	42	0.060	0.060	0.040	0.040
	50	0.059	0.060	0.040	0.040
	100	0.057	0.059	0.038	0.040

Potential accumulation in soil:

The accumulation potential after long term use for all substances with DT_{50} longer than 90 days, metabolites FOE sulfonic acid, FOE methylsulfone and trifluoroacetic acid, was assessed. The results for a standard mixing depth of 5 cm and non-standard mixing depth of 20 cm are presented in the following tables.

Table 9.1.3- 12: PEC_{soil} of flufenacet metabolites for the uses assessed, taking the effect of accumulation into account (standard mixing depth of 5 cm)

Use Pattern	PEC_{soil}	FOE sulfonic acid [mg/kg]	FOE methylsulfone [mg/kg]	Trifluoroacetic acid [mg/kg]
Winter cereals 1 × 240 g a.s./ha	plateau	0.029	0.003	0.213
	total*	0.077	0.015	0.275
Winter cereals 1 × 160 g a.s./ha 1 × 120 g a.s./ha	plateau	0.019	0.002	0.142
	total*	0.051	0.010	0.183

* total = plateau (background concentration after multi-year use) + max. PEC_{soil} (see Table 9.1.3- 4)

Table 9.1.3- 13: PEC_{soil} of flufenacet metabolites for the uses assessed, taking the effect of accumulation into account (non-standard mixing depth of 20 cm)

Use Pattern	PEC_{soil}	FOE sulfonic acid [mg/kg]	FOE methylsulfone [mg/kg]	Trifluoroacetic acid [mg/kg]
Winter cereals 1 × 240 g a.s./ha	plateau	0.007	< 0.001	0.053
	total*	0.055	0.013	0.115
Winter cereals 1 × 160 g a.s./ha 1 × 120 g a.s./ha	plateau	0.005	< 0.001	0.036
	total*	0.037	0.008	0.076

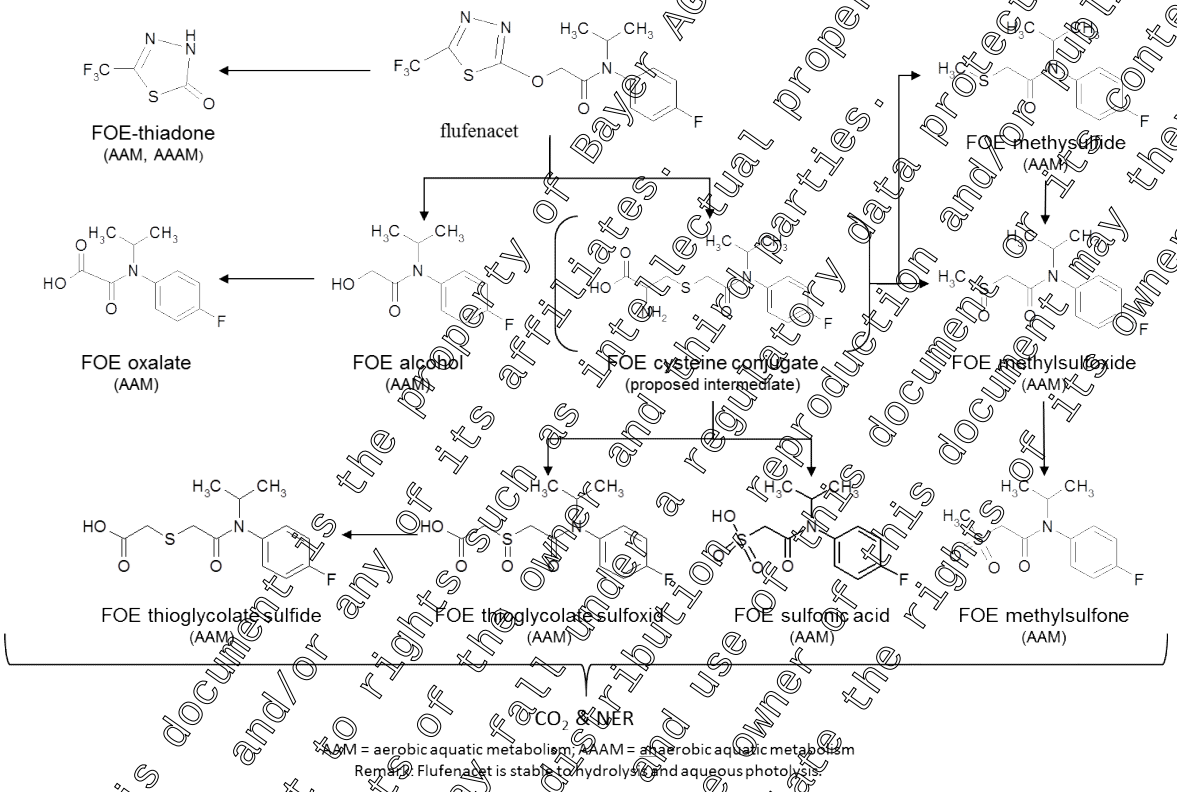
* total = plateau (background concentration after multi-year use) + max. PEC_{soil} (see Table 9.1.3- 4)

9.2 - Fate and behaviour in water and sediment

The proposed degradation pathway of flufenacet in water and sediment is shown below.

For information on the fate and behavior in water and sediment please refer to the MCA Section 7.

Proposed degradation pathway of flufenacet in aquatic systems



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.

9.2.2 - Water/sediment study

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

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.

9.2.4 - Estimation of concentrations in groundwater

Endpoints for PEC_{gw}

Table 9.2.4- 1: Modelling input parameters for flufenacet

End-Point	Flufenacet and metabolites Values used for modelling
Flufenacet	
Aqueous solubility [mg/L]	56 (at pH 7)
Vapour pressure [Pa]	9×10^{-5}
DT_{50} soil [days]	18.5 [a)]
K_{oc}/K_{om} [L/kg]	215 / 125 [b)]
1/n	0.916 [b)]
FOE sulfonic acid	
Aqueous solubility [mg/L] at 20 °C	55000 (at pH4-9)
Vapour pressure [Pa] at 25 °C	1.6×10^{-7}
DT_{50} soil [days]	20.5 c)
K_{oc}/K_{om} [L/kg]	10.3 / 6.3 [b)]
1/n	1.04 [b)]
Formation fraction	0.192 (from flufenacet)
FOE oxalate	
Aqueous solubility [mg/L] at 20 °C	>120000 (at pH 5)
Vapour pressure [Pa] at 20 °C	4.5×10^{-7}
DT_{50} soil [days]	13.7 [a)]
K_{oc}/K_{om} [L/kg]	11.0/ 6.0 [b)]
1/n	0.91 [b)]
Formation fraction	0.414 (from flufenacet)
FOE methylsulfone	
Aqueous solubility [mg/L] at 20 °C	4100
Vapour pressure [Pa] at 20 °C	8.6×10^{-4}
DT_{50} soil [days]	87.7 [a)]
K_{oc}/K_{om} [L/kg]	74.1 / 43.0 [b)]
1/n	0.89 [b)]
Formation fraction	0.066 (from flufenacet)
FOE-thiadone	
Aqueous solubility [mg/L] at 20 °C	30000 (at pH 3)
Vapour pressure [Pa] at 20 °C	2.05
DT_{50} soil [days]	1.6 [a)]
K_{oc}/K_{om} [L/kg]	43.7 / 25.3 [b)]
1/n	0.76 [b)]
Formation fraction	0.570 (from flufenacet)
FOE 5043-trifluoroethanesulfonic acid	
Aqueous solubility [mg/L] at 20 °C	>160000 (at pH 5-7)
Vapour pressure [Pa] at 20 °C	$<1.0 \times 10^{-8}$
DT_{50} soil [days]	9.1 [a)]
K_{oc}/K_{om} [L/kg]	0 (worst case) [d)]
1/n	1.0 (worst case) [d)]
Formation fraction	0.469 (from thiadone)
trifluoroacetic acid	

End-Point	Flufenacet and metabolites
	Values used for modelling
Aqueous solubility [mg/L] at 20 °C	>500000 (at pH 0.4 – 12.6)
Vapour pressure [Pa] at 20 °C	$<1.0 \times 10^{-6}$
DT_{50} soil [days]	1000 (worst case) [e]
K_{oc}/K_{om} [L/kg]	0 (worst case) [d]
1/n	1.0 (worst case) [d]
Formation fraction	0.430 (from flufenacet) / 0.531 (from FOE-thiadone)

[a] Geometric mean based on aerobic soil laboratory studies, normalized to 20°C and 100 % field capacity
[b] Arithmetic mean based on aerobic soil laboratory studies
[c] Median based on field studies, normalized to 20°C and 100 % field capacity
[d] Only low to virtually no adsorption could be determined in laboratory studies, therefore a K_{oc} = 0 together with a Freundlich exponent of 1.0 were used for the simulations to address worst case conditions.
[e] No reliable DT_{50} could be obtained from aerobic soil laboratory studies, therefore a default value of 1000 days was used as worst case assumption in the simulation runs.

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 6 years are intended as a so called 'warm up' period. The following years are taken into account for the assessment of the potential leaching behaviour. 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	Crop stage Interception [%]				
	Bare – emergence	Leaf development	Stem elongation	Flowering	Senescence Ripening
	BBCH#				
	00 - 09	10 - 19	20 - 39	40 - 89	90 - 99
Winter cereals	0	25	50/70*	90	90

* tillering/elongation; BBCH code of 20-29 for tillering and 30-39 for elongation

9.2.4.1 - Calculation of concentrations in groundwater

PEC_{gw} for flufenacet and metabolites

In the PEC_{gw} calculations flufenacet and its metabolites FOE sulfonic acid, FOE oxalate, FOE methylsulfone, FOE-thiadone, FOE 5043-trifluoroethanesulfonic acid and trifluoroacetic acid were assessed.

For metabolites exceeding the groundwater trigger of 0.1 µg/L their relevance according to the EU Guidance Document (SANCO/221/2000 rev 10, 25 February 2003) is addressed in the Document N4 "Relevance of metabolties in groundwater for flufenacet" submitted together with this dossier.

Report:	**KCP 9.2.4.1 / 01, [redacted], G., [redacted], A.; 2014**
Title:	Flufenacet (FOE 5043) and metabolites: PEC_{gw} FOCUS PEARL, PELMO EUR - Autumn use in winter cereals in Europe
Document No:	M-478934-01-1
Guidelines:	FOCUS 2000: SANCO/321/2000 rev.2 FOCUS 2009: SANCO/13144/2010 v. 1 FOCUS 2012, Generic Guidance for FOCUS Groundwater Assessments. v. 2.1
GLP:	No (calculation)

Materials and Methods: The predicted environmental concentrations in groundwater (PEC_{gw}) for flufenacet and its metabolites were calculated using the simulation model 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
		Rate per Season	Interval	Plant Interception	BBCH Stage	
		[g a.s. /ha]	[days]	[%]		[g a.s./ha]
Winter cereals, GAP	-	1 × 240	-	-	10-13	-
Winter cereals, Simulation	Winter cereals	1 × 240	-	25	10-13	1 × 180
Winter cereals, GAP	-	1 × 160	-	-	11-13	-
Winter cereals, Simulation	Winter cereals	1 × 160	-	25	11-13	1 × 120
Winter cereals, GAP	-	1 × 120	-	-	0-22	-
Winter cereals, Simulation	Winter cereals	1 × 120	-	0	0-22	1 × 120

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 (2009). Crop interception was taken into account according to the BBCH growth stage as recommended by FOCUS (2012).

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

Individual crop	Winter cereals 1 × 240 g a.s./ha BBCH 10-13	Winter cereals 1 × 160 g a.s./ha BBCH 11-13	Winter cereals 1 × 120 g a.s./ha BBCH 0-22
Repeat Interval for App. Events	Every Year	Every Year	Every Year
Application Technique	Spray	Spray	Spray
Absolute / Relative to	Emergence	Emergence	Emergence
Scenario	1st App. Date (Julian day) Offset	1st App. Date (Julian day) Offset	1st App. Date (Julian day) Offset
Chateaudun	27 Oct (300) 1	28 Oct (301) 2	16 Oct (289) -10
Hamburg	02 Nov (306) 1	03 Nov (307) 2	22 Oct (295) -10
Jokioinen	21 Sep (264) 1	22 Sep (265) 2	10 Sep (253) -10
Kremsmuenster	06 Nov (310) 1	07 Nov (311) 2	26 Oct (299) -10
Okehampton	18 Oct (291) 1	19 Oct (292) 2	07 Oct (280) -10
Piacenza	02 Dec (336) 1	03 Dec (337) 2	21 Nov (325) -10
Porto	01 Dec (335) 1	02 Dec (336) 2	20 Nov (324) -10
Sevilla	01 Dec (335) 1	02 Dec (336) 2	20 Nov (324) -10
Thiva	01 Dec (335) 1	02 Dec (336) 2	20 Nov (324) -10

Further input parameters for PEC_{gw} modelling of flufenacet and its metabolites are summarised in the following tables.

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

Parameter	Unit	Fufenacet	FOE sulfonic acid	FOE oxalate	FOE methylsulfone
Molar mass	[g/mol]	363.3	275.3	225.2	273.3
Water solubility	[mg/L]	56.0	55000	120000	4100
Vapour pressure	[Pa]	9.00E-05	1.60E-07	4.50E-07	8.60E-04
Freundlich exponent	[-]	0.916	1.040	0.910	0.890
Plant uptake factor	[-]	0.50	0.46	0.50	1.00
Walker exponent	[-]	0.7	0.7	0.7	0.7
PEARL Parameters					
Substance Code	[-]	FFA	FOESA	FOEOX	FOEMS
DT_{50} soil	[days]	18.3	20.5	13.7	67.7
Molar activ. energy	[J/mol]	65400	65400	65400	65400
K_{om}	[mL/g]	125.0	6.3	6.0	43.0
Formation fraction	[-]	-	0.192	0.414	0.066
PELMO Parameters (run 1)					
Substance code		AS	A1	B1	C
Rate constant	[1/day]	0.03788	0.03381	0.05059	0.01024
Q_{10}	[-]	2.58	2.58	2.58	2.58
K_{oc}	[mL/g	215.0	10.3	11.0	74.1

Parameter	Unit	FOE-thiadone	FOE 5043-trifluoroethane sulfonic acid	Trifluoro acetic acid
Molar mass	[g/mol]	170.1	164.1	114.0
Water solubility	[mg/L]	30000	160000	500000
Vapour pressure	[Pa]	2.05	1.00E-08	1.00E-06
Freundlich exponent	[-]	0.760	1.000	1.000
Plant uptake factor	[-]	0.50	1.00	0.59
Walker exponent	[-]	0.7	0.7	0.7
PEARL Parameters				
Substance code	[-]	FOETH	TFESA	TFA
DT_{50} soil	[days]	1.6	9.1	1000.0
Molar activ. energy	[J/mol]	65.4	65.4	65.4
K_{om}	[mL/g]	25.3	0.0	0.0
Formation fraction	[-]	0.570	0.469	0.43 [a] / 0.531 [b]
PELMO Parameters (run 2)				
Substance code	[-]	A1	A2	B1
Rate constant	[1/day]	0.43322	0.07617	0.00069
Q_{10}	[-]	2.58	2.58	2.58
K_{oc}	[mL/g	43.7	0.0	0.0

[a] from flufenacet
[b] from FOE-thiadone

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

Degradation fraction from → to (FOCUS PEARL)	0.192 FFA -> FOESA 0.414 FFA -> FOEOX 0.066 FFA -> FOEMS 0.570 FFA -> FOETH 0.430 FFA -> TFA 0.469 FOETH -> TFESA 0.531 FOETH -> TFA
Degradation rate from → to (FOCUS PELMO) (run1)	0.0072720 Active Substance -> A1 0.0156810 Active Substance -> B1 0.0025000 Active Substance -> C1 0.0124240 Active Substance -> <BR/CO$_2$ 0.0338120 A1 -> <BR/CO$_2$ 0.0505950 B1 -> <BR/CO$_2$ 0.0102390 C1 -> <BR/CO$_2$
Degradation rate from → to (FOCUS PELMO) (run2)	0.0215900 Active Substance -> A1 0.0162870 Active Substance -> B1 0.2300380 A1 -> B1 0.2031790 A1 -> A2 0.0006930 B1 -> <BR/CO$_2$ 0.0761700 A2 -> <BR/CO$_2$

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

Table 9.2.4.1- 5: Winter cereals: PEC_{gw} (PEARL and PELMO) of flufenacet and its metabolites

	Winter cereals, 1 × 240 g a.s./ha, BBCH 10-13							
Scenario	**PEARL**	**PELMO**	**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]**	**PEC_{gw} [µg/L]**	**PEC_{gw} [µg/L]**
	Flufenacet		**FOE sulfonic acid**		**FOE oxalate**		**FOE methylsulfone**	
Châteaudun	<0.001	<0.001	0.398	0.256	0.107	0.055	0.012	0.005
Hamburg	<0.001	<0.001	1.230	1.193	0.619	0.661	0.066	0.056
Jokioinen	<0.001	<0.001	1.601	1.651	0.693	0.744	0.022	0.023
Kremsmuenster	<0.001	<0.001	0.625	0.538	0.264	0.209	0.042	0.033
Okehampton	<0.001	<0.001	1.153	1.152	0.750	0.766	0.070	0.060
Piacenza	<0.001	<0.001	0.393	0.466	0.155	0.222	0.033	0.027
Porto	<0.001	<0.001	0.733	1.141	0.476	0.778	0.036	0.047
Sevilla	<0.001	<0.001	0.017	0.063	0.001	0.017	<0.001	<0.001
Thiva	<0.001	<0.001	0.084	0.097	0.018	0.021	0.004	0.002
	FOE-thiadone		**FOE 5043-trifluoro-ethanesulfonic acid**		**Trifluoroacetic acid**			
Châteaudun	<0.001	<0.001	0.124	0.098	16.90	10.88		
Hamburg	<0.001	<0.001	0.596	0.705	10.71	7.254		
Jokioinen	<0.001	<0.001	1.303	1.303	15.76	10.20		
Kremsmuenster	<0.001	<0.001	0.142	0.157	8.388	6.354		
Okehampton	<0.001	<0.001	0.534	0.582	7.334	6.273		
Piacenza	<0.001	<0.001	0.088	0.228	10.40	6.932		
Porto	<0.001	<0.001	0.388	0.695	5.702	4.343		
Sevilla	<0.001	<0.001	0.001	0.035	7.084	6.891		
Thiva	<0.001	<0.001	0.014	0.037	15.18	9.408		

Table 9.2.4.1- 6: Winter cereals: PEC_{gw} (PEARL and PELMO) of flufenacet and its metabolites

FOCUS Scenario	Winter cereals, 1 × 160 g a.s./ha, BBCH 11-13							
	PEARL	PELMO	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]	PEC_{gw} [µg/L]	PEC_{gw} [µg/L]
	Flufenacet		FOE sulfonic acid		FOE oxalate		FOE methylsulfone	
Châteaudun	<0.001	<0.001	0.261	0.165	0.064	0.030	0.006	0.003
Hamburg	<0.001	<0.001	0.818	0.801	0.385	0.415	0.038	0.033
Jokioinen	<0.001	<0.001	1.074	1.115	0.429	0.467	0.012	0.013
Kremsmuenster	<0.001	<0.001	0.416	0.377	0.165	0.134	0.025	0.019
Okehampton	<0.001	<0.001	0.765	0.772	0.471	0.470	0.042	0.035
Piacenza	<0.001	<0.001	0.236	0.305	0.099	0.135	0.019	0.016
Porto	<0.001	<0.001	0.481	0.767	0.293	0.489	0.021	0.028
Sevilla	<0.001	<0.001	0.012	0.035	<0.001	0.008	<0.001	<0.001
Thiva	<0.001	<0.001	0.056	0.067	0.011	0.012	0.002	0.001
	FOE-thiadone		FOE 5043-trifluoro-ethanesulfonic acid		Trifluoroacetic acid			
Châteaudun	<0.001	<0.001	0.081	0.060	11.24	7.106		
Hamburg	<0.001	<0.001	0.391	0.471	7.133	4.886		
Jokioinen	<0.001	<0.001	0.854	0.852	10.46	6.756		
Kremsmuenster	<0.001	<0.001	0.093	0.101	5.592	4.291		
Okehampton	<0.001	<0.001	0.353	0.374	4.853	4.214		
Piacenza	<0.001	<0.001	0.057	0.148	6.920	4.368		
Porto	<0.001	<0.001	0.250	0.458	3.820	2.931		
Sevilla	<0.001	<0.001	<0.001	0.023	4.748	4.798		
Thiva	<0.001	<0.001	0.009	0.025	10.13	6.185		

Table 9.2.4.1- 7: Winter cereals: PEC_{gw} (PEARL and PELMO) of flufenacet and its metabolites

Scenario	Winter cereals, 1 × 120 g a.s./ha, BBCH 0-22							
	PEARL	PELMO	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]	PEC_{gw} [µg/L]	PEC_{gw} [µg/L]
	Flufenacet		FOE sulfonic acid		FOE oxalate		FOE methylsulfone	
Châteaudun	<0.001	<0.001	0.307	0.229	0.082	0.052	0.007	0.003
Hamburg	<0.001	<0.001	0.894	0.933	0.454	0.507	0.039	0.032
Jokioinen	<0.001	<0.001	1.152	1.201	0.459	0.513	0.012	0.013
Kremsmuenster	<0.001	<0.001	0.440	0.397	0.182	0.147	0.025	0.020
Okehampton	<0.001	<0.001	0.825	0.809	0.535	0.526	0.043	0.036
Piacenza	<0.001	<0.001	0.254	0.296	0.099	0.156	0.019	0.013
Porto	<0.001	<0.001	0.587	0.810	0.385	0.650	0.022	0.029
Sevilla	<0.001	<0.001	0.011	0.141	<0.001	0.045	<0.001	<0.001
Thiva	<0.001	<0.001	0.083	0.107	0.015	0.024	0.002	0.001
	FOE-thiadone		FOE 5043-trifluoro-ethanesulfonic acid		Trifluoroacetic acid			
Châteaudun	<0.001	<0.001	0.105	0.074	11.47	7.292		
Hamburg	<0.001	<0.001	0.474	0.569	7.280	5.373		
Jokioinen	<0.001	<0.001	0.979	0.898	11.11	6.970		
Kremsmuenster	<0.001	<0.001	0.108	0.119	5.608	4.210		
Okehampton	<0.001	<0.001	0.396	0.397	5.327	4.467		
Piacenza	<0.001	<0.001	0.079	0.144	7.013	4.915		
Porto	<0.001	<0.001	0.311	0.458	3.966	3.174		
Sevilla	<0.001	<0.001	0.001	0.073	5.030	3.762		
Thiva	<0.001	<0.001	0.016	0.039	10.47	6.829		

Conclusion: For flufenacet and the metabolites FOE methylsulfone and FOE-thiadone the predicted concentration in groundwater did not exceed 0.1 µg/L for any scenario.
For the metabolites FOE sulfonic acid, FOE oxalate, FOE 5043-trifluoroethanesulfonic acid and trifluoroacetic acid the concentration in groundwater did exceed 0.1 µg/L. This triggers the need to assess the relevance of these metabolites in groundwater.

9.2.4.2 - Additional field tests

No additional field testing was required.

9.2.5 - Estimation of concentrations in surface water and sediment

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.

Derivation of kinetic modelling input values are presented in MCA Section 7.

PEC_{sw} calculations

Endpoints for PEC_{sw}

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

End-Point	Flufenacet and metabolites Values used for modelling
Flufenacet	
Molecular mass [g/mol]	363.3
Aqueous solubility [mg/L] at 20 °C	56 (at pH 7)
Vapour pressure [Pa] at 20 °C	9×10^{-5}
DT_{50} soil [days]	18.3 [a)]
K_{oc}/ K_{om} [L/kg] (arithmetic mean)	215 / 125
1/n (arithmetic mean)	0.916
DT_{50} water [days]	49.6 [b)]
DT_{50} sediment [days]	1000 [c)]
FOE sulfonic acid	
Molecular mass [g/mol]	275.3
Aqueous solubility [mg/L] at 20 °C	55000(at pH 4-9)
DT_{50} soil [days]	20.3 [d)]
K_{oc}/K_{om} [L/kg] (arithmetic mean)	10.3 / 6.3
DT_{50} water [days]	1000 [c)]
DT_{50} sediment [days]	1000 [c)]
Maximum occurrence in soil [%]	26.3 [e)]
Maximum occurrence in water/sediment systems [%]	0 [f)]
Maximum occurrence in aquatic systems [%]	0 [f)]
FOE oxalate	
Molecular mass [g/mol]	225.2
Aqueous solubility [mg/L] at 20 °C	>120000 (at pH 5)
DT_{50} soil [days]	13.7 [a)]
K_{oc}/K_{om} [L/kg] (arithmetic mean)	11.0/ 6.0
DT_{50} water [days]	1000 [c)]
DT_{50} sediment [days]	1000 [c)]
Maximum occurrence in soil [%]	26.5 [e)]
Maximum occurrence in water/sediment systems [%]	0 [f)]
Maximum occurrence in aquatic systems [%]	0 [f)]
FOE methylsulfone	
Molecular mass [g/mol]	273.3
Aqueous solubility [mg/L] at 20 °C	4100
DT_{50} soil [days]	67.7 [a)]
K_{oc}/K_{om} [L/kg] (arithmetic mean)	74.1 / 43.0
DT_{50} water [days]	1000 [c)]
DT_{50} sediment [days]	1000 [c)]
Maximum occurrence in soil [%]	6.6 [e)]
Maximum occurrence in water/sediment systems [%]	0 [f)]
Maximum occurrence in aquatic systems [%]	0 [f)]
FOE methylsulfide	
Molecular mass [g/mol]	241.0
Aqueous solubility [mg/L] at 25 °C	113.3
DT_{50} soil [days]	1000 [c)]
K_{oc} [L/kg] (arithmetic mean)	850.5
DT_{50} water [days]	1000 [c)]
DT_{50} sediment [days]	1000 [c)]
Maximum occurrence in soil [%]	0 [g)]
Maximum occurrence in water/sediment systems [%]	11.4 [h)]
Maximum occurrence in aquatic systems [%]	8.0 [h)]

End-Point	Flufenacet and metabolites Values used for modelling
FOE-thiadone	
Molecular mass [g/mol]	170.1
Aqueous solubility [mg/L] at 20 °C	30000 (at pH 3)
DT_{50} soil [days]	1.6 [a]
K_{oc}/K_{om} [L/kg] (arithmetic mean)	43.7 / 25.3
DT_{50} water [days]	1000 [c]
DT_{50} sediment [days]	1000 [c]
Maximum occurrence in soil [%]	5.9 [e]
Maximum occurrence in water/sediment systems [%]	84.3 [h]
Maximum occurrence in aquatic systems [%]	81.8 [b]
FOE 5043-trifluoroethanesulfonic acid	
Molecular mass [g/mol]	164.1
Aqueous solubility [mg/L] at 20 °C	>160000 (at pH 5-7)
DT_{50} soil [days]	9.1 [a]
K_{oc}/K_{om} [L/kg]	0
DT_{50} water [days]	1000 [c]
DT_{50} sediment [days]	1000 [c]
Maximum occurrence in soil [%]	6.0
Maximum occurrence in water/sediment systems [%]	0 [f]
Maximum occurrence in aquatic systems [%]	0 [f]
Trifluoroacetic acid (M45)	
Molecular mass [g/mol]	114.0
Aqueous solubility [mg/L] at 20 °C	>500000 (at pH 0.4 - 12.6)
DT_{50} soil [days]	1000 [g]
K_{oc}/K_{om} [L/kg]	0 [c]
DT_{50} water [days]	1000 [c]
DT_{50} sediment [days]	1000 [c]
Maximum occurrence in soil [%]	81.5 [e]
Maximum occurrence in water/sediment systems [%]	0 [f]
Maximum occurrence in aquatic systems [%]	0 [f]

[a] Geometric mean based on aerobic soil laboratory studies, normalised to 20°C and field capacity
[b] Geometric mean DT_{50} of total system used for the calculation, value based on laboratory aerobic water/sediment studies
[c] Worst case value
[d] Median value based on aerobic soil laboratory studies, normalised to 20°C and field capacity
[e] Value based on aerobic soil laboratory studies, normalised to 20°C and field capacity
[f] Since the metabolite is not a major metabolite in water sediment system, the value was set to zero.
[g] Since the metabolite is not a major metabolite in soil, the value was set to zero.
[h] Value based on laboratory aerobic water/sediment studies

PECsw for flufenacet and metabolites

Flufenacet and its metabolites FOE sulfonic acid, FOE oxalate, FOE methylsulfone, FOE-thiadone, FOE methylsulfide, FOE 5043-trifluoroethanesulfonic acid and trifluoroacetic acid were considered in this assessment.

Report:	**KCP 9.2.5 / 01, [redacted], G., [redacted], A.; 2014**
Title:	Flufenacet (FOE 5043) and metabolites: $PEC_{sw,sed}$ FOCUS EUR - Autumn use in winter cereals in Europe
Document No:	M 478924-01-1
Guidelines:	FOCUS, 2003: SANCO/4802/2001-rev2 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 flufenacet and its metabolites was calculated for the use in winter cereals in Europe.

At FOCUS Step 2 the application period was set to October to February. Calculations consider the use in Northern and Southern Europe. 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 (according to FOCUS)

Individual Crop	FOCUS Crop Used for Interception	Application			
		Rate per Season [g a.s./ha]	Interval [days]	Plant Interception [%]	Growth Stage
Winter cereals, GAP	-	1 × 240	-	-	10-13
Simulation	cereals, winter (arable crops)	1 × 240	-	25% (Step 1&2) PAT tool (Step 3)	10-13
Winter cereals, GAP	-	1 × 160	-	-	11-13
Simulation	cereals, winter (arable crops)	1 × 160	-	25% (Step 1&2) PAT tool (Step 3)	11-13
Winter cereals, GAP	-	1 × 120	-	-	0-22
Simulation	cereals, winter (arable crops)	1 × 120	-	0% (Step 1&2) PAT tool (Step 3)	0-22

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 flufenacet for the FOCUS Step 3 calculations

Parameter	Winter cereals 1 × 240 g a.s./ha		Winter cereals 1 × 160 g a.s./ha		Winter cereals 1 × 120 g a.s./ha	
PAT start date rel./absolute	Emg., +1 days		Emg., +2 days		Emg., -10 days	
Appl. method (appl. type)	ground spray (CAM 2)		ground spray (CAM 2)		ground spray (CAM 2)	
No of appl.	1		1		1	
PAT window range	30		30		30	
Appl. interval	1		1		1	
Application Details	PAT Start Date/(Julian Day)	Appl. Date	PAT Start Date/(Julian Day)	Appl. Date	PAT Start Date/(Julian Day)	Appl. Date
D1 (1st)	26-Sep/(269)	03-Oct	27-Sep/(270)	03-Oct	15-Sep/(258)	15-Sep
D2 (1st)	26-Oct/(299)	03-Nov	27-Oct/(300)	03-Nov	16-Oct/(288)	15-Oct
D3 (1st)	22-Nov/(326)	22-Nov	23-Nov/(327)	22-Nov	11-Nov/(315)	14-Nov
D4 (1st)	23-Sep/(266)	28-Sep	24-Sep/(267)	28-Sep	12-Sep/(255)	12-Sep
D5 (1st)	11-Nov/(315)	27-Nov	12-Nov/(316)	27-Nov	31-Oct/(304)	27-Nov
D6 (1st)	01-Dec/(335)	06-Dec	02-Dec/(336)	06-Dec	20-Nov/(324)	06-Dec
R1 (1st)	13-Nov/(317)	14-Nov	14-Nov/(318)	14-Nov	02-Nov/(306)	14-Nov
R3 (1st)	02-Dec/(336)	05-Dec	03-Dec/(337)	05-Dec	21-Nov/(325)	21-Nov
R4 (1st)	11-Nov/(315)	10-Dec	12-Nov/(316)	10-Dec	31-Oct/(304)	03-Nov

Compound specific input data for FOCUS Steps 1&2 are summarised in Table 9.2.5- 4 and for Steps 3&4 in Table 9.2.5- 6.

Table 9.2.5- 5: Substance parameters used for flufenacet and its metabolites at Steps 1&2

Parameter	Unit	Flufenacet	FOE sulfonic acid	FOE oxalate	FOE methylsulfone
Molar Mass	g/mol	363.3	275.3	225.2	279.3
Water Solubility	mg/L	56	55000	120000	4100
K_{oc}	mL/g	215	10.3	11	74.1
Degradation					
Soil	days	18.3	205	13.7	67.7
Total System	days	49.6	1000	1000	1000
Water	days	49.6	1000	1000	1000
Sediment	days	1000	1000	1000	1000
Max Occurrence					
Water / Sediment	%	100	0	0	0
Soil	%	100	26.3	26.5	6.6

Parameter	Unit	FOE methylsulfide	FOE-thiadone	FOE 5043-trifluoroethane-sulfonic acid	Trifluoroacetic acid
Molar Mass	g/mol	241	170.1	164.1	114
Water Solubility	mg/L	133.3	30000	160000	500000
K_{oc}	mL/g	850.5	43.7	0	0
Degradation					
Soil	days	1000	1.6	9.1	1000
Total System	days	1000	1000	1000	1000
Water	days	1000	1000	1000	1000
Sediment	days	1000	1000	1000	1000
Max Occurrence					
Water / Sediment	%	11.4	84.3	0	0
Soil	%	0	5.9	6	81.5

Table 9.2.5- 6: Substance parameters used for flufenacet at Steps 3&4

Parameter	Unit	Flufenacet
Molar Mass	g/mol	363.3
Water Solubility	mg/L	56.0
Vapour Pressure	Pa	9.0E-05
Plant Uptake Factor	-	0.5
Wash-Off Factor PRZM	1/cm	0.5
Wash-Off Factor MACRO	1/mm	0.05
Sorption		
K_{oc}	mL/g	215
Freundlich Exponent	-	0.916
Degradation		
Soil	days	18.3
Form. Frac. PRZM	molar basis	-
Form. Frac. MACRO	mass basis	-
Water	days	49.6
Sediment	days	1000
Walker Exponent	-	0.7
Effect of Temperature		
Activation Energy	J/mol	65400
Exponent	1/K	0.095
Q_{10}	-	2.58

Findings:

Step 1 and 2: The maximum PEC values for Steps 1&2 for flufenacet and its metabolites are given in the following tables.

Table 9.2.5- 7: Maximum PEC_{sw} and PEC_{sed} values for flufenacet and its metabolites at Step 1&2

Compound	FOCUS Scenario	Winter cereals 1 × 240 g a.s/ha		Winter cereals 1 × 120 g a.s/ha		Winter cereals 1 × 160 g a.s/ha	
		$PEC_{sw, max}$ [µg/L]	PEC_{sed} [µg/L]	$PEC_{sw, max}$ [µg/L]	PEC_{sed} [µg/L]	$PEC_{sw, max}$ [µg/L]	PEC_{sed} [µg/L]
Flufenacet	**STEP 1**	64.38	133.7	32.19	66.84	42.92	89.12
	STEP 2 - North	21.80	46.57	14.24	30.46	14.53	31.04
	STEP 2 - South	17.79	37.96	10.57	24.72	11.86	25.30
FOE sulfonic acid	**STEP 1**	15.73	1.620	7.864	0.810	10.49	1.080
	STEP 2 - North	5.152	0.531	3.432	0.354	3.435	0.354
	STEP 2 - South	4.121	0.425	2.748	0.283	2.748	0.283
FOE oxalate	**STEP 1**	12.95	1.425	6.476	0.712	8.634	0.950
	STEP 2 - North	3.967	0.436	2.643	0.291	2.645	0.291
	STEP 2 - South	3.174	0.349	2.116	0.233	2.116	0.233
FOE methylsulfone	**STEP 1**	3.615	2.679	1.807	1.339	2.410	1.786
	STEP 2 - North	1.301	0.964	0.867	0.643	0.867	0.643
	STEP 2 - South	1.041	0.771	0.694	0.514	0.694	0.514
FOE methylsulfide	**STEP 1**	0.167	<0.001	0.084	<0.001	0.111	<0.001
	STEP 2 - North	0.167	0.537	0.084	0.269	0.111	0.358
	STEP 2 - South	0.167	0.537	0.084	0.269	0.111	0.358
FOE-thiadone	**STEP 1**	2.959	0.913	1.480	0.456	1.973	0.608
	STEP 2 - North	0.975	0.419	0.510	0.220	0.650	0.279
	STEP 2 - South	0.947	0.407	0.492	0.212	0.631	0.271
FOE 5043 trifluoroethane-sulfonic acid	**STEP 1**	2.168	<0.001	1.084	<0.001	1.445	<0.001
	STEP 2 - North	0.600	<0.001	0.400	<0.001	0.400	<0.001
	STEP 2 - South	0.480	<0.001	0.320	<0.001	0.320	<0.001
trifluoroacetictrifluoroacetic acid	**STEP 1**	20.46	<0.001	10.23	<0.001	13.64	<0.001
	STEP 2 - North	7.651	<0.001	5.101	<0.001	5.101	<0.001
	STEP 2 - South	6.121	<0.001	4.081	<0.001	4.081	<0.001

Step 3: The maximum PEC_{sw} and PEC_{sed} values for relevant FOCUS Step 3 scenarios are given in the table below.

Table 9.2.5- 8: Maximum PEC_{sw} and PEC_{sed} of flufenacet for all scenarios at Step 3 following application to winter cereals

Scenario	Winter cereals 1 × 240 g a.s/ha			Winter cereals 1 × 120 g a.s/ha			Winter cereals 1 × 160 g a.s/ha		
	Entry route*	$PEC_{sw, max}$ [µg/L]	PEC_{sed} [µg/L]	Entry route*	$PEC_{sw, max}$ [µg/L]	PEC_{sed} [µg/L]	Entry route*	$PEC_{sw, max}$ [µg/L]	PEC_{sed} [µg/L]
D1 (ditch, 1st)	D	6.762	21.20	D	2.767	9.004	D	4.460	14.19
D1 (stream, 1st)	D	4.230	11.77	D	1.728	4.808	D	2.782	7.858
D2 (ditch, 1st)	D	7.223	11.54	D	3.750	5.993	D	4.646	7.602
D2 (stream, 1st)	D	4.517	6.836	D	2.343	3.575	D	2.905	4.496
D3 (ditch, 1st)	S	1.513	0.381	S	0.758	0.197	S	1.010	0.258
D4 (pond, 1st)	D	1.245	3.777	D	0.417	1.344	D	0.812	2.505
D4 (stream, 1st)	D	1.892	1.792	S	0.658	0.627	D	1.228	1.185
D5 (pond, 1st)	D	1.176	3.711	D	0.575	1.741	D	0.776	2.460
D5 (stream, 1st)	S	1.419	1.172	S	0.710	0.570	S	0.946	0.779
D6 (ditch, 1st)	D	6.021	4.847	D	2.950	2.320	D	3.969	3.177
R1 (pond, 1st)	R	0.116	0.365	R	0.057	0.191	R	0.077	0.250
R1 (stream, 1st)	R	6.341	1.335	R	3.062	0.658	R	4.142	0.883
R3 (stream, 1st)	R	7.887	1.857	R	4.173	1.830	R	5.448	1.228
R4 (stream, 1st)	R	5.943	1.473	R	1.156	0.299	R	3.936	0.987

* letters S, D, and R before correspond to the dominant entry path – spray drift, drainage, and runoff

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

Table 9.2.5- 9: Maximum PEC_{sw} and PEC_{sed} of flufenacet for all scenarios at Step 4 following application to winter cereals - 1 × 240 g a.s/ha

		flufenacetflufenacet Winter cereals, 1 × 240 g a.s/ha							
Buffer Width & Type	**Scenario**	**PEC_{sw} [µg/L] Drift Reduction**				**PEC_{sed} [µg/kg] Drift Reduction**			
		0%	**50%**	**75%**	**90%**	**0%**	**50%**	**75%**	**90%**
10m SD & RO	D1 (ditch, 1st)	6.762	6.762	6.762	6.762	20.74	20.70	20.68	20.66
	D1 (stream, 1st)	4.230	4.230	4.230	4.230	11.75	11.75	11.75	11.75
	D2 (ditch, 1st)	7.223	7.223	7.223	7.223	11.45	11.44	11.43	11.43
	D2 (stream, 1st)	4.517	4.517	4.517	4.517	6.819	6.817	6.816	6.815
	D3 (ditch, 1st)	0.218	0.109	0.054	0.022	0.058	0.030	0.015	0.006
	D4 (pond, 1st)	1.239	1.233	1.230	1.229	3.741	3.711	3.697	3.688
	D4 (stream, 1st)	1.892	1.892	1.892	1.892	1.783	1.782	1.782	1.781
	D5 (pond, 1st)	1.170	1.165	1.163	1.161	3.676	3.647	3.633	3.624
	D5 (stream, 1st)	1.347	1.347	1.347	1.347	1.160	1.158	1.158	1.157
	D6 (ditch, 1st)	6.021	6.021	6.021	6.021	4.497	4.467	4.452	4.443
	R1 (pond, 1st)	0.056	0.043	0.036	0.032	0.180	0.143	0.124	0.112
	R1 (stream, 1st)	2.845	2.845	2.845	2.845	0.600	0.599	0.598	0.598
	R3 (stream, 1st)	3.562	3.562	3.562	3.562	0.841	0.839	0.837	0.836
	R4 (stream, 1st)	2.683	2.683	2.683	2.683	0.673	0.672	0.671	0.671
20m SD & RO	D1 (ditch, 1st)	6.762	6.762	6.762	6.762	20.70	20.68	20.67	20.66
	D1 (stream, 1st)	4.230	4.230	4.230	4.230	11.75	11.75	11.75	11.75
	D2 (ditch, 1st)	7.223	7.223	7.223	7.223	11.44	11.43	11.43	11.43
	D2 (stream, 1st)	4.517	4.517	4.517	4.517	6.817	6.816	6.815	6.815
	D3 (ditch, 1st)	0.113	0.057	0.028	0.011	0.031	0.016	0.008	0.003
	D4 (pond, 1st)	1.235	1.231	1.229	1.228	3.721	3.702	3.692	3.686
	D4 (stream, 1st)	1.892	1.892	1.892	1.892	1.782	1.782	1.781	1.781
	D5 (pond, 1st)	1.167	1.164	1.162	1.161	3.657	3.638	3.628	3.622
	D5 (stream, 1st)	1.347	1.347	1.347	1.347	1.158	1.158	1.157	1.157
	D6 (ditch, 1st)	6.021	6.021	6.021	6.021	4.468	4.452	4.444	4.440
	R1 (pond, 1st)	0.033	0.024	0.019	0.016	0.106	0.080	0.067	0.059
	R1 (stream, 1st)	1.482	1.482	1.482	1.482	0.317	0.316	0.316	0.316
	R3 (stream, 1st)	1.861	1.861	1.861	1.861	0.447	0.445	0.444	0.444
	R4 (stream, 1st)	1.402	1.402	1.402	1.402	0.357	0.357	0.356	0.356

SD and RO denote spray drift and runoff buffer, respectively

Table 9.2.5- 10: Maximum PEC_{sw} and PEC_{sed} of flufenacet for all scenarios at Step 4 following application to winter cereals – 1 × 120 g a.s/ha

		flufenacetflufenacet Winter cereals, 1 × 120 g a.s/ha							
Buffer Width & Type	**Scenario**	**PEC_{sw} [µg/L] Drift Reduction**				**PEC_{sed} [µg/kg] Drift Reduction**			
		0%	**50%**	**75%**	**90%**	**0%**	**50%**	**75%**	**90%**
10m SD & RO	D1 (ditch, 1st)	2.767	2.767	2.767	2.767	8.564	8.527	8.509	8.498
	D1 (stream, 1st)	1.728	1.728	1.728	1.728	4.797	4.796	4.795	4.795
	D2 (ditch, 1st)	3.750	3.750	3.750	3.750	5.933	5.928	5.926	5.924
	D2 (stream, 1st)	2.343	2.343	2.343	2.343	3.525	3.519	3.516	3.514
	D3 (ditch, 1st)	0.109	0.054	0.027	0.011	0.030	0.015	0.008	0.003
	D4 (pond, 1st)	0.414	0.412	0.411	0.410	1.326	1.311	1.304	1.299
	D4 (stream, 1st)	0.613	0.613	0.613	0.613	0.623	0.623	0.622	0.622
	D5 (pond, 1st)	0.572	0.569	0.568	0.567	1.724	1.709	1.701	1.697
	D5 (stream, 1st)	0.656	0.656	0.656	0.656	0.563	0.563	0.562	0.562
	D6 (ditch, 1st)	2.950	2.950	2.950	2.950	2.140	2.125	2.117	2.112
	R1 (pond, 1st)	0.028	0.021	0.018	0.017	0.094	0.075	0.065	0.059
	R1 (stream, 1st)	1.374	1.374	1.374	1.374	0.295	0.295	0.294	0.294
	R3 (stream, 1st)	1.906	1.906	1.906	1.906	1.155	1.153	1.153	1.152
	R4 (stream, 1st)	0.522	0.522	0.522	0.522	0.137	0.136	0.136	0.136
20m SD & RO	D1 (ditch, 1st)	2.767	2.767	2.767	2.767	8.529	8.510	8.500	8.495
	D1 (stream, 1st)	1.728	1.728	1.728	1.728	4.796	4.795	4.795	4.795
	D2 (ditch, 1st)	3.750	3.750	3.750	3.750	5.929	5.926	5.925	5.924
	D2 (stream, 1st)	2.343	2.343	2.343	2.343	3.519	3.516	3.515	3.514
	D3 (ditch, 1st)	0.057	0.028	0.014	0.006	0.016	0.008	0.004	0.002
	D4 (pond, 1st)	0.412	0.411	0.410	0.410	1.316	1.306	1.301	1.298
	D4 (stream, 1st)	0.613	0.613	0.613	0.613	0.623	0.622	0.622	0.622
	D5 (pond, 1st)	0.570	0.569	0.568	0.567	1.714	1.704	1.699	1.696
	D5 (stream, 1st)	0.656	0.656	0.656	0.656	0.563	0.562	0.562	0.562
	D6 (ditch, 1st)	2.950	2.950	2.950	2.950	2.125	2.117	2.113	2.111
	R1 (pond, 1st)	0.016	0.012	0.009	0.009	0.055	0.042	0.035	0.031
	R1 (stream, 1st)	0.716	0.716	0.716	0.716	0.156	0.155	0.155	0.155
	R3 (stream, 1st)	1.000	1.000	1.000	1.000	0.514	0.513	0.513	0.513
	R4 (stream, 1st)	0.272	0.272	0.272	0.272	0.073	0.072	0.072	0.072

SD and RO denote spray drift and runoff buffer, respectively

Table 9.2.5- 11: Maximum PEC_{sw} and PEC_{sed} of flufenacet for all scenarios at Step 4 following application to winter cereals – 1 × 160 g a.s/ha

		flufenacet Winter cereals, 1 × 160 g a.s/ha							
Buffer Width & Type	**Scenario**	**PEC_{sw} [µg/L] Drift Reduction**				**PEC_{sed} [µg/kg] Drift Reduction**			
		0%	**50%**	**75%**	**90%**	**0%**	**50%**	**75%**	**90%**
10m SD & RO	D1 (ditch, 1st)	4.460	4.460	4.460	4.460	13.87	13.85	13.83	13.82
	D1 (stream, 1st)	2.782	2.782	2.782	2.782	7.849	7.848	7.847	7.847
	D2 (ditch, 1st)	4.646	4.646	4.646	4.646	7.534	7.529	7.526	7.524
	D2 (stream, 1st)	2.905	2.905	2.905	2.905	4.485	4.483	4.483	4.482
	D3 (ditch, 1st)	0.145	0.073	0.036	0.014	0.039	0.020	0.010	0.004
	D4 (pond, 1st)	0.808	0.804	0.802	0.801	2.480	2.460	2.450	2.444
	D4 (stream, 1st)	1.228	1.228	1.228	1.228	1.179	1.179	1.178	1.178
	D5 (pond, 1st)	0.772	0.769	0.767	0.767	2.436	2.417	2.407	2.401
	D5 (stream, 1st)	0.886	0.886	0.886	0.886	0.771	0.770	0.769	0.769
	D6 (ditch, 1st)	3.969	3.969	3.969	3.969	2.940	2.920	2.910	2.904
	R1 (pond, 1st)	0.037	0.028	0.024	0.022	0.123	0.098	0.085	0.077
	R1 (stream, 1st)	1.858	1.858	1.858	1.858	0.396	0.395	0.395	0.395
	R3 (stream, 1st)	2.325	2.325	2.325	2.325	0.556	0.554	0.553	0.552
	R4 (stream, 1st)	1.777	1.777	1.777	1.777	0.451	0.450	0.450	0.449
20m SD & RO	D1 (ditch, 1st)	4.460	4.460	4.460	4.460	13.85	13.83	13.83	13.82
	D1 (stream, 1st)	2.782	2.782	2.782	2.782	7.848	7.847	7.847	7.847
	D2 (ditch, 1st)	4.646	4.646	4.646	4.646	7.529	7.526	7.524	7.523
	D2 (stream, 1st)	2.905	2.905	2.905	2.905	4.483	4.483	4.482	4.482
	D3 (ditch, 1st)	0.075	0.038	0.019	0.008	0.021	0.011	0.005	0.002
	D4 (pond, 1st)	0.806	0.803	0.802	0.801	2.467	2.454	2.447	2.443
	D4 (stream, 1st)	1.228	1.228	1.228	1.228	1.179	1.178	1.178	1.178
	D5 (pond, 1st)	0.770	0.768	0.767	0.766	2.423	2.410	2.404	2.400
	D5 (stream, 1st)	0.886	0.886	0.886	0.886	0.770	0.769	0.769	0.769
	D6 (ditch, 1st)	3.969	3.969	3.969	3.969	2.921	2.910	2.905	2.902
	R1 (pond, 1st)	0.022	0.016	0.012	0.011	0.072	0.055	0.046	0.041
	R1 (stream, 1st)	0.968	0.968	0.968	0.968	0.209	0.209	0.209	0.208
	R3 (stream, 1st)	1.215	1.215	1.215	1.215	0.295	0.294	0.293	0.293
	R4 (stream, 1st)	0.928	0.928	0.928	0.928	0.239	0.239	0.239	0.239

SD and RO denote spray drift and runoff buffer, respectively

Additionally, time weighted average PECsw values are presented for flufenacet, FOCUS Step 3 and FOCUS Step 4.

Table 9.2.5- 12: Summary of TWACsw and TWACsed values of flufenacet after application in winter cereals, 1 × 240 g/ha

Scenario	$PEC_{sw, max}$ [µg/L]	TWACsw [µg/L] 2	3*	7	21	TWACsed [µg/kg] 2	3*	7	21
Step 3									
D1 (ditch, 1st)	6.762	6.668	6.634	6.458	6.221	21.20	21.20	21.19	20.98
D1 (stream, 1st)	4.230	4.159	4.136	4.020	3.856	11.75	11.75	11.74	11.57
D2 (ditch, 1st)	7.223	3.861	3.759	3.497	2.941	11.51	11.50	11.45	11.29
D2 (stream, 1st)	4.517	2.321	2.258	2.092	1.780	6.818	6.811	6.783	6.684
D3 (ditch, 1st)	1.513	0.535	0.403	0.154	0.052	0.299	0.266	0.185	0.113
D4 (pond, 1st)	1.245	1.245	1.244	1.237	1.193	3.777	3.777	3.776	3.775
D4 (stream, 1st)	1.892	1.632	1.601	1.454	0.933	1.789	1.786	1.764	1.641
D5 (pond, 1st)	1.176	1.174	1.172	1.160	1.098	3.711	3.711	3.711	3.705
D5 (stream, 1st)	1.419	0.784	0.760	0.737	0.438	1.168	1.163	1.130	0.989
D6 (ditch, 1st)	6.021	4.356	4.246	3.269	1.645	4.789	4.732	4.467	3.653
R1 (pond, 1st)	0.116	0.114	0.113	0.110	0.101	0.365	0.365	0.365	0.365
R1 (stream, 1st)	6.341	1.324	0.993	0.379	0.135	0.794	0.698	0.474	0.297
R3 (stream, 1st)	7.887	2.046	1.536	0.586	0.291	1.201	1.060	0.728	0.595
R4 (stream, 1st)	5.943	2.212	1.660	0.633	0.218	1.155	1.038	0.735	0.454
Step 4, 10m Buffer									
D1 (ditch, 1st)	6.762	6.668	6.634	6.458	6.221	20.73	20.73	20.71	20.49
D1 (stream, 1st)	4.230	4.159	4.136	4.020	3.856	11.73	11.73	11.72	11.55
D2 (ditch, 1st)	7.223	3.861	3.759	3.497	2.941	11.41	11.40	11.35	11.19
D2 (stream, 1st)	4.517	2.321	2.258	2.092	1.780	6.801	6.794	6.766	6.668
D3 (ditch, 1st)	0.218	0.077	0.058	0.022	0.007	0.046	0.041	0.029	0.018
D4 (pond, 1st)	1.239	1.238	1.237	1.230	1.186	3.741	3.741	3.741	3.739
D4 (stream, 1st)	1.892	1.632	1.601	1.454	0.933	1.780	1.777	1.755	1.632
D5 (pond, 1st)	1.170	1.168	1.166	1.154	1.092	3.676	3.676	3.675	3.669
D5 (stream, 1st)	1.347	0.784	0.760	0.737	0.438	1.156	1.151	1.118	0.977
D6 (ditch, 1st)	6.021	4.356	4.246	3.269	1.645	4.443	4.390	4.134	3.359
R1 (pond, 1st)	0.056	0.055	0.055	0.053	0.049	0.180	0.180	0.180	0.180
R1 (stream, 1st)	2.845	0.591	0.444	0.169	0.058	0.356	0.312	0.210	0.130
R3 (stream, 1st)	3.562	0.924	0.694	0.265	0.131	0.541	0.476	0.323	0.264
R4 (stream, 1st)	2.683	0.995	0.747	0.285	0.096	0.528	0.475	0.335	0.206
Step 4, 20m Buffer									
D1 (ditch, 1st)	6.762	6.668	6.634	6.458	6.221	20.69	20.69	20.67	20.45
D1 (stream, 1st)	4.230	4.159	4.136	4.020	3.856	11.73	11.73	11.72	11.55
D2 (ditch, 1st)	7.223	3.861	3.759	3.497	2.941	11.41	11.39	11.34	11.19
D2 (stream, 1st)	4.517	2.321	2.258	2.092	1.780	6.799	6.792	6.764	6.666
D3 (ditch, 1st)	0.113	0.040	0.030	0.012	0.004	0.025	0.022	0.015	0.009
D4 (pond, 1st)	1.235	1.234	1.233	1.226	1.183	3.721	3.721	3.721	3.719
D4 (stream, 1st)	1.892	1.632	1.601	1.454	0.933	1.779	1.776	1.754	1.631
D5 (pond, 1st)	1.167	1.165	1.163	1.151	1.089	3.657	3.657	3.656	3.649
D5 (stream, 1st)	1.347	0.784	0.760	0.737	0.438	1.154	1.149	1.116	0.975
D6 (ditch, 1st)	6.021	4.356	4.246	3.269	1.645	4.415	4.362	4.106	3.335
R1 (pond, 1st)	0.033	0.032	0.032	0.031	0.028	0.106	0.106	0.106	0.106
R1 (stream, 1st)	1.482	0.308	0.231	0.088	0.030	0.189	0.166	0.111	0.069
R3 (stream, 1st)	1.861	0.483	0.363	0.138	0.069	0.289	0.254	0.172	0.140
R4 (stream, 1st)	1.402	0.519	0.390	0.149	0.050	0.282	0.254	0.179	0.110

* calculated by interpolation

Table 9.2.5- 13: Summary of TWACsw and TWACsed values of flufenacet after application in winter cereals, 1 × 160 g/ha

Scenario	$PEC_{sw\ max}$ [µg/L]	TWACsw [µg/L]				TWACsed [µg/kg]			
		2	3*	7	21	2	3*	7	21
Step 3									
D1 (ditch, 1st)	4.460	4.435	4.410	4.293	4.117	14.19	14.19	14.18	14.03
D1 (stream, 1st)	2.782	2.767	2.750	2.673	2.553	7.842	7.841	7.836	7.718
D2 (ditch, 1st)	4.646	2.487	2.423	2.257	1.903	7.582	7.571	7.538	7.430
D2 (stream, 1st)	2.905	1.494	1.453	1.348	1.151	4.485	4.480	4.462	4.396
D3 (ditch, 1st)	1.010	0.358	0.270	0.103	0.035	0.203	0.181	0.126	0.077
D4 (pond, 1st)	0.812	0.812	0.812	0.807	0.778	2.505	2.505	2.504	2.502
D4 (stream, 1st)	1.228	1.049	1.030	0.939	0.609	1.183	1.181	1.168	1.089
D5 (pond, 1st)	0.776	0.775	0.774	0.765	0.724	2.460	2.460	2.459	2.455
D5 (stream, 1st)	0.946	0.507	0.500	0.485	0.290	0.787	0.773	0.751	0.654
D6 (ditch, 1st)	3.969	2.842	2.767	2.132	1.055	3.142	3.106	2.933	2.396
R1 (pond, 1st)	0.077	0.075	0.074	0.072	0.066	0.250	0.250	0.250	0.250
R1 (stream, 1st)	4.142	0.864	0.649	0.247	0.088	0.527	0.464	0.316	0.198
R3 (stream, 1st)	5.148	1.335	1.002	0.383	0.191	0.798	0.705	0.484	0.398
R4 (stream, 1st)	3.936	1.473	1.105	0.421	0.145	0.780	0.707	0.497	0.307
Step 4, 10m Buffer									
D1 (ditch, 1st)	4.460	4.435	4.410	4.293	4.117	13.87	13.87	13.85	13.7
D1 (stream, 1st)	2.782	2.767	2.750	2.673	2.553	7.833	7.832	7.827	7.708
D2 (ditch, 1st)	4.646	2.487	2.423	2.257	1.903	7.514	7.504	7.471	7.363
D2 (stream, 1st)	2.905	1.494	1.453	1.348	1.151	4.473	4.469	4.45	4.385
D3 (ditch, 1st)	0.145	0.051	0.039	0.015	0.005	0.031	0.028	0.019	0.012
D4 (pond, 1st)	0.808	0.807	0.807	0.803	0.774	2.480	2.480	2.480	2.479
D4 (stream, 1st)	1.228	1.049	1.030	0.939	0.609	1.177	1.175	1.162	1.083
D5 (pond, 1st)	0.772	0.771	0.770	0.762	0.721	2.436	2.436	2.436	2.431
D5 (stream, 1st)	0.886	0.507	0.500	0.485	0.290	0.768	0.765	0.742	0.646
D6 (ditch, 1st)	3.969	2.842	2.767	2.131	1.054	2.908	2.875	2.708	2.196
R1 (pond, 1st)	0.037	0.037	0.036	0.035	0.032	0.123	0.123	0.123	0.123
R1 (stream, 1st)	1.858	0.386	0.290	0.111	0.038	0.236	0.207	0.139	0.086
R3 (stream, 1st)	2.325	0.603	0.453	0.173	0.086	0.359	0.316	0.215	0.176
R4 (stream, 1st)	1.777	0.663	0.498	0.190	0.064	0.357	0.321	0.227	0.139
Step 4, 20m Buffer									
D1 (ditch, 1st)	4.460	4.435	4.410	4.293	4.117	13.84	13.84	13.83	13.67
D1 (stream, 1st)	2.782	2.767	2.750	2.673	2.553	7.832	7.831	7.826	7.707
D2 (ditch, 1st)	4.646	2.487	2.423	2.257	1.903	7.509	7.499	7.465	7.357
D2 (stream, 1st)	2.905	1.494	1.453	1.348	1.151	4.472	4.468	4.449	4.384
D3 (ditch, 1st)	0.076	0.027	0.020	0.008	0.003	0.017	0.015	0.010	0.006
D4 (pond, 1st)	0.806	0.805	0.805	0.800	0.772	2.467	2.467	2.467	2.466
D4 (stream, 1st)	1.228	1.049	1.030	0.939	0.609	1.177	1.175	1.161	1.083
D5 (pond, 1st)	0.770	0.769	0.768	0.760	0.719	2.423	2.423	2.423	2.418
D5 (stream, 1st)	0.886	0.507	0.500	0.485	0.290	0.767	0.764	0.741	0.645
D6 (ditch, 1st)	3.969	2.842	2.767	2.131	1.054	2.888	2.855	2.689	2.179
R1 (pond, 1st)	0.022	0.021	0.021	0.021	0.019	0.072	0.072	0.072	0.072
R1 (stream, 1st)	0.968	0.201	0.151	0.058	0.020	0.125	0.110	0.074	0.046
R3 (stream, 1st)	1.215	0.315	0.237	0.090	0.045	0.191	0.168	0.114	0.094
R4 (stream, 1st)	0.928	0.345	0.259	0.099	0.033	0.190	0.171	0.121	0.074

* calculated by interpolation

Table 9.2.5- 14: Summary of TWACsw and TWACsed values of flufenacet after application in winter cereals, 1 × 120 g/ha

Scenario	$PEC_{sw, max}$ [µg/L]	TWACsw [µg/L] 2	3*	7	21	TWACsed [µg/kg] 2	3*	7	21
Step 3									
D1 (ditch, 1st)	2.767	2.751	2.736	2.667	2.566	9.004	9.004	9.001	8.977
D1 (stream, 1st)	1.728	1.716	1.706	1.660	1.591	4.808	4.808	4.806	4.794
D2 (ditch, 1st)	3.750	2.317	2.269	2.041	1.673	5.954	5.937	5.902	5.828
D2 (stream, 1st)	2.343	1.354	1.326	1.192	0.954	3.543	3.534	3.517	3.473
D3 (ditch, 1st)	0.758	0.273	0.206	0.079	0.026	0.156	0.139	0.097	0.059
D4 (pond, 1st)	0.417	0.417	0.417	0.414	0.400	1.344	1.344	1.344	1.343
D4 (stream, 1st)	0.658	0.531	0.521	0.475	0.312	0.626	0.625	0.619	0.580
D5 (pond, 1st)	0.575	0.574	0.573	0.567	0.536	1.741	1.741	1.741	1.736
D5 (stream, 1st)	0.710	0.375	0.373	0.359	0.216	0.568	0.566	0.548	0.475
D6 (ditch, 1st)	2.950	2.097	2.040	1.572	0.769	2.295	2.270	2.142	1.743
R1 (pond, 1st)	0.057	0.056	0.055	0.054	0.049	0.191	0.191	0.191	0.191
R1 (stream, 1st)	3.062	0.639	0.480	0.183	0.065	0.395	0.348	0.236	0.149
R3 (stream, 1st)	4.173	2.163	1.760	0.778	0.280	4.421	4.282	3.832	3.108
R4 (stream, 1st)	1.156	0.423	0.318	0.121	0.040	0.235	0.212	0.150	0.093
Step 4, 10m Buffer									
D1 (ditch, 1st)	2.767	2.751	2.736	2.667	2.566	8.564	8.564	8.562	8.544
D1 (stream, 1st)	1.728	1.716	1.706	1.660	1.591	4.797	4.797	4.796	4.783
D2 (ditch, 1st)	3.750	2.317	2.269	2.041	1.673	5.893	5.876	5.842	5.767
D2 (stream, 1st)	2.343	1.354	1.326	1.192	0.954	3.494	3.485	3.469	3.425
D3 (ditch, 1st)	0.109	0.039	0.029	0.011	0.004	0.024	0.021	0.015	0.009
D4 (pond, 1st)	0.414	0.414	0.414	0.411	0.397	1.326	1.326	1.326	1.325
D4 (stream, 1st)	0.613	0.531	0.521	0.475	0.312	0.622	0.621	0.615	0.576
D5 (pond, 1st)	0.572	0.571	0.570	0.564	0.533	1.723	1.723	1.723	1.718
D5 (stream, 1st)	0.656	0.375	0.373	0.359	0.216	0.562	0.559	0.542	0.469
D6 (ditch, 1st)	2.950	2.097	2.040	1.572	0.769	2.117	2.094	1.971	1.591
R1 (pond, 1st)	0.028	0.027	0.027	0.026	0.024	0.094	0.094	0.094	0.094
R1 (stream, 1st)	1.374	0.286	0.215	0.082	0.028	0.177	0.155	0.104	0.065
R3 (stream, 1st)	1.906	0.994	0.809	0.357	0.128	1.023	0.979	0.837	0.647
R4 (stream, 1st)	0.522	0.190	0.143	0.054	0.018	0.108	0.097	0.069	0.042
Step 4, 20m Buffer									
D1 (ditch, 1st)	2.767	2.751	2.736	2.667	2.566	8.529	8.529	8.527	8.509
D1 (stream, 1st)	1.728	1.716	1.706	1.660	1.591	4.796	4.796	4.794	4.782
D2 (ditch, 1st)	3.750	2.317	2.269	2.041	1.673	5.888	5.871	5.837	5.763
D2 (stream, 1st)	2.343	1.354	1.326	1.192	0.954	3.488	3.479	3.464	3.419
D3 (ditch, 1st)	0.057	0.020	0.015	0.006	0.002	0.013	0.011	0.008	0.005
D4 (pond, 1st)	0.412	0.412	0.412	0.410	0.396	1.316	1.316	1.316	1.315
D4 (stream, 1st)	0.613	0.531	0.521	0.475	0.312	0.622	0.621	0.614	0.575
D5 (pond, 1st)	0.570	0.569	0.568	0.562	0.532	1.713	1.713	1.713	1.708
D5 (stream, 1st)	0.656	0.375	0.373	0.359	0.216	0.561	0.558	0.541	0.468
D6 (ditch, 1st)	2.950	2.097	2.040	1.572	0.769	2.103	2.080	1.957	1.579
R1 (pond, 1st)	0.016	0.016	0.016	0.015	0.014	0.055	0.055	0.055	0.055
R1 (stream, 1st)	0.716	0.149	0.112	0.043	0.015	0.094	0.082	0.055	0.034
R3 (stream, 1st)	1.000	0.523	0.426	0.188	0.067	0.449	0.428	0.361	0.270
R4 (stream, 1st)	0.272	0.099	0.074	0.028	0.009	0.058	0.052	0.037	0.023

* calculated by interpolation

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.

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

Please refer to point 9.3.

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.

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.