Document Title

Summary of the fate and behaviour in the environment Fluopicolide + Fluoxastrobin FS 350 (200+150 g/L)

Data Requirement(s)

Regulation (EC) No 1107/2009 & Regulation (EU) No 284/2013

Document MCP

Section 9: Fate and behaviour in the environment

According to the Guidance Document SANCO/10181/2013 for applicants on preparing dossiers for the approval of a chemical active substance

Date

2020-08-11

Author(s)

[redacted]

Battelle UK Ltd

on behalf of

Bayer AG

Crop Science Division

OWNERSHIP STATEMENT

This document, the data contained in it and copyright therein are owned by Bayer AG and/or affiliated entities. No part of the document or any information contained therein may be disclosed to any third party without the prior written authorisation of Bayer AG and/or affiliated entities.

The summaries and evaluations contained in this document are based on unpublished proprietary data submitted for the purpose of the assessment undertaken by the regulatory authority. Other registration authorities should not grant, amend, or renew a registration on the basis of the summaries and evaluation of unpublished proprietary data contained in this document unless they have received the data on which the summaries and evaluation are based, either:

- **from Bayer AG or respective affiliate; or**
- **from other applicants once the period of data protection has expired.**

Version history

Date [yyyy-mm-dd]	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'.

Table of Contents

CP 9 FATE AND BEHAVIOUR IN THE ENVIRONMENT

Fluopicolide was included in Annex I to Council Directive 91/414/EEC in 2010 (Commission Directive 2010/15/EU, Entry into Force on June 1, 2010). The expiration of approval of fluopicolide is May 31, 2023 (Commission Implementing Regulation (EU) 2017/1527). The Supplementary Dossier contains only data which were not submitted at the time of the Annex I inclusion of fluopicolide under Council Directive 91/414/EEC and which were therefore not evaluated during the first EU review. All data which were already submitted by Bayer AG (former Bayer CropScience) for the Annex I inclusion under Council Directive 91/414/EEC are contained in the Draft Assessment Report (DAR) and its Addenda, and are included in the Baseline Dossier provided by Bayer AG.

The formulation Fluopicolide + Fluoxastrobin FS 350 (200+150 g/L), abbreviation FLC + FXA FS 350, is a flowable concentrate for seed treatment formulation (FS) containing 200 g/L of fluopicolide. This formulation is registered in Europe under the trade name Scenic Gold. Fluopicolide + Fluoxastrobin FS 350 (200+150 g/L) was not a representative formulation of Bayer AG for the Annex I inclusion of fluopicolide under Council Directive 91/414/EEC.

Fluopicolide (AE C638206) is a fungicidal active substance developed by Bayer. It is the only active substance in Europe representing a class of chemistry (pyridinylmethyl-benzamides) with a unique mode of action via delocalization of a spectrin-like protein in the Oomycetes fungi.

Fluopicolide is active against a wide range of Oomycete fungi low dose rates against a wide range of Oomycete (Phycomycetes) diseases including downy mildews (Pseudoperonospora, Peronospora, Bremia), late blight (Phytophthora). It is also effective against downy mildews and some Pythium species causing damping off at emergence time.

Fluopicolide is redistributed via the xylem and effective disease control can be achieved from foliar and seed applications. Fluopicolide is used in mixture in a range of foliar formulations in potatoes, horticultural crops and industrial crops such as oilseed.

Fluopicolide has a long track record of safe use in a large number of targeted crops within industrial crops.

Fluopicolide can be formulated with other active ingredients in different types of formulations to optimise and complete its activity.

The development of resistances of Oomycetes against existing, well-established fungicide groups represent a threat for European farmers by increasing the complexity of their plant protection programs leading to severe economic impacts. With Fluopicolide, farmers in EU-27 have access to a modern tool for their integrated crop protection programs, contributing to effective and sustainable management of resistance development and preserving high level of protection against Oomycete diseases.

By reducing the Oomycete damages, applications of Fluopicolide + Fluoxastrobin FS 350 on target crops contribute to the achievement of optimum emergence insuring yield and quality, thus securing sufficient supply of high-quality oilseed for European consumer destinations and markets abroad, for the processing industry.

CP 9.1 Fate and behaviour in soil

CP 9.1.1 Rate of degradation in soil

For information on the rate of degradation in soil please refer to Document MCA, Section 7.1.2.

CP 9.1.1.1 Laboratory studies

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

CP 9.1.1.2 Field studies

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

CP 9.1.1.2.1 Soil dissipation studies

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

CP 9.1.1.2.2 Soil accumulation studies

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

CP 9.1.2 Mobility in the soil

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

CP 9.1.2.1 Laboratory studies

For information on laboratory studies please refer to Document MCA, Section 7.1.4.1.

CP 9.1.2.2 Lysimeter studies

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

CP 9.1.2.3 Field leaching studies

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

CP 9.1.3 Estimation of concentrations in soil

Predicted environmental concentrations in soil (PEC_S)

PEC_{soil} for fluopicolide

Data Point:	KCP 9.1.3/01
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluopicolide (FLC): Core PECsoil EUR - Modelling core info document for soil risk assessment in Europe
Report No:	VC/19/041L
Document No:	M-686282-01-1
Guideline(s) followed in study:	FOCUS Degradation Kinetics 2006 & 2014
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

This summary summarises the substance data for fluopicolide and its metabolites, as used for the purpose of soil exposure and soil accumulation calculations (non-scenario based Tier 1). The parameters correspond to standard EU requirements.

Modelling reports utilising the core info document should have the substance data presented in the form as shown in the following table.

Table 9.1.3- 1: Compound and scenario input parameters as used for the calculation

Compound	Molar mass (g/mol)	Max occur. in soil (%)	DT_{50} (days)	Molar mass corr. factor (-)
Fluopicolide	383.59	100	457.6	1
M-01 (AE C653711)	190.03	48	344	0.4954
M-02 (AE C657188)	225.56	16.4	4.4	0.588
M-03 (AE 0608000)	399.58	10.6	1000	1.0417

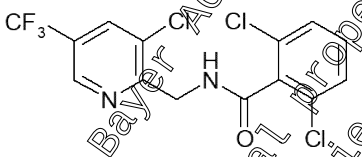
I. Materials and Methods

Calculation of the substance parameters for fluopicolide and its metabolites M-01, M-02 and M-03 is detailed as follows: -

Fluopicolide (AE C638206)

Physico-Chemical Properties

Structural formula



Common name	Fluopicolide (AE C638206)
Chemical name (IUPAC)	2,6-dichloro-N-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]methyl]-benzamide
Molar mass	383.59 g mol^{-1}

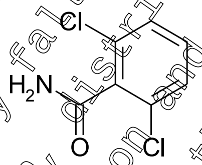
Un-normalised SFO DT_{50} values for fluopicolide have been derived from 12 terrestrial field dissipation studies ([redacted] 2019; M-651636-01-1; [redacted] 2003; M-218667-01-1,; [redacted] 2003; M-220477-02-1; [redacted] 2004; M-234424-01-1; [redacted] 2005; M-247945-01-1; [redacted] 2005; M-251338-01-1; [redacted] 2003; M-218672-01-1,). A summary of the SFO DT_{50} values derived for fluopicolide is given in Table 9.1.3- 2. A worst-case un-normalised field DT_{50} value of **457.6 days** will be used in modelling.

Table 9.1.3- 2: Summary of un-normalised SFO DT_{50} values derived for fluopicolide from terrestrial field dissipation studies ([redacted] 2019; M-651636-01-1; [redacted] 2020; M-685682-01-1)

Soil type	Aerobic field conditions					
	Location (country)	pH ($CaCl_2$)	Depth (cm)	St. (χ^2err) (%)	Method of calculation	DT_{50} (d) un-norm
Silt loam	Burscheid (Germany)	5.9	0 - 120	13.1	SFO	189.9
Clay	Great Chishill (UK)	7.8	0 - 120	11.9	SFO	457.6
Sandy loam	Lignieres de Touraine (France)	6.9	0 - 120	6.9	SFO	284.4
Clay loam	St.Etienne du Grès (France)	8.1	0 - 120	8.0	SFO	370.6
Clay loam	Albaro di Ronco all'Adige (Italy)	7.7	0 - 120	12.6	SFO	284.6
Sandy clay loam	Vilobi d'Onyar (Spain)	6.9	0 - 120	9.0	SFO	208.3
Loamy sand	Philippsburg (Germany)	6.4	0 - 50	18.8	SFO	288.3
Sandy clay loam	Rödelsee (Germany)	7.4	0 - 30	18.5	SFO	256.9
Sand	Huntlosen (Germany)	4.9	0 - 50	16.5	SFO	290.2
Loamy sand	Valencia (Spain)	7.3	0 - 30	21.5	SFO	177.4
Sandy silt	Appilly (France)	7.1	0 - 30	16.3	SFO	194.4
Sandy silt loam	Senas (France)	7.6	0 - 45	14.3	SFO	178.6
					Worst-case	**457.6**

M-01 (BAM; AE C653711)

Physico-Chemical Properties
Structural formula



Common name M-01 (BAM; AE C653711)

Chemical name (IUPAC) 2,6-dichlorobenzamide

Molar mass 190.03 g mol^{-1}

Un-normalised SFO DT_{50} values for M-01 (BAM) have been derived from five terrestrial field dissipation studies (M-650733-02-1, [redacted], 2019b). A summary of the SFO DT_{50} values derived for M-01 is given in Table 9.1.3- 3. A worst-case un-normalised field DT_{50} value of **344 days** will be used in the modelling.

The maximum observed occurrence in soil of M-01 in laboratory studies, expressed as a molar fraction of fluopicolide, was **48%** (M-555570-01-1, [redacted], 2016).

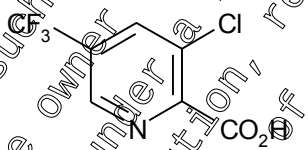
Table 9.1.3- 3: Summary of un-normalised SFO DT_{50} values derived for M-01 (BAM) from terrestrial field dissipation studies (M-650733-02-1, [redacted], 2019b)

Soil type	Aerobic field conditions					
	Location (country)	pH ($CaCl_2$)	Depth (cm)	St. (χ^2err) (%)	Method of calculation	DT_{50} (d) un-norm
Silt loam	Burscheid (Germany)	5.9	0 - 120	17.6	SFO	155
Sandy loam	Lignieres de Touraine (France)	6.9	0 - 120	7.5	SFO	344
Clay loam	St.Etienne du Grès (France)	8.1	0 - 120	10.4	SFO	204
Clay loam	Albarodi Ronco all'Adige (Italy)	7	0 - 120	12.0	SFO	156
Sandy clay loam	Vilobi d'Onyar (Spain)	6.9	0 - 120	9.6	SFO	160
					Worst-case	**344**

M-02 (PCA; AE C657188)

Physico-Chemical Properties

Structural formula



Common name M-02 (PCA; AE C657188)

Chemical name (IUPAC) 3-chloro-5-(trifluoromethyl)pyridine-2-carboxylic acid

Molar mass 225.56 g mol^{-1}

The aerobic degradation and metabolism of M-02 (PCA) in soil was investigated in the laboratory by [redacted] (2003, M-219824-01-1) and [redacted] (2017, M-581364-01-1). A summary of the un-normalised SFO $DegT_{50}$ values derived by [redacted] (2020b, M-685680-01-1) for M-02 is given in Table 9.1.3- 4. A worst-case $DegT_{50}$ value of **4.4 days** will be used in the modelling.

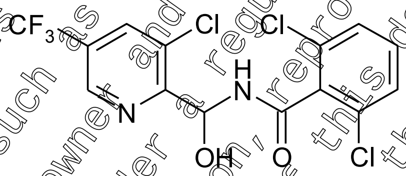
The maximum formation of metabolite M-02 in terrestrial field dissipation studies was **16.4%** (M-220477-02-1, [redacted] 2003).

Table 9.1.3- 4: Summary of un-normalised DegT$_{50}$ values derived for M-02 (PCA) under laboratory conditions (after M-685680-01-1, [redacted] 2020b)

Applied compound	Study	Soil	Model selected	DegT$_{50}$ (d) un-normalised
M-02 (PCA)	M-219824-01-1 [redacted], 2003	Abington	SFO	4.4
		Münster	SFO	3.5
		Sarotti	SFO	4.4
	M-581364-01-1 [redacted] 2017	Dollendorf	SFO	1.1
		[redacted]	SFO	1.1
		[redacted]	SFO	0.7
		[redacted]	SFO	0.7
			Worst-case	**4.4**

M-03 (AE 0608000)

Physico-Chemical Properties
Structural formula



Common name M-03 (AE 0608000)

Chemical name (IUPAC) 2,6-dichloro-N-{[3-chloro-5-(trifluoromethyl)yridine-2-yl](hydroxy)methyl}benzamide

Molar mass 399.58 g mol^{-1}

The aerobic degradation and metabolism of M-03 in soil was investigated in the laboratory by M-241188-01-1, [redacted] (2003) and M-565219-01-1, [redacted] (2016). In addition, M-03 was observed to form from fluopicolide in three studies (M-201230-02-1, [redacted] 2003; M-241052-01-1, [redacted] 2003; M-655056-01-1, [redacted] 2019). A summary of the un-normalised DegT$_{50}$ values derived by M-685680-01-1, [redacted] (2020b) for M-03 is given in Table 9.1.3- 5. A worst-case DegT$_{50}$ value of **1000 days** will be used in the modelling.

The maximum observed occurrence in soil of M-03 in laboratory studies was **10.6%** (M-201230-02-1, [redacted], 2003).

Table 9.1.3- 5: Summary of un-normalised DegT$_{50}$ values derived for M-03 under laboratory conditions (after M-685680-01-1, [redacted]., 2020b)

Applied compound	Study	Soil	Soil pH	Model selected	DegT$_{50}$ (d) un-normalised
Fluopicolide	M-201230-02-1, [redacted] 2003	Münster	4.9	SFO	62.6
	M-241052-01-1, [redacted], 2003	Lamberton	5.9	SFO	49.3
	M-655056-01-1, [redacted] 2019	Pikeville	4.5	SFO	29.3
M-03	M-241188-01-1, [redacted] 2003	Abington	7.2	SFO	0.1
		Münster	4.9	DFOP	1000[a]
		Pikeville	5.4	DFOP	2.7[b]
		Sarotti	7.1	SFO	0.1
	M-565219-01-1, [redacted] 2016	Brierlow (BL)	5.3	SFO	2.5
		[redacted]	6.0	SFO	0.9
				Worst-case	1000

[a] – Derived from DFOP k$_2$ parameter, fixed to conservative default value, [b] – Pseudo-SFO DT$_{50}$ value derived as DT$_{90}$/3.32

II. Results and Discussion

Modelling reports utilising the core info document should have the substance data presented in the form as shown in the following table.

Table 9.1.3- 6: Compound and scenario input parameters as used for the calculation

Compound	Molar mass (g/mol)	Max occur. in soil (%)	DT$_{50}$ (days)	Molar mass corr. factor (-)
Fluopicolide	383.59	100	457.6	1
M-01 (AE C653711)	190.03	48	344	0.4954
M-02 (AE C657188)	225.56	16.4	4.4	0.588
M-03 (AE 0608000)	399.58	10.6	1000	1.0417

III. Conclusion

Soil exposure and soil accumulation calculations should use the input parameters presented in this summary for all calculations.

Assessment and conclusion by applicant:

The modelling report was conducted according to FOCUS Degradation Kinetics (2006, 2014) and is considered valid to assess trigger and modelling endpoints for fluopicolide and its metabolites in soil under laboratory conditions.

Data Point:	KCP 9.1.3/02
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluopicolide (FLC) and metabolites: PECsoil EUR - Use in potatoes, lettuce and oil seed rape (winter) in Europe
Report No:	EnSa-20-0435
Document No:	M-686701-01-1
Guideline(s) followed in study:	Guidance Document on Persistence in Soil EU Commission 9188/VI-97 rev.3 2000 and FOCUS 1997
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

The predicted environmental concentrations in soil (PEC_{soil}) of the active substance fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657188) and M-03 (AE 0608000) were calculated based on a first tier approach using a Microsoft® Excel spreadsheet. The use of fluopicolide in oil seed rape (winter) was assessed according to Good Agricultural Practice (GAP) under Europe cropping conditions. PECsoil values were also calculated for application of fluopicolide to other crops but are not included here as the formulation FLC+FXA SC 350 will be used exclusively as seed treatment on oilseed rape.

Calculations assumed an even distribution of the compound in upper 0 - 5 cm soil layer following application and a soil density of 1.5 g/cm3.

An overview of maximum PECsoil values of fluopicolide and its metabolites for all use patterns under consideration is shown in Table 9.1.3- 7.

Table 9.1.3- 7: Maximum PECsoil of fluopicolide and its metabolites for the uses assessed

Use pattern	Fluopicolide (mg/kg)	M-01 (mg/kg)	M-02 (mg/kg)	M-03 (mg/kg)
Oil Seed Rape (winter) 1 × 12 g a.s./ha	0.016	0.004	0.002	0.002

The accumulation potential of fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657188) and M-03 (AE 0608000) after long term use was also assessed, employing the larger soil depth for the calculation of the background concentration in cases where tillage is relevant. The results are presented in Table 9.1.3- 8. Please note that for technical reasons, accumulation calculation is performed and reported for all substances, even if they do not possess accumulation potential due to short half-life.

Table 9.1.3- 8: PECsoil of fluopicolide and its metabolites for the uses assessed, taking the effect of accumulation into account

Use pattern	PECsoil	Fluopicolide (mg/kg)	M-01 (mg/kg)	M-02 (mg/kg)	M-03 (mg/kg)
Oil Seed Rape (winter) 1 × 12 g a.s./ha	plateau (20 cm) total	0.005 0.021	<0.001 0.005	<0.001 0.002	0.002 0.003

I. Materials and Methods

The predicted environmental concentrations in soil (PEC_{soil}) of the active substance fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657188) and M-03 (AE 0608000) were calculated based on a first tier approach using a Microsoft® Excel spreadsheet. The use of fluopicolide in oil seed rape (winter) was assessed according to Good Agricultural Practice (GAP) under Europe cropping conditions. Calculations assumed an even distribution of the compound in upper 0 - 5 cm soil layer following application and a soil density of 1.5 g/cm^3.

The use of fluopicolide was assessed according to the Good Agricultural Practice (GAP) as summarised below.

Table 9.1.3- 9: Application data of fluopicolide according to the use pattern in Europe

Individual crop	FOCUS crop	Rate (g a.s./ha)	Interval (days)	Plant interception (%)	BBCH stage (-)	Amount reaching soil (g a.s./ha)
Oil Seed Rape (winter)	Oil seed rape (winter)	1 x 12	-	0	00	1 x 12 000

The calculations were based on the maximum intended application rate together with the maximum intended number of applications per season and (for multi-application sequences) the minimum interval between the applications. Crop interception was taken into account according to the BBCH growth stage, as recommended by FOCUS (2014).

For metabolite(s), the (pseudo) application rate is calculated based on the maximum amount of the metabolite observed in soil degradation studies, the interception and the molar mass correction are summarised in Table 9.1.3- 10 and Table 9.1.3- 11.

Table 9.1.3- 10: Summary of properties for metabolite rate calculation

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03 (AE 0608000)
Molar mass	(g/mol)	383.59	190.03	225.56	399.58
Corr. factor	(-)	1	0.4954	0.588	1.0417
Max occ. in soil	(%)	100	48	16.4	10.6

Table 9.1.3- 11: Calculation of metabolite application rates (# = application number)

Compound Crop / rate	#	Fluopicolide (g a.s./ha)	M-01 (g/ha)	M-02 (g/ha)	M-03 (g/ha)
Oil Seed Rape (winter), 1 x 12 g a.s./ha	1	12	2.85	1.16	1.33

Substance parameters used as input in the calculations are based on substance parameters whose derivation is described in detail in the modelling core info document (KCP 9.1.3/01). The modelling parameters used for the calculations are given in Table 9.1.3- 12.

Table 9.1.3- 12: Compound and scenario input parameters as used for the calculation

Compound	Molar mass (g/mol)	Max occur. in soil (%)	DT50 (days)	Molar mass corr. factor (-)
Fluopicolide	383.59	100	457.6	1
M-01 (AE C653711)	190.03	48	344	0.4954

M-02 (AE C657188)	225.56	16.4	4.4	0.588
M-03 (AE 0608000)	399.58	10.6	1000	1.0417
Soil bulk density	1.5 kg/L			
Soil mixing depth	5 cm			
Tillage depth for plateau (if relevant)	20 cm			

The information which mixing depths are employed for individual uses assessed in this report is provided in Table 9.1.3- 13.

Table 9.1.3- 13: Mixing depths used for plateau calculation

Use pattern	Plateau mixing depth
Oil Seed Rape (winter)	20 cm

The details of the calculation can be found below.

Parent compound

1st tier estimation of the initial PEC_{soil} concentration is done using the equation

$$PEC_{soil} = \frac{A \cdot f}{\rho_{soil} \cdot d} \quad (1)$$

with A being the nominal single field application rate, f the fraction reaching soil surface (taking into account crop interception factors according to FOCUS), ρ_{soil} the dry soil bulk density, and d the thickness of the soil layer.

In single application scenarios, the initial PEC_{soil} value is equal to the overall maximum. For multiple (n) applications with constant application rate, crop interception, and application interval, the maximum PEC_{soil} can be written as

$$PEC_{soil,max} = \frac{A \cdot f}{\rho_{soil} \cdot d} \cdot \frac{1 - e^{-k\,n\,\Delta t}}{1 - e^{-k\,\Delta t}} \quad (2)$$

where Δt the application interval and k is the first order degradation rate, calculated from the soil half-life (DT_{50}) as

$$k = \frac{\ln 2}{DT_{50}} \quad (3)$$

For multiple (n) applications with variable application rate, crop interception, or application interval, the PEC_{soil} just after the application (i) can be calculated stepwise as

$$PEC(i)_{soil,max} = \frac{A(i) \cdot f(i)}{\rho_{soil} \cdot d} + PEC(i)_{soil,co} \quad (4)$$

where $PEC_{soil,co}$ represents the residue from the preceding applications at the time of the actual application. For the first application, $PEC_{soil,co}$ is zero, for the following applications it can be written as

$$PEC(i)_{soil,co} = PEC(i-1)_{soil} \cdot e^{-k\,\Delta t(i)} \quad (5)$$

with Δt(i) being the time interval between applications (i-1) and (i). $PEC_{soil,max}$ is then defined as the maximum of the individual PEC_{soil} values.

$$PEC_{soil,max} = \max(PEC(i)_{soil,max}) \quad (6)$$

Metabolites

Maximum soil concentration of a metabolite is calculated in a similar manner to that of the parent compound, taking into account the maximum amount of the metabolite observed in soil ($X_{met,max}$) as well as the different molar masses of the parent (M_{par}) and metabolite (M_{met}).

The value of the initial metabolite concentration $PEC_{soil,met}$ is calculated using

$$PEC_{soil,met} = PEC_{soil,par} \cdot X_{met,max} \cdot \frac{M_{met}}{M_{par}} \quad (7)$$

where $PEC_{soil,par}$ is the respective initial parent concentration.

For a single application, the $PEC_{soil,met}$ value is equal to $PEC_{soil,max,met}$. For multiple applications, the maximum metabolite soil concentration has to be calculated using the equations (4) - (6) given in the previous section, with the parent dissipation rate replaced by that of the metabolite, and with maximum metabolite occurrence in soil and different molar masses of the parent and metabolite taken into account.

Concentrations over time

For first-order kinetics with a degradation rate k the declining PEC values at time t after the maximum can be calculated by

$$PEC(t) = PEC_{max} \cdot e^{-kt} \quad (8)$$

For a better comparison of exposure and effect data time-weighted average concentrations (TWA) may be useful. For first-order kinetics, the TWA are given by the following formula.

$$TWA(t) = PEC_{max} \cdot \frac{1}{k \cdot t} \cdot (1 - e^{-k\,t}) \quad (9)$$

Accumulation after long term use

Potential accumulation after long term use is also assessed, based on the maximum $PEC_{soil,max}$ concentration of the respective compound, obtained as described before.

In case of a single application (or a multiple application sequence leading to the maximum PEC_{soil} after the last application), it can be shown that the maximum concentration in soil after perpetual use ($PEC_{soil,accu}$) can be expressed as

$$PEC_{soil,accu} = PEC_{soil,max} \cdot \frac{1}{1 - e^{-k \cdot t}} \quad (10)$$

where t is the number of days between two events where $PEC_{soil,max}$ is reached, *i.e.*, 365 days for yearly applications, 730 days for bi-yearly applications, *etc*. This PEC_{soil} value is based on a normal mixing depth. In the case of a multiple application sequence leading to the maximum PEC_{soil} before the last application another approach has to be used.

The concentration in soil after an infinite number of applications and immediately before the application in the last year (the so called plateau concentration $PEC_{plateau}$) can be written as

$$PEC_{plateau} = PEC_{soil,accu} \cdot \frac{d}{d_{accu}} \cdot e^{-k \cdot t} \qquad (11)$$

This formula can take the effect of deep soil tillage (or another mixing process) into account by distributing the soil residue amongst larger amounts of soil (larger soil mixing depth d_{accu} of, *e.g.*, 20 cm). In the absence of such mixing process, the factors involving mixing depth cancel out.
The total PEC_{soil} taking the effect of accumulation into account is then the sum of $PEC_{plateau}$ and the maximum PEC_{soil}, as defined previously.

$$PEC_{soil,total} = PEC_{plateau} + PEC_{soil,max} \qquad (12)$$

The plateau concentration is driven by the dissipation DT_{50} in soil. The ratio between maximum PEC_{soil} due to actual application and the respective plateau concentration (taking effect of tillage into account here) can be written as

$$\frac{PEC_{plateau}}{PEC_{soil,max}} = \frac{e^{-k \cdot t}}{1 - e^{-k \cdot t}} \cdot \frac{d}{d_{accu}} \qquad (13)$$

Inspection of Equation (13) shows that this ratio is independent of the application rate. For a DT_{90} of less than a year, the plateau concentration is marginal (< 3% of actual $PEC_{soil,max}$ for d = 5 cm and d_{accu} = 20 cm). It is thus deemed appropriate to neglect the plateau concentration in such a case.

Complex application patterns

If the maximum PEC_{soil} value in a multiple application sequence is reached before the last application (*e.g.*, due to the effects of varying plant interception), a slightly modified calculation procedure has to be used.

Let us assume that the length of the application sequence (the number of days between the first and last applications) is Δt. The maximum concentration in soil after continual use ($PEC_{soil,accu}$) can be expressed as

$$PEC_{soil,accu} = PEC_{soil,last} \cdot \frac{1}{1 - e^{-k \cdot t^*}} \quad (14)$$

where $PEC_{soil,last}$ is the concentration in soil after the last application in the whole sequence and t* is the number of days between two events where $PEC_{soil,last}$ is reached minus the length of the application sequence, *i.e.*, t*=365-Δt days for yearly applications, t*=730-Δt days for bi-yearly applications, *etc.* The same approach (replacing t by t*) is used for all the steps described in the previous section. Other parts of the calculation are not affected.

This provides a conservative assessment since the degradation of the compound in soil is assumed to happen for a shorter time than in reality.

II. Results and Discussion

Detailed results (maximum, short-term and long-term PEC and TWA, and accumulation values) for individual uses are provided in Table 9.2.4- 14 to Table 9.2.4- 17.

Table 9.1.3- 14: PECsoil of fluopicolide, oil seed rape (winter), 1 × 12 g a.s./ha, 0% interception

PECsoil (mg/kg)		**Oil Seed Rape (winter)**			
		Single application		**Multiple applications**	
		Actual	**TWA**	**Actual**	**TWA**
Initial		0.016	-	0.016	-
Short term	24 h	0.016	0.016	0.016	0.016
	2 d	0.016	0.016	0.016	0.016
	4 d	0.016	0.016	0.016	0.016
Long term	7 d	0.016	0.016	0.016	0.016
	14 d	0.016	0.016	0.016	0.016
	21 d	0.015	0.016	0.015	0.016
	28 d	0.015	0.016	0.015	0.016
	42 d	0.015	0.016	0.015	0.016
	50 d	0.015	0.015	0.015	0.015
	100 d	0.014	0.015	0.014	0.015
Plateau concentration (20 cm) after year 5		0.005	-	0.005	-
PECaccumulation (PECact + PECsoil plateau)		0.021	-	0.021	-

Table 9.1.3- 15: PECsoil of M-01, oil seed rape (winter), 1 × 12 g a.s./ha, 0% interception

PECsoil (mg/kg)		Oil Seed Rape (winter)			
		Single application		Multiple applications	
		Actual	TWA	Actual	TWA
Initial		0.004	-	0.004	-
Short term	24 h	0.004	0.004	0.004	0.004
	2 d	0.004	0.004	0.004	0.004
	4 d	0.004	0.004	0.004	0.004
Long term	7 d	0.004	0.004	0.004	0.004
	14 d	0.004	0.004	0.004	0.004
	21 d	0.004	0.004	0.004	0.004
	28 d	0.004	0.004	0.004	0.004
	42 d	0.003	0.004	0.003	0.004
	50 d	0.003	0.004	0.003	0.004
	100 d	0.003	0.003	0.003	0.003
Plateau concentration (20 cm) after year 4		<0.001	-	<0.001	-
PECaccumulation (PECact + PECsoil plateau)		0.005	-	0.005	-

Table 9.1.3- 16: PECsoil of M-02, oil seed rape (winter), 1 × 12 g a.s./ha, 0% interception

PECsoil (mg/kg)		Oil Seed Rape (winter)			
		Single application		Multiple applications	
		Actual	TWA	Actual	TWA
Initial		0.002	-	0.002	-
Short term	24 h	0.001	0.001	0.001	0.001
	2 d	0.001	0.001	0.001	0.001
	4 d	<0.001	0.001	<0.001	0.001
Long term	7 d	<0.001	< 0.001	<0.001	< 0.001
	14 d	<0.001	< 0.001	<0.001	< 0.001
	21 d	<0.001	< 0.001	<0.001	< 0.001
	28 d	<0.001	< 0.001	<0.001	< 0.001
	42 d	<0.001	< 0.001	<0.001	< 0.001
	50 d	<0.001	< 0.001	<0.001	< 0.001
	100 d	<0.001	< 0.001	<0.001	< 0.001
Plateau concentration (20 cm) after year 0		<0.001	-	<0.001	-
PECaccumulation (PECact + PECsoil plateau)		0.002	-	0.002	-

Table 9.1.3- 17: PECsoil of M-03, oil seed rape (winter), 1 × 12 g a.s./ha, 0% interception

PECsoil (mg/kg)		Oil Seed Rape (winter)			
		Single application		Multiple applications	
		Actual	TWA	Actual	TWA
Initial		0.002	-	0.002	-
Short term	24 h	0.002	0.002	0.002	0.002
	2 d	0.002	0.002	0.002	0.002
	4 d	0.002	0.002	0.002	0.002
Long term	7 d	0.002	0.002	0.002	0.002
	14 d	0.002	0.002	0.002	0.002
	21 d	0.002	0.002	0.002	0.002
	28 d	0.002	0.002	0.002	0.002
	42 d	0.002	0.002	0.002	0.002
	50 d	0.002	0.002	0.002	0.002
	100 d	0.002	0.002	0.002	0.002
Plateau concentration (20 cm) after year 10		0.002	-	0.002	-
PECaccumulation (PECact + PECsoil plateau)		0.003	-	0.003	-

An overview of maximum PECsoil values of fluopicolide and its metabolites for all use patterns under consideration is shown in Table 9.1.3- 18.

Table 9.1.3- 18: Maximum PECsoil of fluopicolide and its metabolites for the uses assessed

Use pattern	Fluopicolide (mg/kg)	M-01 (mg/kg)	M-02 (mg/kg)	M-03 (mg/kg)
Oil Seed Rape (winter), 1 × 12 g a.s./ha	0.016	0.004	0.002	0.002

The accumulation potential of fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657188) and M-03 (AE 0608000) after long term use was also assessed, employing the larger soil depth for the calculation of the background concentration in cases where tillage is relevant. The results are presented in Table 9.1.3- 19. Please note that for technical reasons, accumulation calculation is performed and reported for all substances, even if they do not possess accumulation potential due to short half-life.

Table 9.1.3- 19: PECsoil of fluopicolide and its metabolites for the uses assessed, taking the effect of accumulation into account

Use pattern	PEC soil	Fluopicolide (mg/kg)	M-01 (mg/kg)	M-02 (mg/kg)	M-03 (mg/kg)
Oil Seed Rape (winter) 1 × 12 g a.s./ha	plateau (20 cm)	0.005	<0.001	<0.001	0.002
	total	0.021	0.005	0.002	0.003

III. Conclusion

The predicted environmental concentrations in soil (PEC_{soil}) of the active substance fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657188) and M-03 (AE 0608000) were calculated for use in oil seed rape (winter).

Assessment and conclusion by applicant:

The risk assessment report was conducted according to FOCUS (2014) and is considered valid to assess predicted environmental concentrations in soil (PEC_{soil}) for fluopicolide and its metabolites following application to oilseed rape (winter).

PEC_{soil} for fluoxastrobin

Data Point:	KCP 9.1.3/03
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluoxastrobin (FXA): PECsoil EUR - Use in oil seed rape (winter) in Europe
Report No:	EnSa-20-0437
Document No:	M-687159-01-1
Guideline(s) followed in study:	Guidance Documnet on Persistence in Soil EU Commision 9188/VI/97 rev.8 2000 and FOCUS 1997
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

The predicted environmental concentrations in soil (PEC_{soil}) of the active substance fluoxastrobin were calculated based on a first tier approach using a Microsoft® Excel spreadsheet. The use of fluoxastrobin in oilseed rape (winter) was assessed according to Good Agricultural Practice (GAP) under European cropping conditions. Calculations assumed an even distribution of the compound in upper 0 - 5 cm soil layer following application and a soil density of 1.5 g/cm^3.

The maximum PECsoil values of fluoxastrobin for all use patterns under consideration was 0.012 mg/kg.

I. Materials and Methods

The predicted environmental concentrations in soil (PEC_{soil}) of the active substance fluoxastrobin were calculated based on a first tier approach using a Microsoft® Excel spreadsheet. The use of fluoxastrobin in oilseed rape (winter) was assessed according to Good Agricultural Practice (GAP) under European cropping conditions. Calculations assumed an even distribution of the compound in upper 0 - 5 cm soil layer following application and a soil density of 1.5 g/cm^3.

The use of fluoxastrobin in oilseed rape (winter) in Europe was assessed according to the Good Agricultural Practice (GAP) as summarised below.

Table 9.1.3- 20: Application data of fluoxastrobin according to the use pattern in Europe

Individual crop	FOCUS crop	Rate (g a.s./ha)	Interval (days)	Plant interception (%)	BBCH stage (-)	Amount reaching soil (g a.s./ha)
Oilseed Rape	Oil seed rape	1 × 9	-	0	00	1 × 9.000

(winter)	(winter)					

The calculations were based on the maximum intended application rate together with the maximum intended number of applications per season and (for multi-application sequences) the minimum interval between the applications. Crop interception was taken into account according to the BBCH growth stage, as recommended by FOCUS (2014).

Substance parameters used as input in the calculations are based on substance parameters whose derivation is taken from the EFSA LoEP [EFSA Scientific report 102, 13 June 2007]. The modelling parameters used for the calculations are given in Table 9.1.3- 21.

Table 9.1.3- 21: Compound and scenario input parameters as used for the calculation

Compound	Molar mass (g/mol)	Max occur. in soil (%)	DT50 (days)	Molar mass corr. factor (-)
Fluoxastrobin	458.8	100	119	1
Soil bulk density	1.5 kg/L			
Soil mixing depth	5 cm			
Tillage depth for plateau (if relevant)	20 cm			

The information which mixing depths are employed for individual uses assessed in this report is provided in Table 9.1.3- 22.

Table 9.1.3- 22: Mixing depths used for plateau calculation

Use pattern	Plateau mixing depth
Oil Seed Rape (winter)	20 cm

The details of the calculation can be found below.

Parent compound

1st tier estimation of the initial PEC_{soil} concentration is done using the equation

$$PEC_{soil} = \frac{A \cdot f}{\rho_{soil} \cdot d} \qquad (1)$$

with A being the nominal single field application rate, f the fraction reaching soil surface (taking into account crop interception factors according to FOCUS), ρ_{soil} the dry soil bulk density, and d the thickness of the soil layer.

In single application scenarios, the initial PEC_{soil} value is equal to the overall maximum. For multiple (n) applications with constant application rate, crop interception, and application interval, the maximum PEC_{soil} can be written as

$$PEC_{soil,max} = \frac{A \cdot f}{\rho_{soil} \cdot d} \cdot \frac{1 - e^{-k\,n\,\Delta t}}{1 - e^{-k\,\Delta t}} \qquad (2)$$

where Δt the application interval and k is the first order degradation rate, calculated from the soil half-life (DT_{50}) as

$$k = \frac{\ln 2}{DT_{50}} \quad (3)$$

For multiple (n) applications with variable application rate, crop interception, or application interval, the PEC_{soil} just after the application (i) can be calculated stepwise as

$$PEC(i)_{soil,max} = \frac{A(i) \cdot f(i)}{\rho_{soil} \cdot d} + PEC(i)_{soil,co} \quad (4)$$

where $PEC_{soil,co}$ represents the residue from the preceding applications at the time of the actual application. For the first application, $PEC_{soil,co}$ is zero, for the following applications it can be written as

$$PEC(i)_{soil,co} = PEC(i-1)_{soil} \cdot e^{-k\,\Delta t(i)} \quad (5)$$

with $\Delta t(i)$ being the time interval between applications (i-1) and (i). $PEC_{soil,max}$ is then defined as the maximum of the individual PEC_{soil} values.

$$PEC_{soil,max} = \max(PEC(i)_{soil,max}) \quad (6)$$

Metabolites

Maximum soil concentration of a metabolite is calculated in a similar manner to that of the parent compound, taking into account the maximum amount of the metabolite observed in soil ($X_{met,max}$) as well as the different molar masses of the parent (M_{par}) and metabolite (M_{met}).

The value of the initial metabolite concentration $PEC_{soil,met}$ is calculated using

$$PEC_{soil,met} = PEC_{soil,par} \cdot X_{met,max} \cdot \frac{M_{met}}{M_{par}} \quad (7)$$

where $PEC_{soil,par}$ is the respective initial parent concentration.

For a single application, the $PEC_{soil,met}$ value is equal to $PEC_{soil,max,met}$. For multiple applications, the maximum metabolite soil concentration has to be calculated using the equations (4) - (6) given in the previous section, with the parent dissipation rate replaced by that of the metabolite, and with maximum metabolite occurrence in soil and different molar masses of the parent and metabolite taken into account.

Concentrations over time

For first-order kinetics with a degradation rate k the declining PEC values at time t after the maximum can be calculated by

$$PEC(t) = PEC_{max} \cdot e^{-k\,t} \quad (8)$$

For a better comparison of exposure and effect data time-weighted average concentrations (TWA) may be useful. For first-order kinetics, the TWA are given by the following formula.

$$\mathrm{TWA(t)} = \mathrm{PEC_{max}} \cdot \frac{1}{\mathrm{k \cdot t}} \cdot (1 - \mathrm{e^{-k\,t}}) \qquad (9)$$

Accumulation after long term use

Potential accumulation after long term use is also assessed, based on the maximum $PEC_{soil,max}$ concentration of the respective compound, obtained as described before.

In case of a single application (or a multiple application sequence leading to the maximum PEC_{soil} after the last application), it can be shown that the maximum concentration in soil after perpetual use ($PEC_{soil,accu}$) can be expressed as

$$\mathrm{PEC_{soil,accu}} = \mathrm{PEC_{soil,max}} \cdot \frac{1}{1 - \mathrm{e^{-k\,t}}} \qquad (10)$$

where t is the number of days between two events where $PEC_{soil,max}$ is reached, *i.e.* 365 days for yearly applications, 730 days for bi-yearly applications, *etc.* This PEC_{soil} value is based on a normal mixing depth. In the case of a multiple application sequence leading to the maximum PEC_{soil} before the last application another approach has to be used.

The concentration in soil after an infinite number of applications and immediately before the application in the last year (the so called plateau concentration $PEC_{plateau}$) can be written as

$$\mathrm{PEC_{plateau}} = \mathrm{PEC_{soil,accu}} \cdot \frac{\mathrm{d}}{\mathrm{d_{accu}}} \cdot \mathrm{e^{-k \cdot t}} \qquad (11)$$

This formula can take the effect of deep soil tillage (or another mixing process) into account by distributing the soil residue amongst larger amounts of soil (larger soil mixing depth d_{accu} of, *e.g.*, 20 cm). In the absence of such mixing process, the factors involving mixing depth cancel out.
The total PEC_{soil} taking the effect of accumulation into account is then the sum of $PEC_{plateau}$ and the maximum PEC_{soil}, as defined previously.

$$\mathrm{PEC_{soil,total}} = \mathrm{PEC_{plateau}} + \mathrm{PEC_{soil,max}} \qquad (12)$$

The plateau concentration is driven by the dissipation DT_{50} in soil. The ratio between maximum PEC_{soil} due to actual application and the respective plateau concentration (taking effect of tillage into account here) can be written as

$$\frac{\mathrm{PEC_{plateau}}}{\mathrm{PEC_{soil,max}}} = \frac{\mathrm{e^{-k \cdot t}}}{1 - \mathrm{e^{-k \cdot t}}} \cdot \frac{\mathrm{d}}{\mathrm{d_{accu}}} \qquad (13)$$

Inspection of Equation (13) shows that this ratio is independent of the application rate. For a DT_{90} of less than a year, the plateau concentration is marginal (< 3% of actual $PEC_{soil,max}$ for d = 5 cm and d_{accu} = 20 cm). It is thus deemed appropriate to neglect the plateau concentration in such a case.

Complex application patterns

If the maximum PEC_{soil} value in a multiple application sequence is reached before the last application (*e.g.*, due to the effects of varying plant interception), a slightly modified calculation procedure has to be used.
Let us assume that the length of the application sequence (the number of days between the first and

last applications) is Δt. The maximum concentration in soil after continual use ($PEC_{soil,accu}$) can be expressed as

$$PEC_{soil,accu} = PEC_{soil,last} \cdot \frac{1}{1 - e^{-k \cdot t^*}} \qquad (14)$$

where $PEC_{soil,last}$ is the concentration in soil after the last application in the whole sequence and t* is the number of days between two events where $PEC_{soil,last}$ is reached minus the length of the application sequence, *i.e.*, t*=365-Δt days for yearly applications, t*=730-Δt days for bi-yearly applications, *etc.* The same approach (replacing t by t*) is used for all the steps described in the previous section. Other parts of the calculation are not affected.

This provides a conservative assessment since the degradation of the compound in soil is assumed to happen for a shorter time than in reality.

II. Results and Discussion

Detailed results (maximum, short-term and long-term PEC and TWA, and accumulation values) is provided in Table 9.1.3- 23.

Table 9.1.3- 23: PECsoil of fluoxastrobin in oil seed rape (winter), 1 x 9 g a.s./ha, 0% interception

PECsoil (mg/kg)		Oil Seed Rape (winter)			
		Single application		Multiple applications	
		Actual	TWA	Actual	TWA
Initial		0.012	-		
Short term	24 h	0.012	0.012		
	2 d	0.012	0.012		
	4 d	0.012	0.012		
Long term	7 d	0.012	0.012		
	14 d	0.011	0.012		
	21 d	0.011	0.011		
	28 d	0.010	0.011		
	42 d	0.009	0.011		
	50 d	0.009	0.010		
	100 d	0.007	0.009		
Plateau concentration (20 cm) after year 2		<0.001	-		
PECaccumulation (PECact + PECsoil plateau)		0.012	-		

An overview of maximum PECsoil values of fluoxastrobin for all use patterns under consideration is shown in Table 9.1.3- 24.

Table 9.1.3- 24: Maximum PECsoil of fluoxastrobin for the uses assessed

Use pattern	Fluoxastrobin (mg/kg)
Oil Seed Rape (winter), 1 × 9 g a.s./ha	0.012

The accumulation potential of fluoxastrobin after long term use was also assessed, employing the larger soil depth for the calculation of the background concentration in cases where tillage is relevant.

The results are presented in Table 9.1.3- 25.

Table 9.1.3- 25: PECsoil of fluoxastrobin for the uses assessed, taking the effect of accumulation into account

Use pattern	PECsoil	Fluoxastrobin (mg/kg)
Oilseed Rape (winter) 1×9 g a.s./ha	plateau (20 cm) total	<0.001 0.012

III. Conclusion

The predicted environmental concentrations in soil (PEC_{soil}) of the active substance fluoxastrobin were calculated for use in oil seed rape (winter).

Assessment and conclusion by applicant:

The risk assessment report was conducted according to FOCUS (2014) and is considered valid to assess predicted environmental concentrations in soil (PEC_{soil}) for fluoxastrobin in oilseed rape (winter).

CP 9.2 Fate and behaviour in water and sediment

CP 9.2.1 Aerobic mineralisation in surface water

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

CP 9.2.2 Water/sediment study

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

CP 9.2.3 Irradiated water/sediment study

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

CP 9.2.4 Estimation of concentrations in groundwater

CP 9.2.4.1 Calculation of concentrations in groundwater

Predicted environmental concentrations in groundwater (PEC_{GW})

Data Point:	KCP 9.2.4.1/01
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluopicolide (FLC): Core PECgw EUR - Modelling core info document for groundwater risk assessment in Europe
Report No:	VC/19/041J
Document No:	M-688396-01-1
Guideline(s) followed in study:	FOCUS Degradation Kinetics 2006 and 2014
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

This document summarises the substance data for fluopicolide and its metabolites as used for the purpose of groundwater risk assessment. The following deterministic pesticide fate models were used in the calculations:

- FOCUS PEARL
- FOCUS PELMO
- FOCUS MACRO

The parameters correspond to standard EU requirements.

Modelling reports utilising this core info document should have the substance data presented in the form as shown in Table 9.2.4- 1 and Table 9.2.4- 2.

Table 9.2.4- 1: Compound input parameters for fluopicolide and its metabolites – without aged sorption

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03* (AE 0608000)	M-05 (AE 1344122)
Common						
Molar mass	(g/mol)	383.59	190.03	225.56	399.58	253.2
Solubility	(mg/L)	2.8	2220	115000	10	120000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	0.888	0.914	0.889	0.971	0.942
Plant uptake factor	(-)	0.5	0.5	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	FLC	M01	M02	M03	M05
DT50	(days)	182.0	146.0	1.6	17.9	25.2
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	155.3	14.0	3.3	62.0	8.1
PELMO parameters						
Substance code	(-)	Fluopicolide	M-01	M-02	M-03	M-05
Rate constant	(1/day)	0.003809	0.004748	0.433217	0.038723	0.027506
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	267.7	241	5.7	106.9	14.0
MACRO parameters						
Substance code	(-)	Fluopicolide	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948
Parameter	**Unit**	**M-10 (AE 1344123)**	**M-11/12 (AE 1344119/ AE 1344120)**	**M-13 (Fluopicolide-P3)**	**M-14 (AE 1388273)**	**M-15 (AE 1413903)**
Common						
Molar mass	(g/mol)	271.17	287.17	241.55	241.19	463.64
Solubility	(mg/L)	100000	1000	1000	15800	160000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	1.0	1.0	1.0	0.942	0.937
Plant uptake factor	(-)	0	0	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	M10	M11-2	M13	M14	M15
DT50	(days)	35.4	87.6	20.7	9.4	145.0
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	1.1	0	0	5.7	10.9
PELMO parameters						
Substance code	(-)	M-10	M-11/12	M-13	M-14	M-15
Rate constant	(1/day)	0.019580	0.007913	0.033485	0.073739	0.004780
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	1.8	0	0	9.9	18.8
MACRO parameters						
Substance code	(-)	-	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

* Metabolite M-03 not simulated in alkaline soils

Table 9.2.4- 2: Compound input parameters for fluopicolide and metabolites – with aged sorption

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03* (AE 0608000)	M-05 (AE 1344122)
Common						
Molar mass	(g/mol)	383.59	190.03	225.56	399.58	253.2
Solubility	(mg/L)	2.8	2220	115000	10	120000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	0.888	0.914	0.889	0.971	0.942
Plant uptake factor	(-)	0.5	0.5	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	FLC	M01	M02	M03	M05
DT50	(days)	121.0	146.0	1.6	17.9	25.2
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	155.3	14.0	3.3	62.0	8.1
k_{des}	(1/day)	0.0356	0	0	0	0
F_{ne}	(-)	0.508	0	0	0	0
PELMO parameters						
Substance code	(-)	Fluopicolide	M-01	M-02	M-03	M-05
Rate constant	(1/day)	0.005728	0.004748	0.433217	0.038723	0.027506
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	267.7	24.1	5.7	106.9	14.0
MACRO parameters						
Substance code	(-)	Fluopicolide		-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

Parameter	Unit	M-10 (AE 1344123)	M-11/12 (AE 1344119/ AE 1344120)	M-13 (Fluopicolide-P3)	M-14 (AE 1388273)	M-15 (AE 1413903)
Common						
Molar mass	(g/mol)	271.17	287.17	241.55	241.19	463.64
Solubility	(mg/L)	100000	1000	1000	15800	160000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	1.0	1.0	1.0	0.942	0.937
Plant uptake factor	(-)	0	0	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	M10	M11-2	M13	M14	M15
DT50	(days)	35.4	87.6	20.7	9.4	145.0
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	1.1	0	0	5.7	10.9
k_{des}	(1/day)	0	0	0	0	0
F_{ne}	(-)	0	0	0	0	0
PELMO parameters						
Substance code	(-)	M-10	M-11/12	M-13	M-14	M-15
Rate constant	(1/day)	0.019580	0.007913	0.033485	0.073739	0.004780
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	1.8	0	0	9.9	18.8

MACRO parameters						
Substance code	(-)	-	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

* Metabolite M-03 not simulated in alkaline soils

I. Materials and Methods

Calculation of the substance parameters for fluopicolide and its metabolites M-01, M-02, M-03, M-05, M-10, M-11/M-12, M-13, M-14, and M-15 is detailed as follows: -

Figure 9.2.4- 1: Degradation pathway for fluopicolide in acidic soils

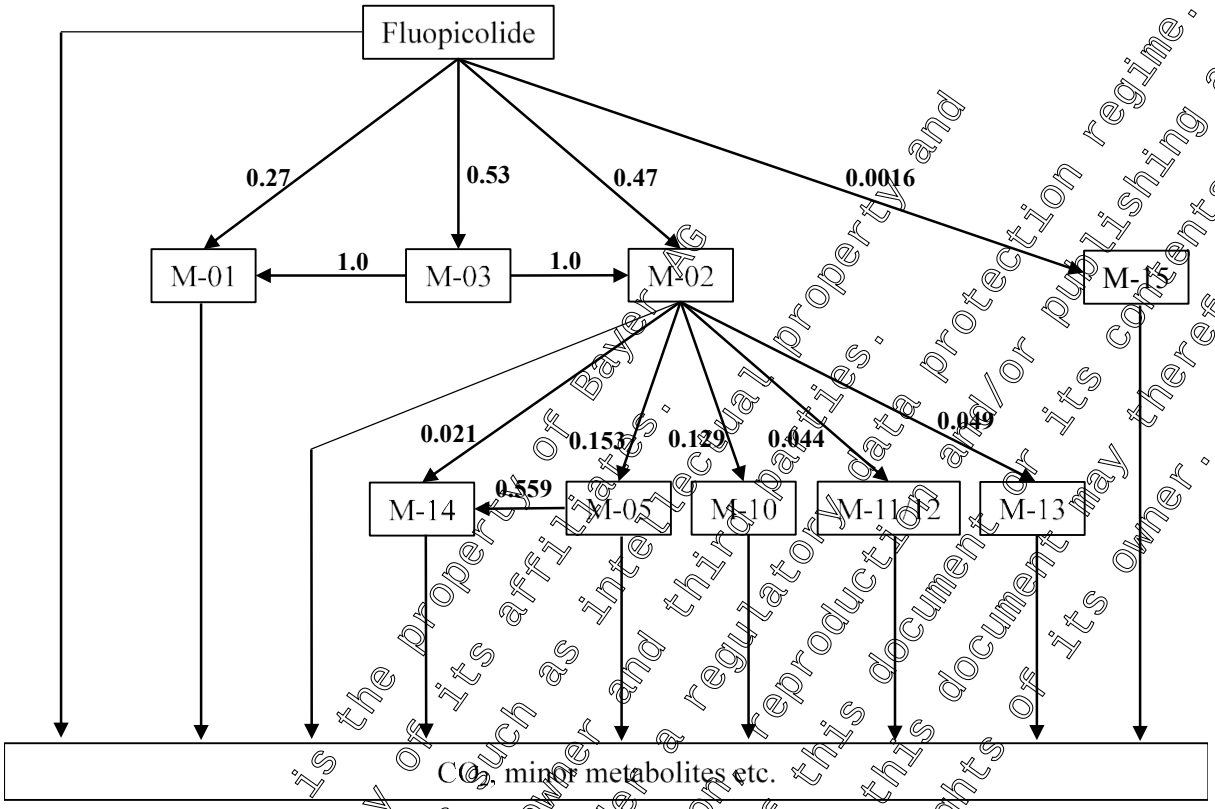


Figure 9.2.4- 2: Degradation pathway for fluopicolide in alkaline soils

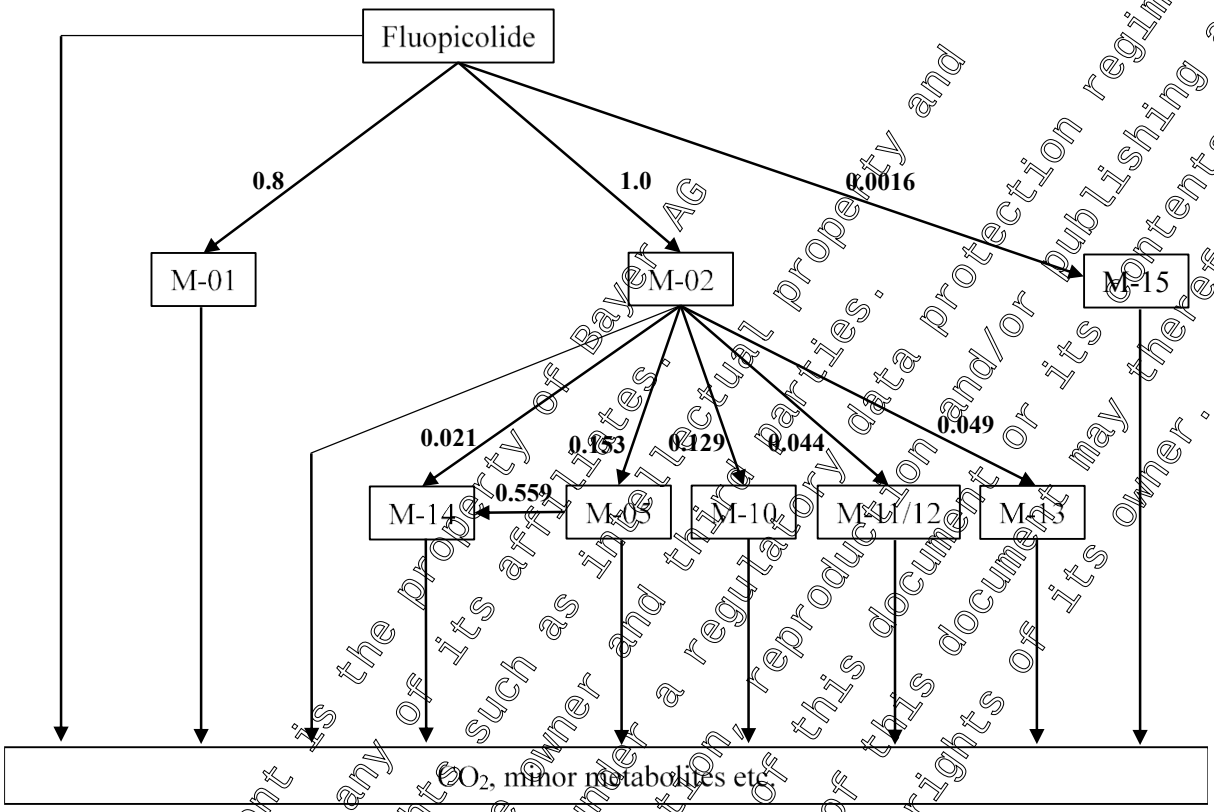


Table 9.2.4- 3: Degradation pathway related parameters for fluopicolide and its metabolites

Degradation fraction from → to (-) (FOCUS PEARL): **acidic soils**	FLC → M01: 0.27 FLC → M02: 0.47 FLC → M03: 0.53 FLC → M15: 0.0016 M03 → M01: 1.0 M03 → M02: 1.0 M02 → M05: 0.153 M02 → M10: 0.129 M02 → M11-2: 0.044 M02 → M13: 0.049 M02 → M14: 0.021 M05 → M14: 0.559
Degradation fraction from → to (-) (FOCUS PEARL): **alkaline soils**	FLC → M01: 0.8 FLC → M02: 1.0 FLC → M15: 0.0016 M02 → M05: 0.153 M02 → M10: 0.129 M02 → M11-2: 0.044 M02 → M13: 0.049 M02 → M14: 0.021 M05 → M14: 0.559

Partial DT_{50}/Degradation rate from → to (day or 1/day) (FOCUS PELMO)[a]: **acidic soils**	Pathway 1: Active Substance → M-02: 387.234 / 0.0017900 Active Substance → M-03: 343.396 / 0.0020190 Active Substance (TDS) → M-02: 257.447 / 0.0026920 Active Substance (TDS) → M-03: 228.302 / 0.0030360 Active Substance → BR/CO2: 0 M-03 → M-02: 17.9 / 0.0387230 M-02 → M-05: 10.458 / 0.0662790 M-02 → M-10: 12.403 / 0.0558850 M-02 → M-14: 76.190 / 0.0090980 M-02 → BR/CO2: 2.296 / 0.3018930 M-05 → M-14: 45.081 / 0.0153760 M-05 → BR/CO2: 57.143 / 0.0121300 M-10 → BR/CO2: 35.4 / 0.0195800 M-14 → BR/CO2: 9.4 / 0.0737390 Pathway 2: Active Substance → M-02: 387.234 / 0.0017900 Active Substance → M-03: 343.396 / 0.0020190 Active Substance (TDS) → M-02: 257.447 / 0.0026920 Active Substance (TDS) → M-03: 228.302 / 0.0030360 Active Substance → BR/CO2: 0 M-03 → M-02: 17.9 / 0.0387230 M-02 → M-11/12: 36.364 / 0.0190610 M-02 → M-13: 32.653 / 0.0212280 M-02 → BR/CO2: 1.764 / 0.3929410 M-11/12 → BR/CO2: 87.6 / 0.0079130 M-13 → BR/CO2: 20.7 / 0.0737390 Pathway 3: Active Substance → M-01: 674.074 / 0.0010280 Active Substance → M-03: 343.396 / 0.0020190 Active Substance → M-15: 113750 / 6.09E-06 Active Substance → BR/CO2: 917.339 / 0.000756 Active Substance (TDS) → M-01: 448.148 / 0.0015470 Active Substance (TDS) → M-03: 228.302 / 0.0030360 Active Substance (TDS) → M-15: 75625 / 9.17E-06 Active Substance (TDS) → BR/CO2: 609.879 / 0.0011370 M-03 → M-01: 17.9 / 0.0387230 M-01 → BR/CO2: 146 / 0.0047480 M-15 → BR/CO2: 145 / 0.0047800
Partial DT_{50}/Degradation rate from → to (day or 1/day) (FOCUS PELMO)[a]: **alkaline soils**	Pathway 1: Active Substance → M-02: 182 / 0.0038090 Active Substance (TDS) → M-02: 121 / 0.0057280 Active Substance → BR/CO2: 0 M-02 → M-05: 10.458 / 0.0662790 M-02 → M-10: 12.403 / 0.0558850 M-02 → M-14: 76.190 / 0.0090980 M-02 → BR/CO2: 2.296 / 0.3018930 M-05 → M-14: 45.081 / 0.0153760 M-05 → BR/CO2: 57.143 / 0.0121300 M-10 → BR/CO2: 35.4 / 0.0195800 M-14 → BR/CO2: 9.4 / 0.0737390 Pathway 2: Active Substance → M-02: 182 / 0.0038090 Active Substance (TDS) → M-02: 121 / 0.0057280 Active Substance → BR/CO2: 0 M-02 → M-11/12: 36.364 / 0.0190610

	M-02 → M-13: 32.653 / 0.0212280 M-02 → BR/CO2: 1.764 / 0.3929410 M-11/12 → BR/CO2: 87.6 / 0.0079130 M-13 → BR/CO2: 20.7 / 0.0737390 Pathway 3: Active Substance → M-01: 227.500 / 0.0030470 Active Substance → M-15: 113750 / 6.09E-06 Active Substance → BR/CO2: 917.339 / 0.000756 Active Substance (TDS) → M-01: 151.250 / 0.0045830 Active Substance (TDS) → M-15: 75625 / 9.17E-06 Active Substance (TDS) → BR/CO2: 609.879 / 0.0011370 M-01 → BR/CO2: 146 / 0.0047480 M-15 → BR/CO2: 145 / 0.0047890
Conversion factor from → to (-) (FOCUS MACRO)[b]: **acidic soils**	-
Conversion factor from → to (-) (FOCUS MACRO)[b]: **alkaline soils**	-

[a] Calculated as *ln(2) / DT50 × formation fraction*
[b] Calculated as *molar mass / molar mass predecessor × formation fraction*

Figure 9.2.4- 3 PELMO simulation pathways for fluopicolide in acidic soils

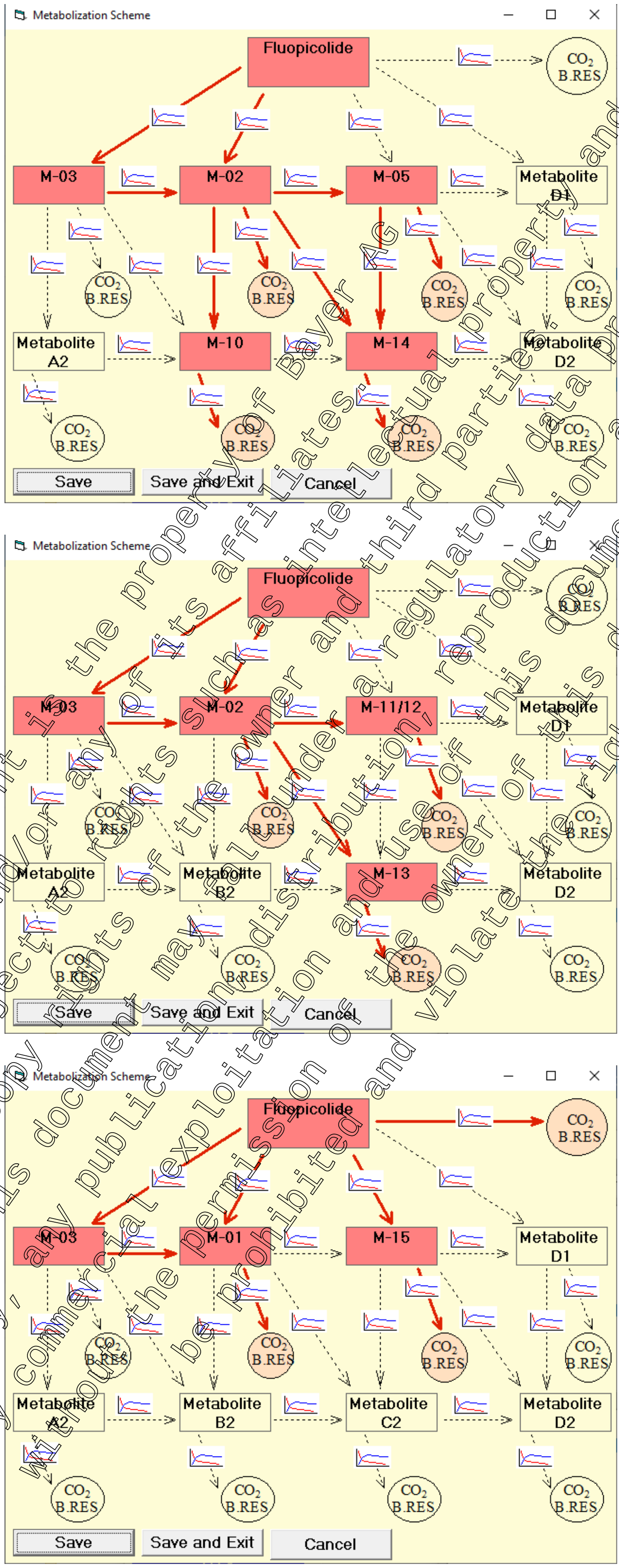
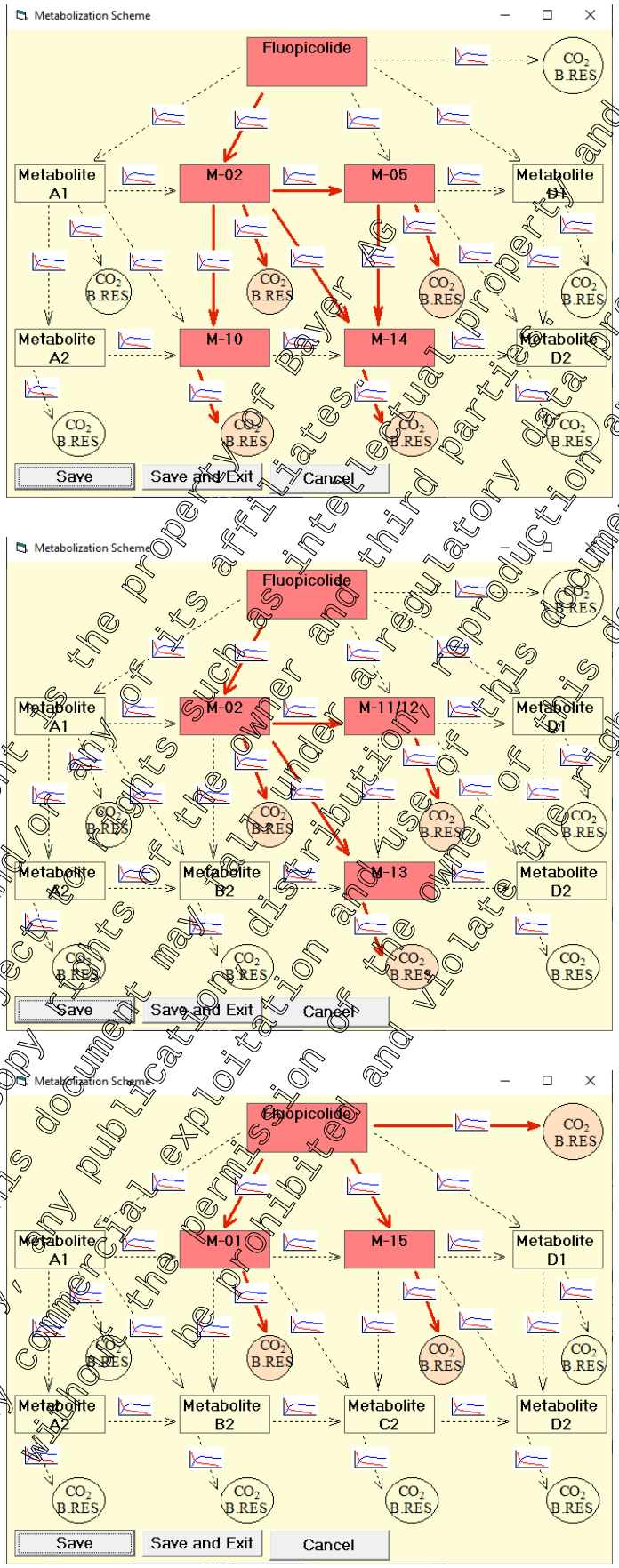


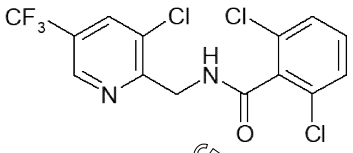
Figure 9.2.4- 4: PELMO simulation pathways for fluopicolide in alkaline soils



Fluopicolide (AE C638206)

Physico-Chemical Properties

Structural formula



Common name	Fluopicolide (AE C638206)
Chemical name (IUPAC)	2,6-dichloro-N-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]methyl]-benzamide
Molar mass	383.59 g mol^{-1}
Water solubility	2.8 mg L^{-1} at 20°C (M-234496-01-1, [redacted], 2003a)
Vapour pressure	3.03 × 10^{-7} Pa at 20°C (M-197457-01-1, [redacted] 2000)

Degradation in Aerobic Soil

Laboratory studies

The aerobic degradation and metabolism of fluopicolide in soil was investigated in the laboratory by M-201230-02-1, [redacted], (2003); M-241049-01-1, [redacted] (2003a); M-241052-01-1, [redacted] (2003b); M-241051-01-1, [redacted] (2003c); M-550687-01-1, [redacted] (2016a); M-555570-01-1, [redacted] (2016b) and M-655056-01-1, [redacted] (2019). A summary of the modelling endpoint DegT$_{50}$ values derived for fluopicolide (KCA 7.1.2.1.1/10; M-685680-01-1, [redacted] 2020), normalised to 20°C and pF2, is given in Table 9.2.4- 4.

Table 9.2.4- 4: Summary of DegT$_{50}$ values derived for fluopicolide under laboratory conditions (after M-685680-01-1, Carnall *et al.*, 2020)

Applied compound	Study	Soil	Model selected	DegT$_{50}$ un-normalised (d)	DegT$_{50}$ normalised to 20°C and pF2 (d)
Fluopicolide	M-201230-02-1, [redacted], 2003	Münster	SFO	212.0	212.0
		Sarotti	SFO	191.2	191.2
	M-241049-01-1, [redacted], 2003a	Abington (non-sterile)	SFO	348.0	340.2
	M-241051-01-1, [redacted], 2003b	Lamberton	SFO	1290.0	1037.9
	M-241052-01-1, [redacted], 2003c	Lamberton	SFO	358.0	395.8
	M-550687-01-1, [redacted], 2016a	Pikeville	DFOP	612.9[a] / 30.1[b]	616.0[a] / 30.3[b]
		Albaro/Marcomcini	DFOP	146.2[a] / 2.8[b]	146.2[a] / 2.8[b]
		Great Chishill	DFOP	312.4[a] / 2.7[b]	312.4[a] / 2.7[b]
		[redacted]	DFOP	155.5[a] / 7.2[b]	155.5[a] / 7.2[b]
		Mas du Coq	DFOP	216.7[a] / 10.5[b]	193.7[a] / 9.4[b]
		Parcey Meslay	DFOP	202.5[a] / 8.1[b]	202.5[a] / 8.1[b]
		Vilobi d'Onyar	DFOP	93.5[a] / 7.8[b]	93.5[a] / 7.8[b]
	M-555570-01-1, [redacted], 2016b	Dollendorf II	DFOP	111.4[a] / 0.6[b]	111.4[a] / 0.6[b]

Applied compound	Study	Soil	Model selected	DegT$_{50}$ un-normalised (d)	DegT$_{50}$ normalised to 20°C and pF2 (d)
	[redacted] 2016b	[redacted]	DFOP	137.7^a / 4.2^b	137.7^a / 4.2^b
		[redacted]	DFOP	141.3^a / 6.3^b	141.3^a / 6.3^b
		[redacted]	DFOP	133.5^a / 9.4^b	133.5^a / 9.4^b
	M-655056-01-1, [redacted] 2019	Abington 2	DFOP	142.1^a / 1.9^b	142.1^a / 1.9^b
		Lamberton	DFOP	176.1^a / 2.8^b	145.1^a / 2.3^b
		Lignieres	DFOP	141.4^a / 1.4^b	141.4^a / 1.4^b
		Münster	DFOP	170.1^a / 5.3^b	124.5^a / 3.9^b
		Pikeville	DFOP	155.2^a / 4.1^b	129.4^a / 3.5^b
		Sarotti 2	DFOP	161.2^a / 1.6^b	143.6^a / 1.4^b
Geometric mean (SFO and DFOP slow phase)					**181.6^c**

a – Pseudo-SFO value based on slow phase of decline (calculated as ln(2)/k_2 and normalised if applicable)
b – Pseudo-SFO value based on fast phase of decline (calculated ln(2)/k_1 and normalised if applicable)
c – Geometric mean calculated of DegT$_{50}$ values from Lamberton soils prior to calculation of overall geometric mean

Field Dissipation Studies

DegT$_{50}$ values for fluopicolide, normalised to 20°C and pF2, have been derived by M-685675-01-1, [redacted] (2020a) and M-685676-01-1, [redacted] (2020b) from 12 terrestrial field dissipation studies (M-651636-01-1, [redacted] (2019a); M-218667-01-1, [redacted] (2003); M-220477-02-1, [redacted] (2003); M-234424-01-1, [redacted] (2004); M-247945-01-1, [redacted] (2005a); M-251338-01-1, [redacted] (2005b); M-218672-01-1, [redacted] (2003)). A summary of the modelling endpoint DegT$_{50}$ values derived for fluopicolide is given in Table 9.2.4- 5.

Table 9.2.4- 5: Summary of DegT$_{50}$ values (normalised to 20°C and pF2) derived for fluopicolide from terrestrial field dissipation studies (after M-685675-01-1, [redacted] 2020a and M-685676-01-1, [redacted] 2020b)

Soil type	Aerobic field conditions					
	Location (country)	**pH (CaCl$_2$)**	**Depth (cm)**	**St. (χ^2err) (%)**	**Method of calculation**	**DegT$_{50}$ (d) norm**
Silt loam	Burscheid (Germany)	5.9	0-120	9.80	SFO	111.9
Clay	Great Chishill (UK)	7.8	0-120	11.64	SFO	216.9
Sandy loam	Lignieres de Touraine (France)	6.9	0-120	4.82	SFO	158.6
Clay loam	St.Etienne du Gres (France)	8.1	0-120	4.90	SFO	303.2
Clay loam	Albaro di Ronco all'Adige (Italy)	7.7	0-120	9.99	SFO	237.3
Sandy clay loam	Vilobi d'Onyar (Spain)	6.9	0-120	6.20	SFO	166.8
Loamy sand	Philippsburg (Germany)	6.4	0-50	9.477	SFO	199.6
Sandy clay loam	Rödelsee (Germany)	7.4	0-30	21.59	SFO	146.4
Sand	Huntlosen (Germany)	4.9	0-50	15.46	SFO	168.4
Loamy sand	Valencia (Spain)	7.3	0-30	13.95	SFO	317.4
Sandy silt	Appilly (France)	7.1	0-30	11.16	SFO	144.2
Sandy silt loam	Senas (France)	7.6	0-45	9.864	SFO	136.5
					Geometric mean	**183**

Degradation in Aerobic Soil: Overall DegT$_{50}$ value

Degradation half-lives for fluopicolide derived from laboratory and field dissipation studies were compared using the EFSA DegT$_{50}$ Endpoint Selector (EFSA, 2014). This comparison indicated that the laboratory and field DegT50 values for fluopicolide should be combined.

An overall geometric mean DegT$_{50}$ value of **182 days** in soil was derived for fluopicolide for use in surface water calculations, including both laboratory and field data.

Plant Uptake

The plant uptake factor for fluopicolide was set to **0.5**. Residues of fluopicolide and metabolites have been found in different plants in a rotational crop study (M-240707-03-1, [redacted] 2003). Fluopicolide is redistributed via the xylem (acropetal systemic activity) but is not phloem mobile. TSCF calculated according to Briggs is 0.47.

The uptake of fluopicolide into potato plants has been investigated in a new study (M-688372-01-1, [redacted] 2020) and the transpiration stream concentration factor (TSCF) determined. The mean TSCF was determined as 0.71 (DAT2), 0.75 (DAT4) and 0.82 (DAT6), thus fully supporting the use of the default value of 0.5 in the PECgw evaluations.

Adsorption

The adsorption and desorption of fluopicolide has been investigated in five studies (M-241425-01-1, [redacted] 2003b; M-233840-01-1, [redacted] 2003b; M-544194-02-1, [redacted] 2015; M-572869-01-1, [redacted] 2016; M-595721-01-1, [redacted] 2017). A summary of K_{OC} and 1/n values derived for fluopicolide from these studies is given in Table 9.2.4- 6.

A geometric mean K_{OC} value of **267.7 mL/g**, corresponding to a K_{OM} value of 155.3 mL/g ($K_{OM} = K_{OC} \div 1.724$), was used for fluopicolide in the modelling, with an arithmetic mean 1/n value of **0.888**.

Table 9.2.4- 6: Summary of sorption parameters derived for fluopicolide

Study reference	Soil	Soil Code	Texture	pH	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-241425-01-1, [redacted] (2003b)	Pikeville Sediment	EFS-54	loam	4.5	2.07	7.73	373*	0.926*
	Pikeville, North Carolina	EFS-65	sand	4.7	0.5	1.42	283	0.924
	Abington	EFS-86	sandy loam	7.5	2.21	7.53 (**3.36)	341 (**151.6)	0.929 (**0.882)
	Sarotti	EFS-88	silty clay loam	7.4	0.9	3.2	356	0.905
	Münster	EFS-93	loamy sand	5.7	1.3	4.54	349	0.929
	Münster	EFS-94	loamy sand	6.2	0.2	0.21	106*	0.931*
	Münster	EFS-95	loamy sand	6.2	0.2	0.17	83*	0.951*
M-233840-01-1, [redacted] (2003b)	Philippsburg	03/02	sandy loam	6.3	0.6	1.49	248	0.841
	Senas	03/03	clay loam	7.6	1.5	3.59	239	0.882
	Huntlosen	03/04	loamy sand	5.3	1.6	9.27	580	0.953
	Rodelsee	03/05	clay	7	1.5	2.59	172	0.859
M-544194-02-1, [redacted] (2015)	[redacted]	WuW	loam	5	1.8	4.65	258.6	0.9258
	[redacted]	HaH	silt loam	6.1	1.9	6.22	327.5	0.8741
	Dollendorf II,	Doll	clay loam	7.3	4.8	11.71	244.1	0.8596
	[redacted]	AXXa	sandy loam	6.5	1.5	4.04	269.3	0.8723

Study reference	Soil	Soil Code	Texture	pH	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-572869-01-1, [redacted] (2016)	Burscheid	VG08	silt loam	6.1	0.7	2.12	303.3	0.8868
	Great Chishill	ENG2	clay	7.3	2.1	5.40	257.0	0.9076
	Parcay Meslay	FR09B	loam	6.7	1.3	3.35	257.4	0.8992
	Tarascon Le Cayades	FR08	clay loam	7.6	0.9	1.84	204.9	0.8668
	Valerio Tomelini	IT09	silty clay	7.2	2.1	3.93	187.0	0.9110
	Vilobi D’Onyar	SPA01	sandy loam	6.3	0.8	2.34	292.0	0.8818
M-595721-01-1, [redacted] (2017)	Abington	AB	sandy loam	7.3	2.6	5.6	214.7	0.868
	Lamberton	LB	loam	5.6	2.6	8.6	331.9	0.844
	Lignieres	LN	sandy loam	5.7	0.8	2.9	363.1	0.888
	Muenster	MS	loamy sand	5.6	1.2	3.4	282.6	0.916
	Pikeville	PV	loamy sand	4.5	1.8	6.2	342.6	0.873
	Sarotti	SR	silty clay loam	6.9	1.4	2.6	185.6	0.851
						Arithmetic mean	-	**0.888**
						Geometric mean	**267.7**	-

*excluded from calculations, **checklist value used for geomean and average

Aged sorption

Data from three aerobic degradation and time-dependent sorption studies in sixteen soils (M-550687-01-1, [redacted] 2016a; M-555570-01-1, [redacted] 2016b and M-655056-01-1, [redacted], 2019) were evaluated by M-685678-02-1, [redacted] (2020a). The aged sorption parameters derived for fluopicolide are summarised in Table 9.2.4-7.

Existing lower-tier degradation study data for fluopicolide from laboratory studies (M-201230-02-1, [redacted], 2003; M-241049-01-1, [redacted], 2003a; M-241052-01-1, [redacted] 2003b; M-241051-01-1, [redacted], 2003c and M-685680-01-1, [redacted] 2020) and field studies (M-651636-01-1, [redacted] 2019a; M-685675-01-1, [redacted] 2020a; M-218667-01-1, [redacted], 2003; M-220477-02-1, [redacted] 2003; M-234424-01-1, [redacted] 2004; M-247945-01-1, [redacted] 2005a; M-251338-01-1, [redacted], 2005b; M-218672-01-1, [redacted] 2003; M-685676-01-1, [redacted] 2020b) were also evaluated to derive DegT50eq values (M-687157-01-1, [redacted], 2020b). When combined with the higher-tier aged-sorption values, this yielded an overall geometric mean DegT50eq of **121 days** (Table 9.2.4- 8) for use in exposure modelling, in combination with the mean aged-sorption parameters: Fne **0.508** and kdes **0.0356 d^{-1}**.

The F_{ne} and k_{des} values require conversion for use in MACRO, resulting in $F_{neMACRO}$ **0.337** and α_{MACRO} **0.0120**.

Table 9.2.4- 7: Aged-sorption parameters derived for fluopicolide (after M-685678-02-1, [redacted] 2020a)

Soil	f_{NE} (-)	K_{des} (1/d)	DT_{50},eq (d)	DT_{50}, eq 20°C, pF2 (d)	Evidence of aged sorption	Robust parameters
[redacted]	0.553	0.0432	80.5	80.5	Yes	Yes
Dollendorf	0.271	0.0433	98.6	98.6	Yes	Yes
[redacted]	0.632	0.0420	69.8	69.8	Yes	Yes
[redacted]	0.785	0.0467	45.4	45.4	Yes	Yes
[redacted]	0.506	0.0507	76.2	76.2	Yes	Yes
Great Chishill	0.571	0.0248	170.9	170.9	Yes	Yes
Parcey Meslay	0.493	0.0524	111.0	111.0	Yes	Yes
Mas du Coq	0.514	0.0310	124.2	108.4	Yes	Yes
Albaro	0.303	0.0287	112.2	112.2	Yes	Yes
Vilobi d'Onyar	0.435	0.0575	52.2	52.2	Yes	Yes
Abington	0.289	0.0885	97.5	97.5	Yes	Yes
Lamberton	0.830	0.0145	111.2	91.6	Yes	Yes
Munster	0.524	0.0163	103.1	75.4	Yes	Yes
Pikeville	0.710	0.0319	80.2	66.8	Yes	Yes
Sarrotti	0.484	0.0534	111.5	99.3	Yes	Yes
Lignieres	0.638	0.0158	96.8	96.8	Yes	Yes
Geometric mean	**0.508**	**0.0356**		**86.6**	-	-

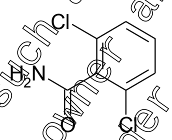
Table 9.2.4- 8: Overall $DegT_{50eq}$ evaluation results (after M-687157-01-1, [redacted] 2020b)

Soil	$DegT_{50}$, eq (days)	Derivation
[redacted]	80.5	TDS – PEARLneq
Dollendorf	98.6	TDS – PEARLneq
[redacted]	69.8	TDS – PEARLneq
[redacted]	45.4	TDS – PEARLneq
[redacted]	76.2	TDS – PEARLneq
Great Chishill	170.9	TDS – PEARLneq
Parcey Meslay	111.0	TDS – PEARLneq
Mas du Coq	108.4	TDS – PEARLneq
Albaro	112.2	TDS – PEARLneq
Vilobi d'Onyar	52.2	TDS – PEARLneq
Abington	97.5	TDS – PEARLneq
Lamberton	91.6	TDS – PEARLneq
Munster	75.4	TDS – PEARLneq
Pikeville	66.8	TDS – PEARLneq
Sarrotti	99.3	TDS – PEARLneq
Lignieres	96.8	TDS – PEARLneq
Munster	178.1	Lab Tier 1 refit
Sarrotti	138.6	Lab Tier 1 refit
Abington	256.4	Lab Tier 1 refit
Lamberton	532.5	Lab Tier 1 refit

Soil	$DegT_{50}$, eq (days)	Derivation
Pikeville	295.2	Lab Tier 1 refit
Burscheid (Germany)	84.3	Field Scaling factor 1
Great Chishill (UK)	155.8	Field Scaling factor 1
Lignieres de Touraine (France)	109.8	Field Scaling factor 1
St.Etienne du Grès (France)	234.2	Field Scaling factor 1
Albaro di Ronco all'Adige (Italy)	205.3	Field Scaling factor 1
Vilobi d'Onyar (Spain)	132.5	Field Scaling factor 1
Philippsburg (Germany)	158.9	Field Scaling factor 1
Rödelsee (Germany)	109.0	Field Scaling factor 1
Huntlosen (Germany)	124.7	Field Scaling factor 1
Valencia (Spain)	234.4	Field Scaling factor 1
Appilly (France)	107.6	Field Scaling factor 1
Senas (France)	101.3	Field Scaling factor 1
Geometric mean	**121**	-

M-01 (BAM; AE C653711)

Physico-Chemical Properties
Structural formula



Common name	M-01 (BAM; AE C653711)
Chemical name (IUPAC)	2,6-dichlorobenzamide
Molar mass	190.03 g mol^{-1}
Water solubility	2220 mg L^{-1} at 20°C (M-505637-01-1, [redacted] 2014)
Vapour pressure	Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

Laboratory studies

The aerobic degradation of M-01 (BAM) in soil was investigated in the laboratory by M-234320-01-1, [redacted] (2002). In addition, M-01 was observed to form from fluopicolide in six studies (M-241049-01-1, [redacted], 2003a; M-241052-01-1, [redacted], 2003b; M-241051-01-1, [redacted] 2003c; M-550687-01-1, [redacted] 2016a; M-555570-01-1, [redacted] 2016b and M-655056-01-1, [redacted] 2019) and from M-03 in one study (M-241188-01-1, [redacted] 2003). A summary of the modelling endpoints derived for M-01 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted] 2020) is given in Table 9.2.4- 9.

Overall formation fractions for M-01 (BAM) from fluopicolide, considering both direct formation and formation *via* metabolite M-03, were also derived by M-685680-01-1, [redacted] (2020), and are summarised in Table 9.2.4- 10. The overall arithmetic mean formation fraction of M-01 from fluopicolide was 0.8. Where metabolite M-03 was included in the groundwater simulations (i.e. for acidic soils), this was implemented by assuming a molar formation fraction of **0.27** from fluopicolide, with a molar formation fraction of **1.0** from metabolite M-03 (where ffm FLC→M-03 = 0.53). Where

M-03 was not included in the simulations (i.e. for alkaline soils), the molar formation fraction of M-01 from fluopicolide was set to **0.8**.

Table 9.2.4- 9: Summary of modelling endpoints derived for M-01 (BAM) under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised to 20°C and pF2 (d)
Fluopicolide	M-201230-02-1 [redacted] 2003	Münster	SFO	1000[a]	1000[a]
		Sarotti	SFO	1000[a]	1000[a]
	M-241049-01-1 [redacted], 2003a	Abington (non-sterile)	SFO	1000[a]	1000[a]
	M-241052-01-1 [redacted], 2003b	Lamberton	SFO	1000[a]	1000[a]
	M-241051-01-1 [redacted], 2003c	Lamberton	SFO	1000[a]	1000[a]
		Pikeville	SFO	173.1	174.0
	M-550687-01-1 [redacted] 2016a	Albaro/Marcomcini	SFO	417.3	417.3
		Great Chishill	SFO	1000[a]	1000[a]
		[redacted]	SFO	571.7	571.7
		Mas du Coq	SFO	472.2	422.2
		Parcey Meslay	SFO	908.4	908.4
		Vilobi d'Onyar	SFO	323.9	323.9
	M-555570-01-1 [redacted] 2016b	Dollendorf II	SFO	159.7	159.7
		[redacted]	SFO	869.3	869.3
		[redacted]	SFO	556.2	556.2
		[redacted]	SFO	1000[a]	1000[a]
	M-655056-01-1 [redacted], 2019	Abington 2	SFO	175.6	175.6
		Lamberton	SFO	1000[a]	1000[a]
		Lignières	SFO	1000[a]	1000[a]
		Münster	SFO	294.7	215.6
		Pikeville	SFO	135.9	113.3
		Sarotti 2	SFO	267.1	237.9
M-01	M-234320-01-1, [redacted] 2002	Bethany	SFO	1858.0	2077.6
		North Dakota	SFO	568.8	913.6
M-03	M-241188-01-1, [redacted] 2003	Münster	SFO	1000[a]	1000[a]
		Pikeville	SFO	1000[a]	1000[a]
				Geometric mean	**569.5[d]**

a – Conservative default value
b – Pseudo-SFO value based on slow phase of decline (calculated as ln(2)/k_2 and normalised if applicable)
c – Pseudo-SFO value based on fast phase of decline (calculated ln(2)/k_1 and normalised if applicable)
d – Geometric mean calculated of DT_{50} values from Lamberton soil prior to calculation of overall geometric mean.

Table 9.2.4- 10: Overall formation fraction of M-01 (BAM) from fluopicolide

Applied compound	Study	Soil	ffm FLC→M-01	ffm FLC→M-03	ffm M-03→M-01	Overall ffm from FLC
Fluopicolide	M-201230-02-1 [redacted] 2003	Münster	0.3914	0.6086	0.3892	0.6283
		Sarotti	0.798	-	-	0.798
	M-241049-01-1 [redacted] 2003a	Abington (non-sterile)	0.8406	-	-	0.8406
	M-241052-01-1 [redacted] 2003b	Lamberton	0.7156	-	-	0.7156
	M-241051-01-1 [redacted] 2003c	Lamberton	0.4067	0.5933	1	1
		Pikeville	1	-	-	1
	M-550687-01-1 [redacted] 2016a	Albaro/Marcomcini	0.8262	-	-	0.8262
		Great Chishill	0.6013	-	-	0.6013
		[redacted]	0.8953	-	-	0.8953
		Mas du Coq	0.8075	-	-	0.8075
		Parcey Meslay	0.8286	-	-	0.8286
		Vilobi d'Onyar	0.9776	-	-	0.9776
	M-555570-01-1 [redacted] 2016b	Dollendorf II	0.819	-	-	0.819
		[redacted]	0.8773	-	-	0.8773
		[redacted]	0.8156	-	-	0.8156
		[redacted]	0.8022	-	-	0.8022
	M-655056-01-1 [redacted] 2019	Abington 2	0.7879	-	-	0.7879
		Lamberton	0.7252	-	-	0.7252
		Lignieres	0.6264	-	-	0.6264
		Münster	0.9101	-	-	0.9101
		Pikeville	0.39	0.4009	1	0.7909
		Sarotti 2	0.6227	-	-	0.6227
					Arithmetic mean	**0.80[a]**

[a] – Arithmetic mean calculated of overall formation fractions from Lamberton soil prior to calculation of overall arithmetic mean.

Field Dissipation Studies

$DegT_{50}$ values for M-01 (BAM), normalised to 20°C and pF2, have been derived by M-685675-01-1, [redacted] (2020a) from five terrestrial field dissipation studies (M-650733-02-1, [redacted] 2019b). A summary of the modelling endpoint $DegT_{50}$ values derived for M-01 Table 9.2.4- 11.

Table 9.2.4- 11: Summary of $DegT_{50}$ values (normalised to 20°C and pF2) derived for M-01 (BAM) from terrestrial field dissipation studies (after M-685675-01-1, [redacted] 2020a)

	Aerobic field conditions					
Soil type	**Location (country)**	**pH ($CaCl_2$)**	**Depth (cm)**	**St. (χ^2err) (%)**	**Method of calculation**	**$DegT_{50}$ (d) norm**
Silt loam	Burscheid (Germany)	5.9	0-120	14.68	SFO	94.0
Sandy loam	Lignieres de Touraine (France)	6.9	0-120	7.82	SFO	191.1
Clay loam	St.Etienne du Grès (France)	8.1	0-120	5.87	SFO	179.9
Clay loam	Albarodi Ronco all'Adige (Italy)	7.7	0-120	13.93	SFO	151.8
Sandy clay loam	Vilobi d'Onyar (Spain)	6.9	0-120	10.94	SFO	136.3
					Geometric mean	**146**

Degradation in Aerobic Soil: Overall $DegT_{50}$ value

Degradation half-lives for M-01 (BAM) derived from laboratory and field dissipation studies were compared using the EFSA $DegT_{50}$ Endpoint Selector (EFSA, 2014). This comparison indicated that the field $DegT_{50}$ values for M-01 were significantly shorter than the laboratory studies, therefore the geometric mean field $DegT_{50}$ value of **146 days** was used in the modelling for M-01 (BAM).

Plant uptake

The plant uptake factor for M-01 was set to **0.5**. Residues of fluopicolide, M-01 and other metabolites have been found in different plants in a rotational crop study (M-240707-03-1, [redacted] 2003). M-01 is described as high xylem systemic, TSCF calculated according to Briggs is 0.49. The uptake of M-01 into potato plants has been investigated in a new study (M-688374-01-1, [redacted], 2020b) and the transpiration stream concentration factor (TSCF) determined. The mean TSCF was determined as 0.86 (DAT2), 0.75 (DAT4) and 0.71 (DAT6), thus fully supporting the use of the default value of 0.5 in the PECgw evaluations.

Adsorption

The adsorption and desorption of M-01 (BAM) has been investigated in ten soils (M-235837-01-1, [redacted] 2001; M-224926-01-2, [redacted] 2003; M-686388-01-1, [redacted] 2020a). A summary of the sorption parameters derived for M-01 from these studies is given in Table 9.2.4- 12. A geometric mean K_{OC} value of **24.1 mL/g**, corresponding to a K_{OM} value of **14.0 mL/g** ($K_{OM} = K_{OC} \div 1.724$), was used for M-01 in the modelling, with an arithmetic mean 1/n value of **0.914**.

Table 9.2.4- 12: Summary of sorption parameters derived for M-01 (BAM)

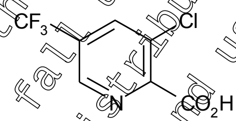
Report reference	Soil	Soil Code	Texture	pH	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-235837-01-1 [redacted] (2001)	Connecticut	RL-51	Sandy loam	4.8	0.9	0.241	26*	1.141*
	North Dakota	RL-81	Sandy loam	7.7	5.7	1.761	31	0.809
	Florida	RM-014	Sand	6.3	1.4	0.529	38	0.916
	Washington	RM-019	Sand	4.9	4.2	1.890	45	0.913
	California	RM-022	Sandy clay loam	6.6	0.4	0.208	51	0.972
M-224926-01-2 [redacted] (2003)	Connecticut	RL-51	Sandy loam	4.8	0.9	0.359	39.9**	0.970**
M-686388-01-1 [redacted] (2020a)	LUFA 2.1	2.1	sand	5.2	0.59	0.103	17.5	0.958
	LUFA 2.3	2.3	sandy loam	6.2	0.61	0.056	9.2	0.859
	LUFA 5M	5M	sandy loam	7.1	1.10	0.162	14.8	0.888
	LUFA 6S	6S	clay loam	7.3	1.78	0.265	14.9	0.872
	Frankenforst	FF	silt loam	6.9	2.4	0.418	17.4	0.980
						Geometric mean	**24.1**	**-**
						Arithmetic mean	**-**	**0.914**

*Excluded from calculations
**Recalculated and used for calculations

M-02 (PCA; AE C657188)

Physico-Chemical Properties

Structural formula



Common name M-02 (PCA; AE C657188)

Chemical name (IUPAC) 3-chloro-5-(trifluoromethyl)pyridine-2-carboxylic acid

Molar mass 225.56 g mol^{-1}

Water solubility 115000 mg L^{-1} at 20°C (M-653965-01-1, [redacted], 2019)

Vapour pressure Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-02 (PCA) in soil was investigated in the laboratory by M-219824-01-1, [redacted] (2003) and M-581364-01-1, [redacted] (2017). A summary of the modelling endpoints derived for M-02 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted]., 2020) is given in Table 9.2.4- 13. A geometric mean $DegT_{50}$ value of 1.6 days was used in the modelling for M-02 (PCA).

The overall formation fraction of M-02 (PCA) from fluopicolide was set to 1.0 as a conservative assumption. Where metabolite M-03 was included in the groundwater simulations (i.e. for acidic soils), this was implemented by assuming a molar formation fraction of 0.47 from fluopicolide, with a molar formation fraction of 1.0 from metabolite M-03 (where ffm FLC→M-03 = 0.53). Where M-03

was not included in the groundwater simulations (i.e. for alkaline soils), the molar formation fraction of M-02 from fluopicolide was set to 1.0.

Table 9.2.4- 13: Summary of modelling endpoints derived for M-02 (PCA) under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised to 20°C and pF2 (d)
M-02 (PCA)	M-219824-01-1 [redacted] 2003	Abington	SFO	4.4	4.4
		Münster	SFO	3.5	3.5
		Sarotti	SFO	4.4	4.1
	M-581364-01-1 [redacted] 2017	Dollendorf	SFO	1.1	1.1
		[redacted]	SFO	1.1	0.9
		[redacted]	SFO	0.7	0.7
		[redacted]	SFO	0.7	0.7
				Geometric mean	**1.6**

Plant uptake

The plant uptake factor for M-02 was set to **0**. Residues of fluopicolide, M-01, M-02 and other metabolites have been found in different plants in a rotational crop study (M-240707-03-1, [redacted] 2003). M-02 is described as phloem mobile.

Adsorption

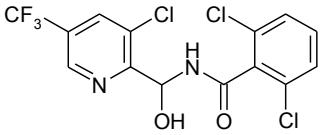
The adsorption and desorption of M-02 (PCA) has been investigated in eight soils (M-219828-01-1, [redacted] 2003; M-686387-01-1, [redacted], 2020b). A summary of the sorption parameters derived for M-02 from these studies is given in Table 9.2.4- 14. A geometric mean K_{OC} value of **5.7 mL/g,** corresponding to a K_{OM} value of **3.3 mL/g** ($K_{OM} = K_{OC} \div 1.724$) was used for M-02 in the modelling, with an arithmetic mean 1/n value of **0.889.**

Table 9.2.4- 14: Summary of sorption parameters derived for M-02 (PCA)

Report reference	Soil	Soil Code	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-219828-01-1 [redacted] (2003)	Abington	03/06	Sandy loam	7.2	2.6	0.029	1.1	0.725
	Munster	03/07	Loamy sand	5.4	1.1	0.116	10.5	0.887
	Sarotti	03/10	Silt loam	7.5	1.3	0.082	6.3	0.709
M-686387-01-1 [redacted] (2020b)	LUFA 2.1	2.1	Sand	5.2	0.59	0.047	8.0	1.031
	LUFA 2.3	2.3	Sandy loam	6.2	0.61	0.038	6.2	0.853
	LUFA 5M	5M	Sandy loam	7.1	1.1	0.154	14.0	0.989
	LUFA 6S	6S	Clay loam	7.3	1.78	0.145	8.2	1.105
	Frankenforst	FF	Silt loam	6.9	2.4	0.059	2.5	0.814
						Geometric mean	**5.7**	**-**
						Arithmetic mean	**-**	**0.889**

M-03 (AE 0608000)

Physico-Chemical Properties
Structural formula



Common name	M-03 (AE 0608000)
Chemical name (IUPAC)	2,6-dichloro-N-{[3-chloro-5-(trifluoromethyl)pyridine-2-yl](hydroxy)methyl}benzamide
Molar mass	399.58 g mol^{-1}
Water solubility	10 mg L^{-1} at 20°C (M-223201-01-1, [redacted] 2003)
Vapour pressure	Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-03 in soil was investigated in the laboratory by M-241188-01-1, [redacted] (2003) and M-565219-01-1, [redacted] (2016a). In addition, M-03 was observed to form from fluopicolide in three studies (M-201230-02-1, [redacted] 2003; M-241052-01-1, [redacted] 2003; M-655056-01-1, [redacted] 2019). A summary of the modelling endpoints derived for M-03 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted]., 2020b) is given in Table 9.2.4-15.

The half-lives derived indicate that M-03 is transient in alkaline soils, and this metabolite was therefore simulated for acidic conditions only. A geometric mean $DegT_{50}$ value of **17.9 days** was used in the groundwater modelling derived from acidic soils (pH<6), with an arithmetic mean formation fraction from fluopicolide of **0.53**.

Table 9.2.4- 15: Summary of modelling endpoints derived for M-03 under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Soil pH	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised (d)	ffm from FLC
Fluopicolide	M-201230-02-1, [redacted] 2003	Münster	4.9	SFO	62.6	62.6	0.6086
	M-241052-01-1, [redacted] 2003	Lamberton	5.9	SFO	49.3	54.5	0.5933
	M-655056-01-1, [redacted] 2019	Pikeville	4.5	SFO	29.3	24.4	0.4009
M-03	M-241188-01-1, [redacted], 2003	Abington	7.2	SFO	0.1	0.1	-
		Münster	4.9	DFOP	1000[a]	1000[a]	-
		Pikeville	5.4	DFOP	2.7[b]	2.2[b]	-
		Sarotti	7.1	SFO	0.1	0.08	-
	M-565219-01-1, [redacted] 2016	Brierlow (BL)	5.3	SFO	2.5	2.5	-
		[redacted]	6.0	SFO	0.9	0.9	-
					Geometric mean (pH <6)	17.9[c]	-
					Arithmetic mean (pH <6)	-	0.53
					Geometric mean (soil pH ≥6)	0.19	-
					Arithmetic mean (pH ≥6)	-	-

a – DFOP k_2 parameter fixed to conservative default value
b – Pseudo-SFO DT_{50} value derived as DT_{90}/3.32 (and normalised if applicable)
c – Geometric mean calculated for Münster soils prior to calculation of overall value

Plant uptake

As the metabolite M-03 (AE 0608000) has not been detected in the plants from rotational crop studies, the uptake factor was set to a conservative default of 0.

Adsorption

The adsorption and desorption of M-03 has been investigated in three soils by M-221107-01-2, [redacted] (2003). A summary of the sorption parameters derived for M-03 is given in Table 9.2.4- 16. A geometric mean K_{OC} value of **106.9 mL/g**, corresponding to a K_{OM} value of **62.0 mL/g** ($K_{OM} = K_{OC} \div 1.724$), was used for M-03 in the modelling, with an arithmetic mean 1/n value of **0.971**.

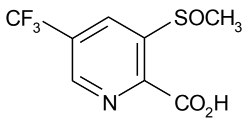
Table 9.2.4- 16: Summary of sorption parameters derived for M-03

Report reference	Soil	Soil Code	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-221107-01-2 [redacted] (2003)	Ingleby	02/03	Sandy loam	4.1	3.5	2.86	82	0.961
	Huntlosen	03/04	Loamy sand	4.7	1.7	2.26	133	1.012
	Münster	03/07	Loamy sand	5.4	1.1	1.23	112	0.939
						Geometric mean	106.9	-
						Arithmetic mean	-	0.971

M-05 (AE 1344122)

Physico-Chemical Properties

Structural formula



Common name	M-05 (AE 1344122)
Chemical name (IUPAC)	3-methylsulfinyl-5-(trifluoromethyl)pyridine-2-carboxylic acid
Molar mass	253.2 g mol^{-1}
Water solubility	120000 mg L^{-1} at 20°C (M-507655-01-1, [redacted]., 2015)
Vapour pressure	Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-05 in soil was investigated in the laboratory by M-241410-01-2, [redacted] (2003a) and M-565223-01-1, [redacted] (2016b). In addition, M-05 was observed to form from M-02 in two studies (M-219824-01-1, [redacted] 2003; M-581364-01-1, [redacted], 2017).

A summary of the modelling endpoints derived for M-05 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted] 2020) is given in Table 9.2.4- 17. A geometric mean $DegT_{50}$ value of **25.2 days** was used in the modelling for M-05, with an arithmetic mean molar formation fraction from M-02 of **0.153**.

Table 9.2.4- 17: Summary of modelling endpoints derived for M-05 under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised (d)	ffm from M-02 (PCA)
M-02	M-219824-01-1 [redacted] 2003	Abington	SFO	29.4	29.4	0.2581[a]
		Münster	SFO	172.1	172.1	0.1557[a]
		Sarotti	SFO	45.5	42.3	0.1811[a]
	M-581364-01-1 [redacted] 2017	Dollendorf	SFO	9.3	9.3	0.1528
		[redacted]	SFO	11.2	9.3	0.0859
		[redacted]	SFO	5.6	5.6	0.1438
		[redacted]	SFO	8.1	8.1	0.0918
M-05	M-241410-01-2 [redacted] 2003a	Abington	SFO	62.2	62.2	-
		Münster	SFO	136.1	136.1	-
		Sarotti	SFO	34.9	32.5	-
	M-565223-01-1 [redacted] 2016b	[redacted]	SFO	22.5	22.5	-
		[redacted]	SFO	16.8	16.8	-
		[redacted]	SFO	19.0	19.0	-
				Geometric mean	**25.2**	
				Arithmetic mean	**-**	**0.153**

a – Factored formation fraction: ff M-02-ghost × ff ghost-M-05

Plant uptake

The plant uptake factor for M-05 (AE 1344122) was set to **0**. Residues of fluopicolide, M-01, M-02

and other metabolites have been found in different plants in a rotational crop study (M-240707-03-1, [redacted] 2003).

Adsorption

The adsorption and desorption of M-05 has been investigated in seven soils by M-241403-01-2, [redacted] (2003a) and M-587780-01-1, [redacted] (2017). A summary of the sorption parameters derived for M-05 is given in Table 9.2.4- 18. These data indicate that the sorption of M-05 is pH-dependent, with greater sorption observed in acidic soils (pH <7).

As a conservative approach at Tier 1, a geometric mean K_{OC} value of **14.0 mL/g** was used in the modelling, based on alkaline soils (pH ≥7), with a corresponding arithmetic mean 1/n value of **0.942**. A corresponding K_{OM} value of **8.1 mL/g** was calculated by dividing the K_{OC} value by 1.724.

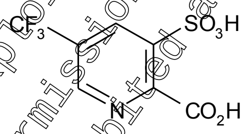
Table 9.2.4- 18: Summary of sorption parameters derived for M-05

Report reference	Soil	Soil Code	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-241403-01-2 [redacted] (2003a)	Abington	n/a	Sandy loam	7.2	2.6	0.294	11	0.883
	Munster	n/a	Loamy sand	5.4	1.1	0.544	49	0.954
	Sarotti	n/a	Silt loam	7.7	1.3	0.218	17	0.918
M-587780-01-1 [redacted] (2017)	[redacted]	331	Sandy loam	5.3	1.9	1.4793	77.9	0.974
	[redacted]	329	Silt loam	6.3	2	0.4915	24.6	0.985
	Dollendorf	330	Loam	7.3	4.5	0.6629	14.7	1.025
	[redacted]	327	Loamy sand	6.3	1.6	0.4671	29.2	0.984
Geometric mean (pH <7)							**40.7**	**-**
Arithmetic mean (pH <7)							**-**	**0.974**
Geometric mean (pH ≥7)							**14.0**	**-**
Arithmetic mean (pH ≥7)							**-**	**0.942**

M-10 (AE 1344123)

Physico-Chemical Properties

Structural formula



Common name M-10 (AE 1344123)

Chemical name (IUPAC) 3-sulfo-5-(trifluoromethyl)pyridine-2-carboxylic acid

Molar mass 271.17 g mol^{-1}

Water solubility 100000 mg L^{-1} at 20°C (M-517618-01-1, [redacted] 2015)

Vapour pressure Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-10 in soil was investigated in the laboratory by M-241411-01-2, [redacted]. (2003b) and M-565224-01-1, [redacted] (2016c). In addition, M-10 was observed to form from M-02 in two studies (M-219824-01-1, [redacted] 2003; M-581364-01-1, [redacted] 2017).

A summary of the modelling endpoints derived for M-10 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted]., 2020) is given in Table 9.2.4- 19. A geometric mean $DegT_{50}$ value of **35.4 days** was used in the modelling for M-10, with an arithmetic mean molar formation fraction from M-02 of **0.129**.

Table 9.2.4- 19: Summary of modelling endpoints derived for M-10 under laboratory conditions (after M-685680-01-1, [redacted]., 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised (d)	ffm from M-02 (PCA)
M-02 (PCA)	M-219824-01-1 [redacted] 2003	Abington	SFO	5.4	5.4	0.1436[a]
		Münster	SFO	1000[b]	1000[a]	0.0335
		Sarotti	SFO	14.6	13.6	0.0796[a]
	M-581364-01-1 [redacted], 2017	Dollendorf	SFO	3.5	3.5	0.1997
		[redacted]	SFO	20.2	16.8	0.1265
		[redacted]	SFO	88.2	88.2	0.1502
		[redacted]	SFO	5.8	5.8	0.1686
M-10	M-241411-01-2 [redacted] 2003b	Abington	SFO	31.6	31.6	-
		Münster	SFO	241.9	241.9	-
		Sarotti	SFO	21.3	19.8	-
	M-565224-01-1 [redacted] 2016c	[redacted]	SFO	21.6	21.6	-
		[redacted]	SFO	83.9	83.9	-
		[redacted]	HS	228.8	228.8	-
				Geometric mean	**35.4**	**-**
				Arithmetic mean	**-**	**0.129**

a – Factored formation fraction: ff M-02-ghost × ff ghost-M-05
b – Conservative default value

Plant uptake

As the metabolite M-10 (AE 1344123) has not been detected in the plants from rotational crop studies, the uptake factor was set to a conservative default of **0**.

Adsorption

The adsorption and desorption of M-10 has been investigated in three soils by M-241404-01-2, [redacted] (2003b). A summary of the sorption parameters derived for M-10 is given in Table 9.2.4- 20. A geometric mean K_{OC} value of **1.8 mL/g**, corresponding to a K_{OM} value of **1.1 mL/g** ($K_{OM} = K_{OC} / 1.724$), was used for M-10 in the modelling, with a default 1/n value of **1.0**.

Table 9.2.4- 20: Summary of sorption parameters derived for M-10

Report reference	Soil	Soil Code	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n

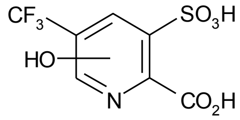
M-241404-01-2 [redacted] (2003b)	Abington	n/a	Sandy loam	7.2	2.6	0.003[a]	0.07[a]	n/a
	Munster	n/a	Loamy sand	5.4	1.1	0.09[a]	8.2[a]	n/a
	Sarotti	n/a	Silt loam	7.5	1.3	0.14[a]	10.7[a]	n/a
						Geometric mean	**1.8**	**-**

a – EFSA value

M-11 and M-12 (AE 1344119 and AE 1344120)

Physico-Chemical Properties

Structural formula



Common name	M-11 and M-12 (two isomers; AE 1344119 and AE 1344120)
Chemical name (IUPAC)	6-hydroxy-3-sulfo-5-(trifluoromethyl)pyridine-2-carboxylic acid; 4-hydroxy-3-sulfo-5-(trifluoromethyl)pyridine-2-carboxylic acid
Molar mass	287.17 g mol^{-1}
Water solubility	1000 mg L^{-1} at 20°C (default)
Vapour pressure	Assumed 0 Pa as worst case for modelling
Mixture of two isomers	M-11:M-12 ≈ 60:40

Degradation in Aerobic Soil

Metabolites M-11/12 were observed to form from M-02 in a study by M-219824-01-1, [redacted] 2003.

A summary of the modelling endpoints derived for M-11/12 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted] 2020) is given in Table 9.2.4- 21. A geometric mean $DegT_{50}$ value of **87.6 days** was used in the modelling for M-11/12, with an arithmetic mean molar formation fraction from M-02 of **0.044**.

Additional supporting information for M-11/12 was obtained from inverse model fitting of lysimeter study data (M-687853-01-1, [redacted], 2020b), where an overall ffm value of 0.054 was derived considering a fixed DT_{50} of 87.6 days.

M-11/12 is a mixture of two isomers M-11 and M-12 in the ratio M-11:M-12 ≈ 60:40. PECgw calculations are conducted for M-11/12 and the results then split in the ratio 60:40 to derive PECgw values for M-11 and M-12.

Table 9.2.4- 21: Summary of modelling endpoints derived for M-11/12 under laboratory conditions (after M-685680-01-1, [redacted]., 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised (d)	ffm from M-02 (PCA)
M-02 (PCA)	M-219824-01-1 [redacted] 2003	Abington	SFO	31.7	31.7	0.0177
		Münster	SFO	242.5	242.5	0.0711
				Geometric mean	**87.6**	-
				Arithmetic mean		**0.044**

Plant uptake

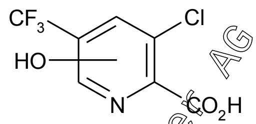
As the metabolites M-11/M-12 have not been detected in the plants from rotational crop studies, the uptake factor was set to a conservative default of **0**.

Adsorption

No reliable sorption parameters have been derived for M-11/12. A worst-case K_{OC}/K_{OM} value of **0 mL/g** was therefore used in the groundwater modelling, with a default 1/n value of **1.0**.

M-13 (Fluopicolide-P3)

Physico-Chemical Properties

Structural formula	
Common name	M-13 (Fluopicolide-P3)
Chemical name (IUPAC)	3-chloro-4-hydroxy-5-(trifluoromethyl)pyridine-2-carboxylic acid; 3-chloro-6-hydroxy-5-(trifluoromethyl)pyridine2-carboxylic acid
Molar mass	241.55 g mol^{-1}
Water solubility	1000 mg L^{-1} at 20°C (default)
Vapour pressure	Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

Metabolite M-13 was observed to form from M-02 in a study by M-219824-01-1, [redacted] 2003.

A summary of the modelling endpoints derived for M-13 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted]., 2020) is given in Table 9.2.4- 22. A geometric mean $DegT_{50}$ value of **20.7 days** was used in the modelling for M-13, with an arithmetic mean molar formation fraction from M-02 of **0.049**.

Additional supporting information for M-13 was obtained from inverse model fitting of lysimeter study data (M-687853-01-1, [redacted], 2020b), where an overall ffm value of 0.023 was derived considering a fixed DT_{50} of 20.7 days.

Table 9.2.4- 22: Summary of modelling endpoints derived for M-13 under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised (d)	ffm from M-02 (PCA)
M-02 (PCA)	M-219824-01-1 [redacted] 2003	Abington	SFO	13.3	13.3	0.0667
		Münster	SFO	48.4	48.4	0.0286
		Sarotti	SFO	14.8	13.8	0.0507
				Geometric mean	**20.7**	-
				Arithmetic mean	-	**0.049**

Plant uptake

As the metabolite M-13 has not been detected in the plants from rotational crop studies, the uptake factor was set to a conservative default of **0**.

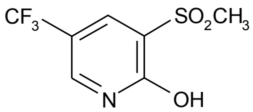
Adsorption

No reliable sorption parameters have been derived for M-13. A worst-case K_{OC}/K_{OM} value of **0 mL/g** was therefore used in the groundwater modelling, with a default 1/n value of **1.0**.

M-14 (AE 1388273)

Physico-Chemical Properties

Structural formula



Common name	M-14 (AE 1388273)
Chemical name (IUPAC)	3-Methylsulfonyl-5-(trifluoromethyl)-1H-pyridin-2-one
Molar mass	241.19 g mol^{-1}
Water solubility	15800 mg L^{-1} at 20°C (M-505731-01-1, [redacted], 2014)
Vapour pressure	Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-14 in soil was investigated in the laboratory by M-234149-01-2, [redacted] (2003). In addition, M-14 was observed to form from M-05 in a study by M-241410-01-2, [redacted]. (2003a).

A summary of the modelling endpoints derived for M-14 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted], 2020) is given in Table 9.2.4- 23. A geometric mean DegT$_{50}$ value of **9.4 days** was used in the modelling for M-14, along with a formation fraction of **0.559** from M-05 and **0.021** from M-02 (PCA). These values represent overall formation fractions for M-14 *via* metabolite M-20, which was not included in the groundwater simulations.

Table 9.2.4- 23: Summary of modelling endpoints derived for M-14 under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	DegT$_{50}$ un-normalised (d)	DegT$_{50}$ normalised (d)	ffm from M-20[a]
M-05	M-241410-01-2 [redacted] 2003a	Abington	SFO	16.4	16.4	1
		Sarotti	SFO	21.7	20.1	1
M-14	M-234149-01-2 [redacted], 2003	Abington	SFO	4.9	4.9	-
		Münster	SFO	8.2	8.2	-
		Sarotti (SLS)	SFO	5.8	5.4	-
				Geometric mean	**9.4**	**-**
				Arithmetic mean	**-**	**1**

a – Metabolite M-20 is formed from M-05 with an arithmetic mean formation fraction of 0.559, and from M-02 (PCA) with an arithmetic mean formation fraction of 0.021 (M-685680-01-1, [redacted] 2020). As shown above, metabolite M-14 is formed from M-20 with a formation fraction of 1.0. The overall formation fractions of M-14 were therefore set to 0.559 and 0.021, respectively, from M-05 from M-02. Metabolite M-20 was not included in the simulations.

Plant uptake

As the metabolite M-14 (AE 1388273) has not been detected in the plants from rotational crop studies, the uptake factor was set to a conservative default of **0**.

Adsorption

The adsorption and desorption of M-14 has been investigated by OECD 121 and in nine soils by M-223531-01-2, [redacted] (2004), M-572869-01-1, [redacted] (2016) and M-686386-01-1, [redacted] (2020c). A summary of the sorption parameters derived for M-14 is given in Table 9.2.4- 24.

A geometric mean K_{OC} value of **9.9 mL/g**, corresponding to a K_{OM} value of **5.7 mL/g** (K_{OM} = K_{OC} ÷ 1.724), was used for M-14 in the modelling, with an arithmetic mean 1/n value of **0.942**.

Table 9.2.4- 24: Summary of sorption parameters derived for M-14

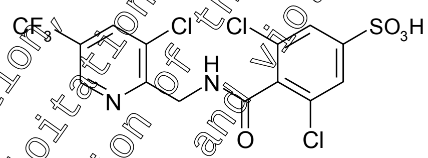
Report reference	Soil	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-223531-01-2 [redacted] (2004)	n/a	n/a	6	n/a	n/a	1.28*	n/a
	n/a	n/a	2.5	n/a	n/a	2.13*	n/a
M-572869-01-1 [redacted] (2016)	[redacted]	Loam	5	1.8	0.1765	9.8	0.964
	[redacted]	Silt loam	6.1	1.9	0.2834	14.9	0.937
	Dollendorf II	Clay loam	7.3	4.8	0.5601	11.7	0.941
	[redacted]	Sandy loam	6.5	1.5	0.1848	12.3	0.956
M-686386-01-1 [redacted] (2020c)	LUFA 2.1	Sand	5.2	0.59	0.031	5.3	1.022
	LUFA 2.3	Sandy loam	6.2	0.61	0.028	4.6	0.908
	LUFA 5M	Sandy loam	7.1	1.1	0.117	10.7	0.892
	LUFA 6S	Clay loam	7.3	1.78	0.3	16.9	0.936
	Frankenforst	Silt loam	6.9	2.4	0.238	9.9	0.923
					Geometric mean	**9.9**	**-**
					Arithmetic mean	**-**	**0.942**

* Excluded from calculations

M-15 (AE 1413903)

Physico-Chemical Properties

Structural formula



Common name M-15 (AE 1413903; BCS-BA91072)

Chemical name (IUPAC) 3,5-dichloro-4-({[3-chloro-5-(trifluoromethyl)57yridine-2-yl]methyl}carbamoyl)benzenesulfonic acid

Molar mass 463.64 g mol^{-1}

Water solubility 160000 mg L^{-1} at 20°C (M-633477-01-1, [redacted], 2018)

Vapour pressure Assumed 0 Pa as worst case for modelling

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-15 in soil was investigated in the laboratory by M-585202-01-1, [redacted] (2016d).

A summary of the modelling endpoints derived for M-15 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted], 2020) is given in Table 9.2.4- 25. A geometric mean $DegT_{50}$ value of **145 days** was used in the modelling for M-15.

A molar formation fraction of **0.0016** from fluopicolide was estimated by inverse modelling of a lysimeter study (M-687165-01-1, [redacted], 2020c) based on a fixed DT_{50} of 145 days.

Table 9.2.4- 25: Summary of modelling endpoints derived for M-15 under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised (d)
M-15	M-585202-01-1 [redacted] 2016d	Dollendorf II	DFOP	172.5[a]	172.5[a]
		[redacted]	DFOP	137.9[a]	137.9[a]
		[redacted]	DFOP	139.6[a]	139.6[a]
		[redacted]	DFOP	132.4[a]	132.4[a]
				Geometric mean	**145**

a – Pseudo-SFO value based on slow phase of decline (calculated as $\ln(2)/k_2$)

Plant uptake

As the metabolite M-15 (AE 1413903) has not been detected in the plants from rotational crop studies, the uptake factor was set to a conservative default of **0**.

Adsorption

The adsorption and desorption of M-15 has been investigated in four soils by M-585208-01-1, [redacted] (2017). A summary of the sorption parameters derived for M-15 is given in Table 9.2.4- 26

A geometric mean K_{OC} value of **18.8 mL/g**, corresponding to a K_{OM} value of **10.9 mL/g** ($K_{OM} = K_{OC} \div 1.724$), was used for M-15 in the modelling, with an arithmetic mean 1/n value of **0.937**.

Table 9.2.4- 26: Summary of sorption parameters derived for M-15

Report reference	Soil	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-585208-01-1 [redacted] (2017)	[redacted]	loamy sand	5.4	1.8	0.431	23.9	0.953
	Dollendorf II	clay loam	7.3	5.2	0.728	14.0	0.920
	[redacted]	silt loam	6.0	2.4	0.500	20.8	0.923
		sandy loam	5.1	2.1	0.380	18.1	0.950
					Geometric mean	**18.8**	**-**
					Arithmetic mean	**-**	**0.937**

* Excluded from calculations

II. Results and Discussion

Modelling reports utilising the core info document should have the substance data presented in the form as shown in Table 9.2.4- 1 and Table 9.2.4- 2.

Table 9.2.4- 27: Compound input parameters for fluopicolide and its metabolites – without aged sorption

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03* (AE 0608000)	M-05 (AE 1344122)
Common						
Molar mass	(g/mol)	383.59	190.03	225.56	399.58	253.2
Solubility	(mg/L)	2.8	2220	115000	10	120000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	0.888	0.913	0.889	0.971	0.942
Plant uptake factor	(-)	0.5	0.5	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	FLC	M01	M02	M03	M05
DT50	(days)	182.0	146.0	1.6	17.9	25.2
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	155.3	14.0	3.3	62.0	8.1
PELMO parameters						
Substance code	(-)	Fluopicolide	M-01	M-02	M-03	M-05
Rate constant	(1/day)	0.003809	0.004748	0.433217	0.038723	0.027506
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	267.1	24.1	5.4	106.9	14.0
MACRO parameters						
Substance code	(-)	Fluopicolide	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

Parameter	Unit	M-10 (AE 1344123)	M-11/12 (AE 1344119/ AE 1344120)	M-13 (Fluopicolide P3)	M-14 (AE 1388273)	M-15 (AE 1413903)
Common						
Molar mass	(g/mol)	271.17	287.17	241.65	241.19	463.64
Solubility	(mg/L)	106000	1000	1000	15800	160000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	1.0	1.0	1.0	0.942	0.937
Plant uptake factor	(-)	0	0	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	M10	M11-2	M13	M14	M15
DT50	(days)	35.4	87.6	20.7	9.4	145.0
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	1	0	0	5.7	10.9
PELMO parameters						
Substance code	(-)	M-10	M-11/12	M-13	M-14	M-15
Rate constant	(1/day)	0.019580	0.007913	0.033485	0.073739	0.004780
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	1.8	0	0	9.9	18.8
MACRO parameters						
Substance code	(-)	-	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

* Metabolite M-03 not simulated in alkaline soils

Table 9.2.4- 28: Compound input parameters for fluopicolide and metabolites – with aged sorption

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03* (AE 0608000)	M-05 (AE 1344122)
Common						
Molar mass	(g/mol)	383.59	190.03	225.56	399.58	253.2
Solubility	(mg/L)	2.8	2220	115000	10	120000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	0.888	0.914	0.889	0.971	0.942
Plant uptake factor	(-)	0.5	0.5	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	FLC	M01	M02	M03	M05
DT50	(days)	121.0	146.0	1.6	17.9	25.2
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	155.3	14.0	3.3	62.0	8.1
k_{des}	(1/day)	0.0356	0	0	0	0
F_{ne}	(-)	0.508	0	0	0	0
PELMO parameters						
Substance code	(-)	Fluopicolide	M-01	M-02	M-03	M-05
Rate constant	(1/day)	0.005728	0.004748	0.433217	0.038723	0.027506
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	267.7	24.1	5.7	106.9	14.0
MACRO parameters						
Substance code	(-)	Fluopicolide	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

Parameter	Unit	M-10 (AE 1344123)	M-11/12 (AE 1344119/ AE 1344120)	M-13 (Fluopicolide-P3)	M-14 (AE 1388273)	M-15 (AE 1413903)
Common						
Molar mass	(g/mol)	271.17	287.17	241.55	241.19	463.64
Solubility	(mg/L)	100000	1000	1000	15800	160000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	1.0	1.0	1.0	0.942	0.937
Plant uptake factor	(-)	0	0	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	M10	M11-2	M13	M14	M15
DT50	(days)	35.4	87.6	20.7	9.4	145.0
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	1.1	0	0	5.7	10.9
k_{des}	(1/day)	0	0	0	0	0
F_{ne}	(-)	0	0	0	0	0
PELMO parameters						
Substance code	(-)	M-10	M-11/12	M-13	M-14	M-15
Rate constant	(1/day)	0.019580	0.007913	0.033485	0.073739	0.004780
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	1.8	0	0	9.9	18.8

MACRO parameters						
Substance code	(-)	-	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

* Metabolite M-03 not simulated in alkaline soils

III. Conclusion

For the groundwater risk assessment of fluopicolide and its metabolites M-01, M-02, M-03, M-05, M-10, M-11/M-12, M-13, M-14, and M-15 the input parameters presented in this summary should be used in all calculations.

Assessment and conclusion by applicant:

This core modelling report was conducted according to FOCUS Degradation Kinetics (2006, 2014) and is considered valid to assess trigger and modelling endpoints for fluopicolide and its metabolites in groundwater.

PEC_{gw} for fluopicolide

Data Point:	KCP 9.2.4.1/02
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluopicolide (FLC) and metabolites: PECgw FOCUS PEARL, PELMO and MACRO - Use as seed treatment application in WOSR in Europe
Report No:	VC/19/041P
Document No:	M-688512-01-1
Guideline(s) followed in study:	FOCUS 2014
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

Predicted environmental concentrations of the active substance fluopicolide and its metabolites M-01, M-02, M-03, M-05, M-10, M-11/M-12, M-13, M-14, and M-15 in groundwater recharge (PECgw) were calculated for the use in winter oilseed rape in Europe, using the simulation models FOCUS PEARL 4.4.4 (Leistra *et al.* 2001), FOCUS PELMO 5.5.3 (Jene 1998; Klein 1995, 1999, 2011), and FOCUS MACRO 5.5.4 (Jarvis 1994; Jarvis and Larsbo 2012). PECgw were evaluated as the 80th percentile of the mean annual leachate concentration at 1 m soil depth. Model parameters and scenarios consisting of weather, soil, and crop data were used as proposed by FOCUS (2014b).

I. Materials and Methods

Use of fluopicolide in winter oilseed rape was investigated in the report. Detailed application parameters are presented in Table 9.2.4- 29

Table 9.2.4- 29: Application data of fluopicolide according to the use pattern in Europe

Individual crop	FOCUS crop	Rate g/ha	Interval (days)	Plant interception (%)	BBCH stage (-)	Amount reaching soil g/ha
Winter oilseed rape	Winter oilseed rape	12	-	0	Seed treatment	12

The calculations were based on the maximum intended application rate together with the maximum intended number of applications per season and the minimum interval between applications (where applicable).

The relative application dates were taken as the 7 days before the emergence date of winter oilseed rape. For winter oilseed rape, an injection depth of 3cm was used to simulate seed treatment applications.

Input parameters for PEC groundwater modelling are fully evaluated and derived in the Core Modelling Information document (M-688396-01-1; [redacted], 2020) and are summarised in Table 9.2.4- 30 and Table 9.2.4- 31.

Table 9.2.4- 30: Input parameters related to active substance fluopicolide and metabolites for PEC_{gw} calculations – with aged-sorption

Parameter		Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03* (AE 0608000)	M-05 (AE 1344122)
Molar mass		(g/mol)	383.59	190.03	225.56	399.58	253.2
Solubility		(mg/L)	2.8	2220	115000	10	120000
at temp.		(°C)	20	20	20	20	20
Vapour pressure		(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.		(°C)	20	20	20	20	20
Freundlich		(-)	0.888	0.914	0.889	0.971	0.942
exponent		(-)	0.5	0.5	0	0	0
Plant uptake		(-)	0.7	0.7	0.7	0.7	0.7
factor							
Walker exponent		(-)	FLC	M01	M02	M03	M05
PEARL		(days)	121.0	146.0	1.6	17.9	25.2
parameters		(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Substance code		(mL/g)	155.3	14.0	3.3	62.0	8.1
DT50		(1/day)	0.0356	0	0	0	0
Molar activ.		(-)	0.508	0	0	0	0
energy							
Kom		(-)	Fluopicolide	M-01	M-02	M-03	M-05
k_{des}		(1/day)	0.005728	0.004748	0.433217	0.038723	0.027506
F_{ne}		(-)	2.58	2.58	2.58	2.58	2.58
PELMO		(mL/g)	267.7	24.1	5.7	106.9	14.0
parameters							
Substance code							
Rate constant							
Q10							
Koc							
MACRO							
parameters		(-)	Fluopicolide	-	-	-	-
Substance code		(-)	0.49	0.49	0.49	0.49	0.49
Exponent		(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948
moisture							
Exponent temp							

Parameter		Unit	M-10 (AE 1344123)	M-11/12 (AE 1344119/ AE 1344120)	M-13 (Fluopicolide-P3)	M-14 (AE 1388273)	M-15 (AE 1413903)
Molar mass		(g/mol)	271.17	287.17	241.55	241.19	463.64
Solubility		(mg/L)	100000	1000	1000	15800	160000
at temp.		(°C)	20	20	20	20	20
Vapour pressure		(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.		(°C)	20	20	20	20	20
Freundlich		(-)	1.0	1.0	1.0	0.942	0.937
exponent		(-)	0	0	0	0	0
Plant uptake factor		(-)	0.7	0.7	0.7	0.7	0.7
Walker exponent		(-)	M10	M11-2	M13	M14	M15
PEARL		(days)	35.4	87.6	20.7	9.4	145.0
parameters		(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Substance code		(mL/g)	1.1	0	0	4.7	10.9
DT50		(1/day)	0	0	0	0	0
Molar activ. energy		(-)	0	0	0	0	0
Kom		(-)	M-10	M-11/12	M-13	M-14	M-15
k_{des}		(1/day)	0.019580	0.007913	0.033485	0.073739	0.004780
F_{ne}		(-)	2.58	2.58	2.58	2.58	2.58
PELMO		(mL/g)	1.8	0	0	9.9	18.8
parameters							
Substance code							
Rate constant							
Q10							
Koc							
MACRO parameters		(-)			-	-	-
Substance code		(-)	0.49	0.49	0.49	0.49	0.49
Exponent moisture		(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948
Exponent temp							

* Metabolite M-03 not simulated in alkaline soils

Table 9.2.4- 31: Input parameters related to active substance fluopicolide and metabolites for PECgw calculations – without aged-sorption

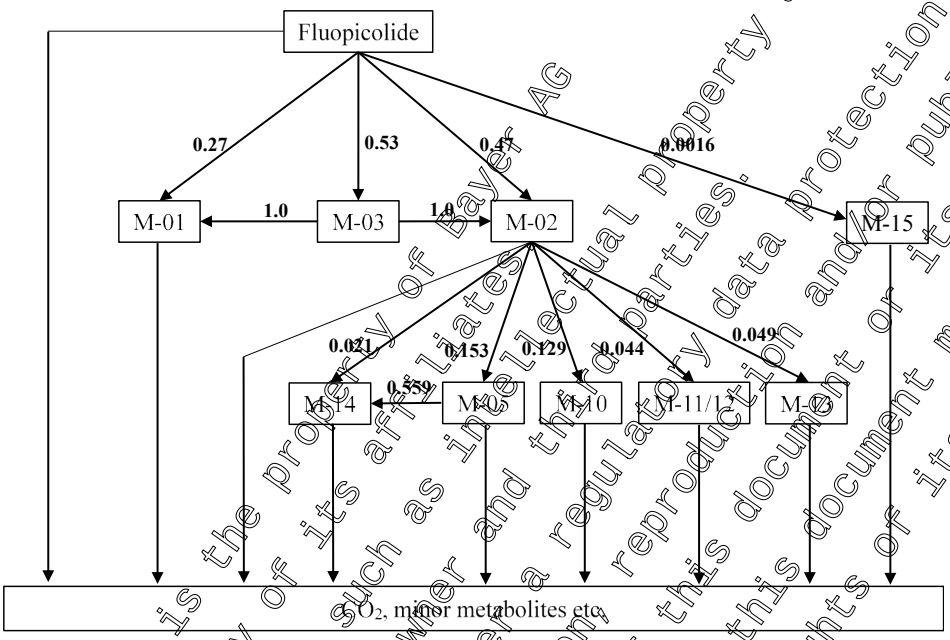
Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03* (AE 0608000)	M-05 (AE 1344122)
Molar mass	(g/mol)	383.59	190.03	225.56	399.58	253.2
Solubility	(mg/L)	2.8	2220	115000	10	120000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	0.888	0.914	0.889	0.971	0.942
Plant uptake factor	(-)	0.5	0.5	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	FLC	M01	M02	M03	M05
DT50	(days)	182.0	146.0	1.6	17.9	25.2
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	155.3	14.0	3.3	62.0	8.1
PELMO parameters						
Substance code	(-)	Fluopicolide	M-01	M-02	M-03	M-05
Rate constant	(1/day)	0.003809	0.004748	0.433217	0.038723	0.027506
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	267.7	24.1	5.7	106.9	14.0
MACRO parameters						
Substance code	(-)	Fluopicolide	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

Parameter	Unit	M-10 (AE 1344123)	M-11/12 (AE 1344119/ AE 1344120)	M-13 (Fluopicolide-P3)	M-14 (AE 1388273)	M-15 (AE 1413903)
Molar mass	(g/mol)	201.17	287.17	341.55	241.19	463.64
Solubility	(mg/L)	100000	1000	1000	15800	160000
at temp.	(°C)	20	20	20	20	20
Vapour pressure	(Pa)	0 (default)	0 (default)	0 (default)	0 (default)	0 (default)
at temp.	(°C)	20	20	20	20	20
Freundlich exponent	(-)	1.0	1.0	1.0	0.942	0.937
Plant uptake factor	(-)	0	0	0	0	0
Walker exponent	(-)	0.7	0.7	0.7	0.7	0.7
PEARL parameters						
Substance code	(-)	M10	M11/12	M13	M14	M15
DT50	(days)	35.4	87.6	20.7	9.4	145.0
Molar activ. energy	(kJ/mol)	65.4	65.4	65.4	65.4	65.4
Kom	(mL/g)	1.1	0	0	5.7	10.9
PELMO parameters						
Substance code	(-)	M-10	M-11/12	M-13	M-14	M-15
Rate constant	(1/day)	0.019580	0.007913	0.033485	0.073739	0.004780
Q10	(-)	2.58	2.58	2.58	2.58	2.58
Koc	(mL/g)	1.8	0	0	9.9	18.8
MACRO parameters						
Substance code	(-)	-	-	-	-	-
Exponent moisture	(-)	0.49	0.49	0.49	0.49	0.49
Exponent temperature	(1/K)	0.0948	0.0948	0.0948	0.0948	0.0948

* Metabolite M-03 not simulated in alkaline soils

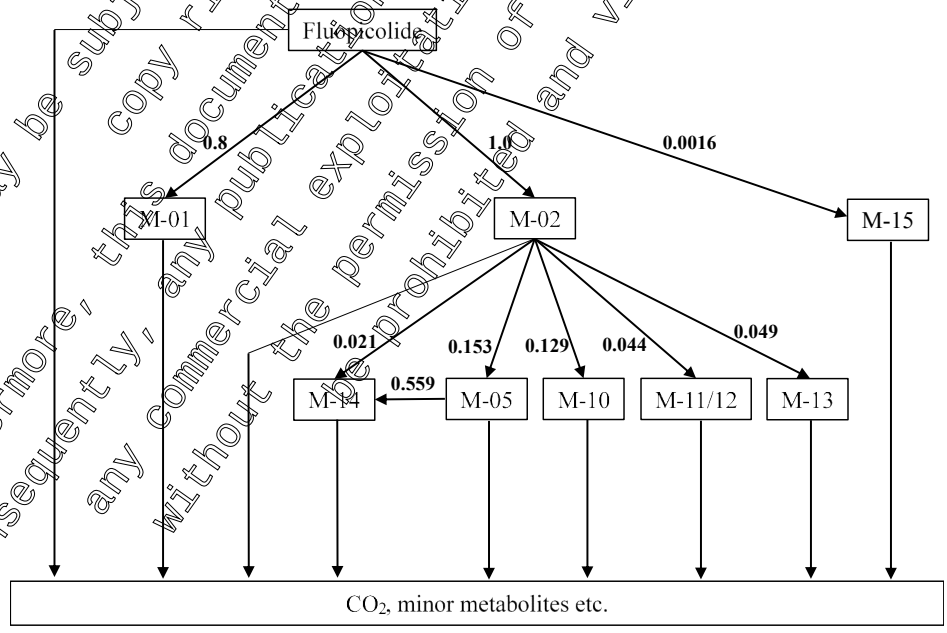
In acidic soils, the principle breakdown of fluopicolide in soil proceeds via formation of the M-03 metabolite, which splits to form the M-01 and M-02 metabolites, with M-01 and M-02 additionally being formed direct from fluopicolide [Figure 9.2.4- 5].

Figure 9.2.4- 5: Degradation pathway for fluopicolide in acidic soils



In alkaline soils, degradation of M-03 is very rapid (DT_{50} << 1day) and no kinetic formation information can be derived. Therefore simulations for alkaline soil conditions are made assuming only direct formation of M-01 and M-02 from fluopicolide [Figure 9.2.4- 6].

Figure 9.2.4- 6: Degradation pathway for fluopicolide in alkaline soils



These two pathways can be fully parameterised directly in FOCUS PEAR 4.4.4. However, due to the pathway limitations in FOCUS PELMO 5.5.3, three separate evaluations are required for each. Aged-sorption is significant for fluopicolide, and thus two sets of evaluations are conducted – with/without the use of aged-sorption. Thus, for PEARL four sets of model evaluations are conducted per GAP, whereas twelve sets of model evaluations are required for PELMO.

Table 9.2.4- 32: Degradation pathway related parameters for fluopicolide and its metabolites

Degradation fraction from → to (-) (FOCUS PEARL): **acidic soils**	FLC → M01: 0.27 FLC → M02: 0.47 FLC → M03: 0.53 FLC → M15: 0.0016 M03 → M01: 1.0 M03 → M02: 1.0 M02 → M05: 0.153 M02 → M10: 0.129 M02 → M11-2: 0.044 M02 → M13: 0.049 M02 → M14: 0.021 M05 → M14: 0.559
Degradation fraction from → to (-) (FOCUS PEARL): **alkaline soils**	FLC → M01: 0.8 FLC → M02: 1.0 FLC → M15: 0.0016 M02 → M05: 0.153 M02 → M10: 0.129 M02 → M11-2: 0.044 M02 → M13: 0.049 M02 → M14: 0.021 M05 → M14: 0.559
Partial DT_{50}/Degradation rate from → to (day or 1/day) (FOCUS PELMO)*: **acidic soils**	Pathway 1: Active Substance → M-02: 387.234 / 0.0017900 Active Substance → M-03: 343.396 / 0.0020190 Active Substance (TDS) → M-02: 257.447 / 0.0026920 Active Substance (TDS) → M-03: 228.302 / 0.0030360 Active Substance → BR/CO2: 0 M-03 → M-02: 17.9 / 0.0387230 M-02 → M-05: 10.458 / 0.0662790 M-02 → M-10: 12.403 / 0.0558850 M-02 → M-14: 76.190 / 0.0090980 M-02 → BR/CO2: 2.296 / 0.3018930 M-05 → M-14: 45.081 / 0.0153760 M-05 → BR/CO2: 57.143 / 0.0121300 M-10 → BR/CO2: 35.4 / 0.0195800 M-14 → BR/CO2: 9.4 / 0.0737390 Pathway 2: Active Substance → M-02: 387.234 / 0.0017900 Active Substance → M-03: 343.396 / 0.0020190 Active Substance (TDS) → M-02: 257.447 / 0.0026920 Active Substance (TDS) → M-03: 228.302 / 0.0030360 Active Substance → BR/CO2: 0 M-03 → M-02: 17.9 / 0.0387230 M-02 → M-11/12: 36.364 / 0.0190610 M-02 → M-13: 32.653 / 0.0212280 M-02 → BR/CO2: 1.764 / 0.3929410 M-11/12 → BR/CO2: 87.6 / 0.0079130 M-13 → BR/CO2: 20.7 / 0.0737390

	Pathway 3: Active Substance → M-01: 674.074 / 0.0010280 Active Substance → M-03: 343.396 / 0.0020190 Active Substance → M-15: 113750 / 6.09E-06 Active Substance → BR/CO2: 917.339 / 0.000756 Active Substance (TDS) → M-01: 448.148 / 0.0015470 Active Substance (TDS) → M-03: 228.302 / 0.0030360 Active Substance (TDS) → M-15: 75625 / 9.17E-06 Active Substance (TDS) → BR/CO2: 609.879 / 0.0011370 M-03 → M-01: 17.9 / 0.0387230 M-01 → BR/CO2: 146 / 0.0047480 M-15 → BR/CO2: 145 / 0.0047800
Partial DT$_{50}$/Degradation rate from → to (day or 1/day) (FOCUS PELMO)[a]: **alkaline soils**	Pathway 1: Active Substance → M-02: 182 / 0.0038090 Active Substance (TDS) → M-02: 121 / 0.0057280 Active Substance → BR/CO2: 0 M-02 → M-05: 10.458 / 0.0662790 M-02 → M-10: 12.403 / 0.0558850 M-02 → M-14: 76.190 / 0.0090980 M-02 → BR/CO2: 2.296 / 0.3018930 M-05 → M-14: 45.081 / 0.0153760 M-05 → BR/CO2: 57.143 / 0.0121300 M-10 → BR/CO2: 35.4 / 0.0195800 M-14 → BR/CO2: 9.4 / 0.0737390 Pathway 2: Active Substance → M-02: 182 / 0.0038090 Active Substance (TDS) → M-02: 121 / 0.0057280 Active Substance → BR/CO2: 0 M-02 → M-11/12: 36.364 / 0.0190610 M-02 → M-13: 32.653 / 0.0212280 M-02 → BR/CO2: 1.764 / 0.3929410 M-11/12 → BR/CO2: 87.6 / 0.0079130 M-13 → BR/CO2: 20.7 / 0.0737390 Pathway 3: Active Substance → M-01: 227.500 / 0.0030470 Active Substance → M-15: 113750 / 6.09E-06 Active Substance → BR/CO2: 917.339 / 0.000756 Active Substance (TDS) → M-01: 151.250 / 0.0045830 Active Substance (TDS) → M-15: 75625 / 9.17E-06 Active Substance (TDS) → BR/CO2: 609.879 / 0.0011370 M-01 → BR/CO2: 146 / 0.0047480 M-15 → BR/CO2: 145 / 0.0047800
Conversion factor from → to (-) (FOCUS MACRO)[b]: **acidic soils**	-
Conversion factor from → to (-) (FOCUS MACRO)[b]: **alkaline soils**	-

[a] Calculated as *ln(2) / DT50 × formation fraction*
[b] Calculated as *molar mass / molar mass predecessor × formation fraction*

Plant uptake parameters, in different leaching models, define the ability of plant roots to transport a solute into the plant, in comparison to the water uptake (that is, the ratio between pesticide mass uptake flux and water volume uptake flux, normalised to the aqueous concentration of the pesticide outside the root). For fluopicolide and M-01 the plant uptake factor was set to the value of 0.5; for all the other metabolites the plant uptake factors were set at 0.

M-11/12 is a mixture of two isomers M-11 and M-12 in the ratio M-11:M-12 ≈ 60:40. PECgw calculations are conducted for M-11/12 and the results then split in the ratio 60:40 to derive PECgw values for M-11 and M-12. Groundwater simulations using MACRO 5.5.4 was carried out for fluopicolide only.

Following the proposal of the FOCUS working group on groundwater scenarios (FOCUS 2014b), the concentrations in the percolate at 1 m depth were evaluated. This shallow depth reflects a worst case with respect to the assessment of a potential groundwater contamination. The effective long-term groundwater concentrations will be even lower due to dilution in the upper groundwater layer.

II. Results and Discussion

An overview of the PECgw values obtained with individual FOCUS models is given in Table 9.2.4- 33 to Table 9.2.4- 36 (PEARL), Table 9.2.4- 37 to Table 9.2.4- 40 (PELMO).

Table 9.2.4- 33: Maximum FOCUS PEARL PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – acidic soils, with aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL										
	FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.006	0.752	0.002	0.065	0.022	0.150	0.028	0.019	0.222	0.008	0.006

Table 9.2.4- 34: Maximum FOCUS PEARL PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – acidic soils, without aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL										
	FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.043	0.771	0.004	0.020	0.072	0.225	0.092	0.061	0.049	0.023	0.006

Table 9.2.4- 35: Maximum FOCUS PEARL PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – alkaline soils, with aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL									
	FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.006	0.730	0.001	0.061	0.218	0.089	0.060	0.047	0.021	0.006

Table 9.2.4- 36: Maximum FOCUS PEARL PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – alkaline soils, without aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL									
	FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.043	0.752	0.003	0.067	0.222	0.091	0.061	0.048	0.022	0.006

Table 9.2.4- 37: Maximum FOCUS PELMO PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – acidic soils, with aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PELMO										
	FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.006	1.024	0.005	0.009	0.062	0.184	0.078	0.052	0.015	0.020	0.005

Table 9.2.4- 38: Maximum FOCUS PELMO PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – acidic soils, without aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PELMO										
	FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.038	1.021	0.008	0.018	0.067	0.186	0.078	0.052	0.015	0.021	0.003

Table 9.2.4- 39: Maximum FOCUS PELMO PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – alkaline soils, with aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PELMO									
	FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.006	1.002	0.003	0.058	0.180	0.077	0.052	0.005	0.015	0.019

Table 9.2.4- 40: Maximum FOCUS PELMO PECgw results of fluopicolide and its metabolites in µg/L for the uses assessed – alkaline soils, without aged-sorption

Use pattern	80th percentile PECgw at 1 m soil depth (µg/L) - PELMO									
	FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR, 12 g/ha	0.038	1.001	0.005	0.063	0.182	0.077	0.052	0.015	0.020	0.005

Detailed results for all scenarios for FOCUS PEARL, FOCUS PELMO and FOCUS MACRO are listed in the following subsections Table 9.2.4- 41 to Table 9.2.4- 49.

Winter oilseed rape 12g / ha

Annual application

Table 9.2.4- 41: FOCUS PEARL, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – acidic soils, with aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL										
		FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	<0.001	0.663	<0.001	0.025	0.009	0.150	0.010	0.006	0.106	0.000	0.006
	Hamburg	0.005	0.752	0.002	0.065	0.022	0.147	0.028	0.019	0.222	0.008	0.005
	Kremsmunster	0.003	0.546	0.001	0.037	0.012	0.076	0.013	0.008	0.111	0.004	0.003
	Okehampton	0.006	0.509	0.002	0.044	0.014	0.073	0.014	0.009	0.113	0.008	0.003
	Piacenza	0.003	0.448	0.001	0.024	0.007	0.057	0.007	0.005	0.064	0.004	0.003
	Porto	0.001	0.443	0.002	0.033	0.010	0.071	0.011	0.007	0.091	0.004	0.003

Table 9.2.4- 42: FOCUS PEARL, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – acidic soils, without aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL										
		FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	0.005	0.698	<0.001	0.003	0.029	0.111	0.092	0.061	0.017	0.010	0.006
	Hamburg	0.043	0.771	0.004	0.020	0.072	0.225	0.087	0.058	0.049	0.023	0.005
	Kremsmunster	0.030	0.560	0.002	0.012	0.041	0.113	0.045	0.030	0.022	0.013	0.004
	Okehampton	0.041	0.515	0.003	0.018	0.047	0.115	0.044	0.029	0.024	0.015	0.003
	Piacenza	0.022	0.465	0.002	0.010	0.027	0.066	0.035	0.023	0.013	0.008	0.003
	Porto	0.017	0.456	0.004	0.011	0.036	0.095	0.043	0.029	0.019	0.011	0.003

Table 9.2.4- 43: FOCUS PEARL, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – alkaline soils, with aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL									
		FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	<0.001	0.644	<0.001	0.023	0.105	0.089	0.060	0.016	0.008	0.006
	Hamburg	0.005	0.730	0.001	0.061	0.218	0.088	0.058	0.047	0.021	0.005
	Kremsmunster	0.003	0.530	0.000	0.034	0.109	0.045	0.030	0.020	0.011	0.003
	Okehampton	0.006	0.494	0.001	0.041	0.111	0.044	0.029	0.023	0.013	0.003
	Piacenza	0.003	0.435	0.000	0.023	0.064	0.034	0.023	0.013	0.007	0.003
	Porto	0.001	0.431	0.001	0.030	0.090	0.043	0.028	0.017	0.010	0.003

Table 9.2.4- 44: FOCUS PEARL, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – alkaline soils, without aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - PEARL									
		FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	0.005	0.670	<0.001	0.026	0.108	0.091	0.061	0.017	0.009	0.006
	Hamburg	0.043	0.752	0.002	0.067	0.222	0.087	0.058	0.048	0.022	0.005
	Kremsmunster	0.030	0.544	0.001	0.038	0.111	0.045	0.030	0.021	0.012	0.004
	Okehampton	0.041	0.503	0.002	0.044	0.113	0.044	0.029	0.024	0.014	0.003
	Piacenza	0.022	0.451	0.001	0.026	0.066	0.034	0.023	0.013	0.008	0.003
	Porto	0.017	0.444	0.003	0.034	0.094	0.043	0.029	0.019	0.011	0.003

Table 9.2.4- 45: FOCUS PELMO, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – acidic soils, with aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - PELMO										
		FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	<0.001	0.979	<0.001	<0.001	0.021	0.095	0.078	0.052	0.003	0.007	0.005
	Hamburg	0.003	1.024	0.003	0.006	0.062	0.184	0.073	0.049	0.015	0.020	0.005
	Kremsmunster	0.002	0.776	0.001	0.003	0.037	0.119	0.049	0.033	0.007	0.012	0.004
	Okehampton	0.006	0.624	0.002	0.009	0.046	0.114	0.044	0.030	0.009	0.015	0.003
	Piacenza	0.002	0.644	0.002	0.004	0.031	0.076	0.041	0.027	0.006	0.010	0.003
	Porto	0.003	0.575	0.005	0.008	0.042	0.098	0.044	0.030	0.009	0.012	0.003

Table 9.2.4- 46: FOCUS PELMO, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – acidic soils, without aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) – PELMO										
		FLC	M-01	M-02	M-03	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	0.001	0.985	<0.001	0.001	0.024	0.096	0.078	0.052	0.004	0.008	0.005
	Hamburg	0.029	1.021	0.006	0.015	0.067	0.186	0.071	0.048	0.015	0.021	0.005
	Kremsmunster	0.021	0.774	0.002	0.009	0.041	0.119	0.048	0.032	0.007	0.013	0.004
	Okehampton	0.038	0.610	0.004	0.018	0.049	0.114	0.043	0.028	0.010	0.015	0.003
	Piacenza	0.018	0.649	0.003	0.010	0.033	0.077	0.040	0.027	0.007	0.010	0.003
	Porto	0.025	0.567	0.008	0.017	0.043	0.104	0.044	0.030	0.009	0.013	0.003

Table 9.2.4- 47: FOCUS PELMO, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – alkaline soils, with aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - PELMO									
		FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	<0.001	0.953	<0.001	0.020	0.093	0.077	0.052	0.005	0.003	0.007
	Hamburg	0.003	1.002	0.002	0.058	0.180	0.073	0.049	0.005	0.015	0.019
	Kremsmunster	0.002	0.756	<0.001	0.034	0.117	0.049	0.033	0.004	0.007	0.012
	Okehampton	0.006	0.614	0.001	0.044	0.112	0.044	0.029	0.003	0.009	0.014
	Piacenza	0.002	0.628	0.001	0.029	0.076	0.041	0.027	0.003	0.007	0.009
	Porto	0.003	0.564	0.003	0.039	0.095	0.044	0.029	0.003	0.008	0.012

Table 9.2.4- 48: FOCUS PELMO, PECgw results of fluopicolide and its metabolites – 12 g/ha annual seed treatment application – alkaline soils, without aged-sorption

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - PELMO									
		FLC	M-01	M-02	M-05	M-10	M-11	M-12	M-13	M-14	M-15
WOSR	Chateaudun	0.001	0.959	<0.001	0.022	0.094	0.077	0.052	0.003	0.008	0.005
	Hamburg	0.029	1.001	0.004	0.063	0.182	0.071	0.048	0.015	0.020	0.005
	Kremsmunster	0.021	0.756	0.001	0.038	0.117	0.048	0.032	0.007	0.012	0.004
	Okehampton	0.038	0.601	0.003	0.046	0.112	0.043	0.028	0.009	0.015	0.003
	Piacenza	0.018	0.633	0.002	0.032	0.076	0.040	0.027	0.007	0.010	0.003
	Porto	0.025	0.559	0.005	0.041	0.101	0.044	0.029	0.009	0.012	0.003

Table 9.2.4- 49: FOCUS MACRO, PECgw results of fluopicolide – 12 g/ha annual seed treatment application

Crop	Scenario	80th percentile PECgw at 1 m soil depth (µg/L) - MACRO Fluopicolide
WOSR	Chateaudun	<0.001

III. Conclusion

The predicted environmental concentrations in groundwater (PEC_{gw}) of the active substance fluopicolide and its metabolites M-01, M-02, M-03, M-05, M-10, M-11, M-12, M-13, M-14, and M-15 were calculated for use in oil seed rape (winter).

The overall maximum PEC_{gw} value for fluopicolide was 0.042 µg/L. The metabolites M-02, M-03, M-05, M-11, M-12, M-13, M-14 and M-15 were also predicted to reach groundwater at concentrations below 0.1 µg/L. Two metabolites M-01 and M-10 were predicted to reach groundwater at concentrations in excess of 0.1 µg/L. The overall maximum concentrations were 1.024 µg/L for M-01 and 0.225 µg/L for M-10. The non-relevance of these metabolites has been addressed in Document N4 using the assessment scheme described in the Guidance Document On The Assessment Of The Relevance Of Metabolites In Groundwater Of Substances Regulated Under Council Directive 91/414/EEC (Sanco/221/2000 – Revision 10 – Final, 25 February 2003).

Assessment and conclusion by applicant:

The risk assessment report was conducted according to FOCUS (2014) and is considered valid to assess predicted environmental concentrations in groundwater (PEC_{GW}) for fluopicolide and its metabolites in oil seed rape (winter).

PEC_{gw} for fluoxastrobin

No groundwater assessment was required for fluoxastrobin.

CP 9.2.4.2 Additional field tests

Given the results of the calculations for predicted environmental concentrations in groundwater for this seed treatment show no concerns for fluopicolide and its metabolites no further field tests are needed or required for this formulation.

CP 9.2.5 Estimation of concentrations in surface water and sediment

Predicted environmental concentrations fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657488) and M-03 (AE 0608000) in surface water (PECsw) and sediment (PECsed) were calculated for the use in Europe using the tiered FOCUS Surface Water approach. All relevant entry routes of a compound into surface water (principally a combination of spray drift and runoff/erosion or drain flow) were considered in these calculations. FOCUS Steps 1-3 calculations were performed for

fluopicolide and M-03 (AE 0608000) and FOCUS Step 1-2 calculations for the metabolites M-01 (AE C653711) and M-02 (AE C657188).

Metabolites M-01, M-02 and M-03 are relevant for the aquatic risk assessment. No metabolite is relevant for sediment risk assessment.

M-01 was the only major metabolite detected in water sediment systems reaching a maximum of 20.3% in the total system (sediment compartment maximum 3.9%, water compartment maximum 18.2%). M-02 (AE C657188) was also detected as a significant minor metabolite, >5% at 3 consecutive timepoints and increasing at final timepoint, reaching a maximum of 8.2% in the total system (sediment compartment maximum 0.8%, water compartment maximum 7.4%). The metabolite M-03 (AE 0608000) was not detected as an aquatic metabolite. All three metabolites have been included in FOCUS surface water and sediment modelling, as exposure from formation of a metabolite in soil, with subsequent exposure of surface water and sediment from drainage or runoff from soil, has to be considered in addition to the formation of a metabolite in aquatic systems. However, M-03 is unstable in aquatic systems making aquatic ecotoxicological testing unfeasible (see KCA 7.2.1.1/03 and KCA 8.2.6.2/11 for further details).

Predicted environmental concentrations in surface water (PEC_{SW})

PEC_{sw} for fluopicolide

Data Point:	KCP 9.2.5/01
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluopicolide (FLC): Core PECsw EUR - Modelling core info document for surface water risk assessment in Europe
Report No:	VC/19/041K
Document No:	M-686283-01-1
Guideline(s) followed in study:	FOCUS 2014 Generic guidance for FOCUS Surface Water Scenarios Version 1.4 May 2015
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

This summary summarises the substance data for fluopicolide and its metabolites as used for the purpose of surface water risk assessment employing the following deterministic pesticide fate models:

- STEP 1 in FOCUS
- STEP 2 in FOCUS
- STEP 3 in FOCUS
- STEP 4 in FOCUS

The parameters correspond to standard EU requirements.

Modelling reports utilising the core info document should have the substance data presented as shown in the following tables.

Table 9.2.5- 1: Substance parameters used at FOCUS Steps 1-2 level

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03 (AE 0608000)
Molar mass	(g/mol)	383.59	190.03	225.56	399.58
Water solubility	(mg/L)	2.8	1830	9721	10
Koc	(mL/g)	267.7	24.1	5.7	106.9
Degradation					
Soil	(days)	182	146	1.6	17.9
Total system	(days)	1000	1000	1000	1.9
Water	(days)	1000	1000	1000	1.9
Sediment	(days)	1000	1000	1000	1000
Max occurrence					
Water / sediment	(%)	100	20.3	8.2	0.001
Soil	(%)	100	48	16.4	10.6

Table 9.2.5- 2: Substance parameters used for fluopicolide and its metabolite M-03 (AE 0608000) at Step 3/4 level

Parameter	Unit	Parent	Metabolite
Substance		Fluopicolide	M-03 (AE 0608000)
SWASH code		FLC	M03
General			
Molar mass	(g/mol)	383.59	399.58
Water solubility (temp.)	(mg/L)	2.8 (20 °C)	10 (20 °C)
Vapour pressure (temp.)	(Pa)	3.03E-07 (20 °C)	0 (20 °C)
Crop processes			
Coefficient for uptake by plant (TSCF)	(-)	0.5	0
Wash-off factor	(1/m)	50	50
Sorption			
K_{OC}	(mL/g)	267.74	106.89
K_{OM}	(mL/g)	155.3	62
Freundlich exponent ($1/n$)	(-)	0.888	0.971
Transformation			
DT$_{50}$ in soil	(days)	182	17.9
temperature	(°C)	20	20
moisture content (pF)	(log(cm))	2	2
formation fraction in soil	(-)	-	0.53
DT$_{50}$ in water	(days)	1000	1.9
temperature	(°C)	20	20
formation fraction in water	(-)	-	-
DT$_{50}$ in sediment	(days)	1000	1000
temperature	(°C)	20	20
formation fraction in sediment	(-)	-	-
DT$_{50}$ on canopy	(days)	10	10
Exponent for the effect of moisture			
PRZM and TOXSWA (Walker exp.)	(-)	0.7	0.7
MACRO (calibrated value)	(-)	0.49	0.49
Effect of temperature			
TOXSWA (molar activation energy)	(kJ/mol)	65.4	65.4
MACRO (effect of temperature)	(1/K)	0.0948	0.0948
PRZM (Q_{10})	(-)	2.58	2.58

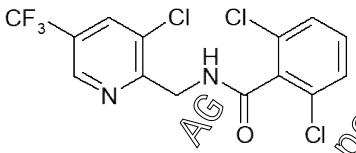
I. Materials and Methods

Calculation of the substance parameters for fluopicolide and its metabolites M-01, M-02 and M-03 is detailed as follows: -

Fluopicolide (AE C638206)

Physico-Chemical Properties

Structural formula



Common name	Fluopicolide (AE C638206)
Chemical name (IUPAC)	2,6-dichloro-N-[[3-chloro-5-(trifluoromethyl)-2-pyridinyl]methyl]-benzamide
Molar mass	383.59 g mol^{-1}
Water solubility	2.8 mg L^{-1} at 20°C (M-234496-01-1, [redacted] 2003a)
Vapour pressure	3.03 × 10^{-7} Pa at 20°C (M-197457-01-1, [redacted] 2000)

Degradation in Aerobic Soil

Laboratory studies

The aerobic degradation and metabolism of fluopicolide in soil was investigated in the laboratory by M-201230-02-1, [redacted] (2003); M-241049-01-1, [redacted] (2003a); M-241052-01-1, [redacted] (2003b); M-241051-01-1, [redacted] (2003c); M-550687-01-1, [redacted] (2016a); M-555570-01-1, [redacted] (2016b) and M-655056-01-1, [redacted] (2019). A summary of the modelling endpoint $DegT_{50}$ values derived for fluopicolide (KCA 7.1.2.1.1/10; M-685680-01-1, [redacted], 2020), normalised to 20°C and pF2, is given in Table 9.2.5-3.

Table 9.2.5-3: Summary of $DegT_{50}$ values derived for fluopicolide under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised to 20°C and pF2 (d)
Fluopicolide	M-201230-02-1, [redacted] 2003	Münster	SFO	212.0	212.0
		Sarotti	SFO	191.2	191.2
	M-241049-01-1, [redacted] 2003a	Abington (non-sterile)	SFO	348.0	340.2
	M-241051-01-1, [redacted] 2003b	Lamberton	SFO	1290.0	1037.9
	M-241052-01-1, [redacted] 2003c	Lamberton	SFO	358.0	395.8
	M-550687-01-1, [redacted] 2016a	Pikeville	DFOP	612.9[a] / 30.1[b]	616.0[a] / 30.3[b]
		Albaro/Marcomcini	DFOP	146.2[a] / 2.8[b]	146.2[a] / 2.8[b]
		Great Chishill	DFOP	312.4[a] / 2.7[b]	312.4[a] / 2.7[b]
		[redacted]	DFOP	155.5[a] / 7.2[b]	155.5[a] / 7.2[b]
		Mas du Coq	DFOP	216.7[a] / 10.5[b]	193.7[a] / 9.4[b]
		Parcey Meslay	DFOP	202.5[a] / 8.1[b]	202.5[a] / 8.1[b]
		Vilobi d'Onyar	DFOP	93.5[a] / 7.8[b]	93.5[a] / 7.8[b]
	M-555570-01-1,	Dollendorf II	DFOP	111.4[a] / 0.6[b]	111.4[a] / 0.6[b]

Applied compound	Study	Soil	Model selected	DegT$_{50}$ un-normalised (d)	DegT$_{50}$ normalised to 20°C and pF2 (d)
	[redacted] 2016b	[redacted]	DFOP	137.7[a] / 4.2[b]	137.7[a] / 4.2[b]
		[redacted]	DFOP	141.3[a] / 6.3[b]	141.3[a] / 6.3[b]
		[redacted]	DFOP	133.5[a] / 9.4[b]	133.5[a] / 9.4[b]
	M-655056-01-1, [redacted] 2019	Abington 2	DFOP	142.1[a] / 1.9[b]	142.1[a] / 1.9[b]
		Lamberton	DFOP	176.1[a] / 2.8[b]	145.1[a] / 2.3[b]
		Lignieres	DFOP	141.4[a] / 1.4[b]	141.4[a] / 1.4[b]
		Münster	DFOP	170.1[a] / 5.3[b]	124.5[a] / 3.9[b]
		Pikeville	DFOP	155.2[a] / 4.1[b]	129.4[a] / 3.5[b]
		Sarotti 2	DFOP	161.2[a] / 1.6[b]	143.6[a] / 1.4[b]
Geometric mean (SFO and DFOP slow phase)					**181.6[c]**

a – Pseudo-SFO value based on slow phase of decline (calculated as ln(2)/k_2 and normalised if applicable)
b – Pseudo-SFO value based on fast phase of decline (calculated ln(2)/k_1 and normalised if applicable)
c – Geometric mean calculated of DegT$_{50}$ values from Lamberton soils prior to calculation of overall geometric mean

Field Dissipation Studies

DegT$_{50}$ values for fluopicolide, normalised to 20°C and pF2, have been derived by M-685675-01-1, [redacted]. (2020a) and M-685676-01-1, [redacted]. (2020b) from 12 terrestrial field dissipation studies (M-651636-01-1, [redacted], 2019a; M-218667-01-1, [redacted] 2003; M-220477-02-1, [redacted] 2003; M-234424-01-1, [redacted] 2004; M-247945-01-1, [redacted] 2005a; M-251338-01-1, [redacted] 2005b; M-218672-01-1, [redacted], 2003). A summary of the modelling endpoint DegT$_{50}$ values derived for fluopicolide is given in Table 9.2.5- 4.

Table 9.2.5- 4: Summary of DegT$_{50}$ values (normalised to 20°C and pF2) derived for fluopicolide from terrestrial field dissipation studies (after M-685675-01-1, [redacted] 2020a and M-685676-01-1, [redacted] 2020b)

Soil type	Aerobic field conditions					
	Location (country)	**pH (CaCl$_2$)**	**Depth (cm)**	**St. (χ^2err) (%)**	**Method of calculation**	**DegT$_{50}$ (d) norm**
Silt loam	Burscheid (Germany)	5.9	0-120	9.80	SFO	111.9
Clay	Great Chishill (UK)	7.8	0-120	11.64	SFO	216.9
Sandy loam	Lignieres de Touraine (France)	6.9	0-120	4.82	SFO	158.6
Clay loam	St.Etienne du Grès (France)	8.1	0-120	4.90	SFO	303.2
Clay loam	Albaro di Ronco all'Adige (Italy)	7.7	0-120	9.99	SFO	237.3
Sandy clay loam	Vilobi d'Onyar (Spain)	6.9	0-120	6.20	SFO	166.8
Loamy sand	Philippsburg (Germany)	6.4	0-50	9.477	SFO	199.6
Sandy clay loam	Rödelsee (Germany)	7.4	0-30	21.59	SFO	146.4
Sand	Huttlosen (Germany)	4.9	0-50	15.46	SFO	168.4
Loamy sand	Valencia (Spain)	7.3	0-30	13.95	SFO	317.4
Sandy silt	Appilly (France)	7.1	0-30	11.16	SFO	144.2
Sandy silt loam	Senas (France)	7.6	0-45	9.864	SFO	136.5
					Geometric mean	**183**

Degradation in Aerobic Soil: Overall DegT$_{50}$ value

Degradation half-lives for fluopicolide derived from laboratory and field dissipation studies were compared using the EFSA $DegT_{50}$ Endpoint Selector (EFSA, 2014). This comparison indicated that the laboratory and field DegT50 values for fluopicolide should be combined.

An overall geometric mean $DegT_{50}$ value of **182 days** in soil was derived for fluopicolide for use in surface water calculations, including both laboratory and field data.

Degradation in Water-Sediment Systems

The degradation of fluopicolide in water sediment systems was investigated in the laboratory by M-241425-01-1, [redacted] (2003a). Limited degradation of fluopicolide was observed, and a default $DegT_{50}$ value of **1000 days** was used in the modelling to describe the degradation of fluopicolide in the water compartment, sediment compartment and total water sediment system.

Plant Uptake

The plant uptake factor for fluopicolide was set to 0.5. Residues of fluopicolide and metabolites have been found in different plants in a rotational crop study (M-240707-03-1, [redacted] 2003). Fluopicolide is redistributed via the xylem (acropetal systemic activity) but is not phloem mobile. TSCF calculated according to Briggs is 0.47.

The uptake of fluopicolide into potato plants has been investigated in a new study (M-688372-01-1, [redacted] 2020) and the transpiration stream concentration factor (TSCF) determined. The mean TSCF was determined as 0.71 (DAT2), 0.75 (DAT4) and 0.82 (DAT6), thus fully supporting the use of the default value of 0.5 in the PECsw evaluations.

Foliar Wash-off and Canopy Degradation

Plant wash-off was set to the default value of **50 m^{-1}**, and the canopy degradation DT_{50} value was set to the default value of **10 days** (FOCUS, 2014).

Adsorption

The adsorption and desorption of fluopicolide has been investigated in five studies (M-241425-01-1, [redacted] 2003b; M-233840-01-1, [redacted] 2003b; M-544194-02-1, [redacted] 2015; M-572869-01-1, [redacted] 2016; M-595721-01-1, [redacted], 2017). A summary of K_{OC} and 1/n values derived for fluopicolide from these studies is given in Table 9.2.5- 5.

A geometric mean K_{OC} value of **267.7 mL/g**, corresponding to a K_{OM} value of 155.3 mL/g ($K_{OM} = K_{OC} \div 1.724$), was used for fluopicolide in the modelling, with an arithmetic mean 1/n value of **0.888**.

Table 9.2.5- 5: Summary of sorption parameters derived for fluopicolide

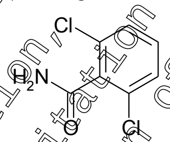
Study reference	Soil	Soil Code	Texture	pH	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-241425-01-1, [redacted] (2003b)	Pikeville Sediment	EFS-54	loam	4.5	2.07	7.73	373*	0.926*
	Pikeville, North Carolina	EFS-65	sand	4.7	0.5	1.42	283	0.924
	Abington	EFS-86	sandy loam	7.5	2.21	7.53 (**3.36)	341 (**151.6)	0.929 (**0.882)
	Sarotti	EFS-88	silty clay loam	7.4	0.9	3.2	356	0.905
	Münster	EFS-93	loamy sand	5.7	1.3	4.54	349	0.929
	Münster	EFS-94	loamy sand	6.2	0.2	0.21	106*	0.931*
	Münster	EFS-95	loamy sand	6.2	0.2	0.17	83*	0.951*
M-233840-01-1, [redacted]	Philippsburg	03/02	sandy loam	6.3	0.6	1.49	248	0.841
	Senas	03/03	clay loam	7.6	1.5	3.59	239	0.882

(2003b)	Huntlosen	03/04	loamy sand	5.3	1.6	9.27	580	0.953
	Rodelsee	03/05	clay	7	1.5	2.59	172	0.859
M-544194-02-1, [redacted] (2015)	[redacted]	WuW	loam	5	1.8	4.65	258.6	0.9258
	[redacted]	HaH	silt loam	6.1	1.9	6.22	327.5	0.8741
	Dollendorf II,	Doll	clay loam	7.3	4.8	11.71	244.1	0.8596
	[redacted]	AXXa	sandy loam	6.5	1.5	4.04	269.3	0.8723
M-572869-01-1, [redacted] (2016)	Burscheid	VG08	silt loam	6.1	0.7	2.12	303.3	0.8868
	Great Chishill	ENG2	clay	7.3	2.1	5.40	257.0	0.9076
	Parcay Meslay	FR09B	loam	6.7	1.3	3.35	257.4	0.8992
	Tarascon Le Cayades	FR08	clay loam	7.6	0.9	1.84	204.9	0.8668
	Valerio Tomelini	IT09	silty clay	7.2	2.1	3.93	187.0	0.9110
	Vilobi D'Onyar	SPA01	sandy loam	6.3	0.8	2.34	292.0	0.8818
M-595721-01-1, [redacted] (2017)	Abington	AB	sandy loam	7.3	2.6	5.6	214.7	0.868
	Lamberton	LB	loam	5.6	2.6	8.6	334.9	0.844
	Lignieres	LN	sandy loam	5.7	0.8	2.9	363.1	0.888
	Muenster	MS	loamy sand	5.6	1.2	3.4	282.6	0.916
	Pikeville	PV	loamy sand	4.5	1.8	6.2	342.6	0.873
	Sarotti	SR	silty clay loam	6.9	1.4	2.6	185.6	0.851
						Arithmetic mean	-	**0.888**
						Geometric mean	**267.7**	-

*excluded from calculations, **checklist value used for geomean and average

M-01 (BAM; AE C653711)

Physico-Chemical Properties
Structural formula



Common name M-01 (BAM; AE C653711)

Chemical name (IUPAC) 2,6-dichlorobenzamide

Molar mass 190.03 g mol^{-1}

Water solubility 2220 mg L^{-1} at 20°C ([redacted] 2014, M-505637-01-1)

Laboratory studies

The aerobic degradation of M-01 (BAM) in soil was investigated in the laboratory by M-234320-01-1, [redacted] (2002). In addition, M-01 was observed to form from fluopicolide in six studies (M-241049-01-1, [redacted] 2003a; M-241052-01-1, [redacted] 2003b; M-241051-01-1, [redacted] 2003c; M-550687-01-1, [redacted] 2016a; M-555570-01-1, [redacted] 2016b and M-655056-01-1, [redacted] 2019) and from M-03 in one study (M-241188-01-1, [redacted], 2003). A summary of the modelling endpoints derived for M-01 b (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted] 2020) is given in Table 9.2.5- 6.

The maximum observed occurrence in soil of M-01 in laboratory studies, expressed as a molar fraction of applied fluopicolide, was **48%** (M-555570-01-1, [redacted], 2016b).

Table 9.2.5- 6: Summary of modelling endpoints derived for M-01 (BAM) under laboratory conditions (after M-685680-01-1, [redacted]., 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised to 20°C and pF2 (d)
Fluopicolide	M-201230-02-1 [redacted] 2003	Münster	SFO	1000[a]	1000[a]
		Sarotti	SFO	1000[a]	1000[a]
	M-241049-01-1 [redacted] 2003a	Abington (non-sterile)	SFO	1000[a]	1000[a]
	M-241052-01-1 [redacted] 2003b	Lamberton	SFO	1000[a]	1000[a]
	M-241051-01-1 [redacted] 2003c	Lamberton	SFO	1000[a]	1000[a]
		Pikeville	SFO	173.1	174.0
	M-550687-01-1 [redacted] 2016a	Albaro/Marcomcini	SFO	417.3	417.3
		Great Chishill	SFO	1000[a]	1000[a]
		[redacted]	SFO	571.7	571.7
		Mas du Coq	SFO	472.2	422.2
		Parcey Meslay	SFO	908.4	908.4
		Vilobi d'Ònyar	SFO	323.9	323.9
	M-555570-01-1 [redacted] 2016b	Dollendorf II	SFO	159.7	159.7
		[redacted]	SFO	869.3	869.3
		[redacted]	SFO	556.2	556.2
		[redacted]	SFO	1000[a]	1000[a]
	M-655056-01-1 [redacted] 2019	Abington 2	SFO	175.6	175.6
		Lamberton	SFO	1000[a]	1000[a]
		Lignières	SFO	1000[a]	1000[a]
		Münster	SFO	294.7	215.6
		Pikeville	SFO	135.9	113.3
		Sarotti 2	SFO	267.1	237.9
M-01	M-234320-01-1, [redacted] 2002	Bethany	SFO	1858.0	2077.6
		North Dakota	SFO	568.8	913.6
M-03	M-241188-01-1, [redacted], 2003	Münster	SFO	1000[a]	1000[a]
		Pikeville	SFO	1000[a]	1000[a]
				Geometric mean	**569.5[d]**

a – Conservative default value
b – Pseudo-SFO value based on slow phase of decline (calculated as $\ln(2)/k_2$ and normalised if applicable)
c – Pseudo-SFO value based on fast phase of decline (calculated $\ln(2)/k_1$ and normalised if applicable)
d – Geometric mean calculated of DT_{50} values from Lamberton soil prior to calculation of overall geometric mean.

Field Dissipation Studies

$DegT_{50}$ values for M-01 (BAM), normalised to 20°C and pF2, have been derived by M-685675-01-1, [redacted]. (2020a) from five terrestrial field dissipation studies (M-650733-02-1, [redacted], 2019b). A summary of the modelling endpoint $DegT_{50}$ values derived for M-01 is given in Table 9.2.5- 7.

Table 9.2.5- 7: Summary of $DegT_{50}$ values (normalised to 20°C and pF2) derived for M-01 (BAM) from terrestrial field dissipation studies (after M-685675-01-1, [redacted] 2020a)

	Aerobic field conditions					
Soil type	**Location (country)**	**pH ($CaCl_2$)**	**Depth (cm)**	**St. (χ^2err) (%)**	**Method of calculation**	**$DegT_{50}$ (d) norm**
Silt loam	Burscheid (Germany)	5.9	0-120	14.68	SFO	94.0
Sandy loam	Lignieres de Touraine (France)	6.9	0-120	7.82	SFO	191.1
Clay loam	St.Etienne du Grès (France)	8.1	0-120	5.87	SFO	179.9
Clay loam	Albarodi Ronco all'Adige (Italy)	7.7	0-120	13.93	SFO	151.8
Sandy clay loam	Vilobi d'Onyar (Spain)	6.9	0-120	10.94	SFO	136.3
					Geometric mean	**146**

Degradation in Aerobic Soil: Overall $DegT_{50}$ value

Degradation half-lives for M-01 (BAM) derived from laboratory and field dissipation studies were compared using the EFSA $DegT_{50}$ Endpoint Selector (EFSA, 2014). This comparison indicated that the field $DegT_{50}$ values for M-01 were significantly shorter than the laboratory studies, therefore the geometric mean field $DegT_{50}$ value of **146 days** was used in the modelling for M-01 (BAM).

Degradation in Water-Sediment Systems

The degradation of fluopicolide in water sediment systems was investigated in the laboratory by M-241425-01-1, [redacted] (2003a). In this study, metabolite M-01 (BAM) was observed to form up to a maximum of **20.3%** of applied radioactivity.

Limited degradation was observed in the study by M-241425-01-1, [redacted] (2003a), and no reliable $DegT_{50}$ values were derived for M-01. A default $DegT_{50}$ value of **1000 days** was therefore used in the modelling to describe the degradation of M-01 in the water compartment, sediment compartment and total water sediment system.

Adsorption

The adsorption and desorption of M-01 (BAM) has been investigated in ten soils (M-235837-01-1, [redacted] 2001; M-224926-01-2, [redacted] 2003; M-686388-01-1, [redacted] 2020a). A summary of the sorption parameters derived for M-01 from these studies is given in Table 9.2.5- 8. A geometric mean K_{OC} value of **24.1 mL/g** was used for M-01 in the modelling.

Table 9.2.5- 8: Summary of sorption parameters derived for M-01 (BAM)

Report reference	**Soil**	**Soil Code**	**Texture**	**pH**	**OC [%]**	**K_f (mL/g)**	**K_{OC} (mL/g)**
M-235837-01-1 [redacted] (2001)	Connecticut	RL-51	Sandy loam	4.8	0.9	0.241	26*
	North Dakota	RL-81	Sandy loam	7.7	5.7	1.761	31
	Florida	RM-014	Sand	6.3	1.4	0.529	38
	Washington	RM-019	Sand	4.9	4.2	1.890	45
	California	RM-022	Sandy clay loam	6.6	0.4	0.208	51
M-224926-01-2 [redacted] (2003)	Connecticut	RL-51	Sandy loam	4.8	0.9	0.359	39.9**
M-686388-01-1 [redacted] (2020a)	LUFA 2.1	2.1	sand	5.2	0.59	0.103	17.5
	LUFA 2.3	2.3	sandy loam	6.2	0.61	0.056	9.2
	LUFA 5M	5M	sandy loam	7.1	1.10	0.162	14.8

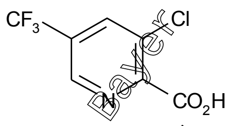
Report reference	Soil	Soil Code	Texture	pH	OC [%]	K_f (mL/g)	K_{OC} (mL/g)
	LUFA 6S	6S	clay loam	7.3	1.78	0.265	14.9*
	Frankenforst	FF	silt loam	6.9	2.4	0.418	17.4
						Geometric mean	**24.1**

*excluded from calculations, **recalculated and used for calculations

M-02 (PCA; AE C657188)

Physico-Chemical Properties

Structural formula



Common name: M-02 (PCA; AE C657188)

Chemical name (IUPAC): 3-chloro-5-(trifluoromethyl)pyridine-2-carboxylic acid

Molar mass: 225.56 g mol^{-1}

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-02 (PCA) in soil was investigated in the laboratory by M-219824-01-1, [redacted] (2003) and M-581364-01-1, [redacted] (2017). A summary of the modelling endpoints derived for M-02 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted] 2020) is given in Table 9.2.5- 9. A geometric mean $DegT_{50}$ value of **1.6 days** was used in the modelling for M-02 (PCA).

The maximum formation of metabolite M-02 in terrestrial field dissipation studies was **16.4%** (M-220477-02-1, [redacted] 2003).

Table 9.2.5- 9: Summary of modelling endpoints derived for M-02 (PCA) under laboratory conditions (after M-685680-01-1, [redacted] 2020)

Applied compound	Study	Soil	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised to 20°C and pF2 (d)
M-02 (PCA)	M-219824-01-1 [redacted] 2003	Abington	SFO	4.4	4.4
		Münster	SFO	3.5	3.5
		Sarotti	SFO	4.4	4.1
	M-581364-01-1 [redacted] 2017	Dollendorf	SFO	1.1	1.1
		[redacted]	SFO	1.1	0.9
		[redacted]	SFO	0.7	0.7
		[redacted]	SFO	0.7	0.7
				Geometric mean	**1.6**

Degradation in Water-Sediment Systems

The degradation of fluopicolide in water sediment systems was investigated in the laboratory by M-241425-01-1, [redacted] (2003a). In this study, metabolite M-02 (PCA) was observed to form up to a maximum of **8.2%** of applied radioactivity.

Limited degradation was observed in the study by M-241425-01-1, [redacted] (2003a), and no reliable $DegT_{50}$ values were derived for M-02. A default $DegT_{50}$ value of **1000 days** was used in the modelling

to describe the degradation of M-02 in the water compartment, sediment compartment and total water sediment system.

Adsorption

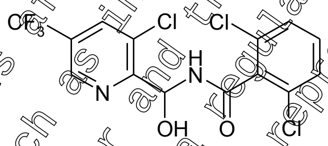
The adsorption and desorption of M-02 (PCA) has been investigated in eight soils (M-219828-01-1, [redacted], 2003; M-686387-01-1, [redacted] 2020b). A summary of the sorption parameters derived for M-02 from these studies is given in Table 9.2.5- 10. A geometric mean K_{OC} value of **5.7 mL/g** was used for M-02 in the modelling.

Table 9.2.5- 10: Summary of sorption parameters derived for M-02 (PCA)

Report reference	Soil	Soil Code	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{Foc} (mL/g)
M-219828-01-1 [redacted] (2003)	Abington	03/06	Sandy loam	7.2	2.6	0.029	1.1
	Munster	03/07	Loamy sand	5.4	1.1	0.116	10.5
	Sarotti	03/10	Silt loam	7.5	1.3	0.082	6.3
M-686387-01-1 [redacted] (2020b)	LUFA 2.1	2.1	Sand	5.2	0.59	0.047	8.0
	LUFA 2.3	2.3	Sandy loam	6.2	0.61	0.038	6.2
	LUFA 5M	5M	Sandy loam	7.1	1.1	0.154	14.0
	LUFA 6S	6S	Clay loam	7.3	1.78	0.145	8.2
	Frankenforst	FF	Silt loam	6.9	2.4	0.059	2.5
						Geometric mean	**5.7**

M-03 (AE 0608000)

Physico-Chemical Properties
Structural formula



Common name M-03 (AE 0608000)

Chemical name (IUPAC) 2,6-dichloro-N-{[3-chloro-5-(trifluoromethyl)yridine-2-yl](hydroxy)methyl}benzamide

Molar mass 399.58 g mol^{-1}

Degradation in Aerobic Soil

The aerobic degradation and metabolism of M-03 in soil was investigated in the laboratory by M-241188-01-1, [redacted] (2003) and M-565219-01-1, [redacted] (2016a). In addition, M-03 was observed to form from fluopicolide in three studies (M-201230-02-1, [redacted] 2003; M-241052-01-1, [redacted] 2003; M-655056-01-1, [redacted] 2019). A summary of the modelling endpoints for M-03 (KCA 7.1.2.1.1/10, M-685680-01-1, [redacted], 2020b) is given in Table 9.2.5- 11.

A geometric mean DegT$_{50}$ value of **17.9 days** was used in the modelling for M-03, with an arithmetic mean molar formation fraction from fluopicolide of **0.53**. These values were derived from acidic soils (pH<6), where the degradation of M-03 occurs more slowly and provide a conservative assessment for M-03.

The maximum observed occurrence in soil of M-03 in laboratory studies was **10.6%** (M-201230-02-1, [redacted] 2003).

Table 9.2.5- 11: Summary of un-normalised $DegT_{50}$ values derived for M-03 under laboratory conditions (after [redacted] 2020b)

Applied compound	Study	Soil	Soil pH	Model selected	$DegT_{50}$ un-normalised (d)	$DegT_{50}$ normalised (d)	ffm from FLC
Fluopicolide	M-201230-02-1, [redacted] 2003	Münster	4.9	SFO	62.6	62.6	0.6086
	M-241052-01-1, [redacted] 2003	Lamberton	5.9	SFO	49.3	54.5	0.5933
	M-655056-01-1, [redacted] 2019	Pikeville	4.5	SFO	29.3	24.4	0.4009
M-03	M-241188-01-1, [redacted] 2003	Abington	7.2	SFO	0.1	0.1	-
		Münster	4.9	DFOP	1000[a]	1000[a]	-
		Pikeville	5.4	DFOP	2.7[b]	2.2[b]	-
		Sarotti	7.1	SFO	0.1	0.08	-
	M-565219-01-1, [redacted] 2016	Brierlow (BL)	5.3	SFO	2.5	2.5	-
		[redacted]	6.0	SFO	0.9	0.9	-
					Geometric mean (pH <6)	**17.9[c]**	**-**
					Arithmetic mean (pH <6)	**-**	**0.53**
					Geomtric mean (soil pH ≥6)	**0.19**	**-**
					Arithmetic mean (pH ≥6)	**-**	**-**

a – DFOP k_2 parameter fixed to conservative default value
b – Pseudo-SFO DT_{50} value derived as $DT_{90}/3.32$ (and normalised if applicable)
c – Geometric mean calculated for Münster soils prior to calculation of overall value

Degradation in Water-Sediment Systems

Metabolite M-03 has not been observed to form in water sediment systems, however an aqueous hydrolysis study has been performed for this compound (M-236241-01-2, [redacted] 2004). The half-life of M-03 in sterile, aqueous buffered solutions ranged from 8.4 minutes at pH 8.1 to 45.5 hours at pH 5.1. A DT_{50} value of **1.9 days** (i.e. 45.5 hours) was used in the modelling to describe the degradation of M-03 in the water compartment and the total water sediment system. The DT_{50} value for M-03 in the sediment compartment was set to a default value of **1000 days**.

The maximum occurrence of M-03 in water sediment systems was set to **0.001%**, as the STEP1-2 calculator requires an input greater than zero for this parameter.

Plant uptake

The plant uptake factor for M-03 was set to a conservative default value of 0. As the metabolite M-03 (AE 0608000) has not been detected in the plants from rotational crop studies, the uptake factor was set to 0.

Foliar Wash-off and Canopy Degradation

Plant wash-off was set to the default value of **50 m^{-1}**, and the canopy degradation DT_{50} value was set to the default value of **10 days** (FOCUS, 2014).

Adsorption

The adsorption and desorption of M-03 has been investigated in three soils by M-221107-01-2, [redacted] (2003). A summary of the sorption parameters derived for M-03 is given in Table 9.2.5- 12. A geometric mean K_{OC} value of **106.9 mL/g**, corresponding to a K_{OM} value of 62.0 mL/g ($K_{OM} = K_{OC} \div 1.724$), was used for M-03 in the modelling, with an arithmetic mean 1/n value of **0.971**.

Table 9.2.5- 12: Summary of sorption parameters derived for M-03

Report reference	Soil	Soil Code	Texture	pH ($CaCl_2$)	OC [%]	K_f (mL/g)	K_{OC} (mL/g)	1/n
M-221107-01-2 [redacted] (2003)	Ingleby	02/03	Sandy loam	4.1	3.5	2.86	82	0.961
	Huntlosen	03/04	Loamy sand	4.7	1.7	2.26	133	1.012
	Munster	03/07	Loamy sand	5.4	1.1	1.23	112	0.939
						Geometric mean	**106.9**	-
						Arithmetic mean	-	**0.971**

II. Results and Discussion

Modelling reports utilising the core info document should have the substance data presented as shown in the following tables.

Table 9.2.5- 13: Substance parameters used at FOCUS Steps 1-2 level

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03 (AE 0608000)
Molar mass	(g/mol)	383.59	190.03	225.56	399.58
Water solubility	(mg/L)	2.8	1830	9721	10
Koc	(mL/g)	267.7	24.7	5.7	106.9
Degradation					
Soil	(days)	182	146	1.6	17.9
Total system	(days)	1000	1000	1000	1.9
Water	(days)	1000	1000	1000	1.9
Sediment	(days)	1000	1000	1000	1000
Max occurrence					
Water / sediment	(%)	100	20.3	8.2	0.001
Soil	(%)	100	48	16.4	10.6

Table 9.2.5- 14: Substance parameters used for fluopicolide and its metabolite M-03 (AE 0608000) at Step 3/4 level

Parameter	Unit	Parent	Metabolite
Substance		Fluopicolide	M-03 (AE 0608000)
SWASH code		FLC	M03
General			
Molar mass	(g/mol)	383.59	399.58
Water solubility (temp.)	(mg/L)	2.8 (20 °C)	10 (20 °C)
Vapour pressure (temp.)	(Pa)	3.03E-07 (20 °C)	0 (20 °C)
Crop processes			
Coefficient for uptake by plant (TSCF)	(-)	0.5	0
Wash-off factor	(1/m)	50	50
Sorption			
K_{OC}	(mL/g)	267.74	106.89
K_{OM}	(mL/g)	155.3	62
Freundlich exponent ($^1/_n$)	(-)	0.888	0.971
Transformation			
DT_{50} in soil	(days)	182	17.9
temperature	(°C)	20	20
moisture content (pF)	(log(cm))	2	2
formation fraction in soil	(-)	-	0.53
DT_{50} in water	(days)	1000	1.9
temperature	(°C)	20	20
formation fraction in water	(-)	-	-

Parameter	Unit	Parent	Metabolite
DT_{50} in sediment	(days)	1000	1000
temperature	(°C)	20	20
formation fraction in sediment	(-)	-	-
DT_{50} on canopy	(days)	10	10
Exponent for the effect of moisture			
PRZM and TOXSWA (Walker exp.)	(-)	0.7	0.7
MACRO (calibrated value)	(-)	0.49	0.49
Effect of temperature			
TOXSWA (molar activation energy)	(kJ/mol)	65.4	65.4
MACRO (effect of temperature)	(1/K)	0.0948	0.0948
PRZM (Q_{10})	(-)	2.58	2.58

III. Conclusion

For the surface water and sediment risk assessment of fluopicolide and its metabolites M-01, M-02, and M-03 the input parameters presented in this summary should be used in all calculations.

<u>Assessment and conclusion by applicant:</u>

This core modelling report was conducted according to FOCUS Degradation Kinetics (2006, 2014) and is considered valid to assess trigger and modelling endpoints for fluopicolide and its metabolites in surface water and sediment under laboratory conditions.

Data Point:	KCP 9.2.5/02
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluopicolide (FLC) and metabolites: PECsw,sed FOCUS EUR - Use in winter oilseed rape in Europe
Report No:	EnSa-20-0397
Document No:	M-687154-01-1
Guideline(s) followed in study:	FOCUS 2015 Generic guidance for FOCUS Surface Water Scenarios Version 1.4 May 2015
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

Predicted environmental concentrations of the fungicide fluopicolide and its metabolites in surface water (PECsw) and sediment (PECsed) were calculated for the use in Europe, employing the tiered FOCUS Surface Water (SW) approach (FOCUS 2001, 2015). All relevant entry routes of a compound into surface water (principally a combination of spray drift and runoff/erosion or drain flow) were considered in these calculations.

The uses of fluopicolide in winter oilseed rape were assessed according to the Good Agricultural Practice (GAP) in Europe.

I. Materials and Methods

Intended GAPs for the use of fluopicolide in Europe were analysed and consolidated according to regulatory and modelling requirements. As a result, one or more uses may be covered by a single modelling GAP row (DGR). The translation of the regulatory GAP for modelling purposes is shown in Table 9.2.5-15.

Table 9.2.5-15: GAP translation for modelling purposes

GAP group ID	GAP group name (DGR) and use IDs	Covered crop(s)	Growth stage	Max. apps	Interval (days)	Rate (kg a.s./ha)
DGR I	winter oilseed rape	winter oilseed rape	BBCH 00	1	-	1 × 0.012

The implementation of the modelling GAP (Table 9.2.5-15) at Steps 1-2 level is shown in Table 9.2.5-16. One or more calculations (modelling tasks, PMT) are necessary to fully cover the use assessed. The number and name of the respective DGR is provided for easier reference.

Table 9.2.5- 16: FOCUS Steps 1-2 specific data for the GAPs assessed

Run IDs (DGR / PMT)	GAP group name (DGR)	Assessment name (PMT)	FOCUS crop (crop group)	Season	Crop cover
DGR I PMT I	winter oilseed rape	Seed treatment	no drift (incorp or seed trtmt) (arable crops)	autumn (Oct.- Feb.)	no interception

This section provides the implementation of the modelling GAP (Table 9.2.5-15) at Step 3 level. Also, here one or more calculations (modelling tasks, PMT) are necessary to fully cover the use assessed. The number and name of the respective DGR is provided for easier reference.

Please note that PMTs at Steps 1-2 and Step 3 do not necessarily fully correspond to each other due to inherent differences in the models.

The application dates for this assessment were set with the help of the tool AppDate (Klein 2018), which proposes dates for specific crop stages (given as BBCH code) based on the crop development as defined in the FOCUS model scenarios for groundwater and surface water.

The summary of all Step 3 PMTs is provided in Table 9.2.5- 17. The detailed information on individual uses is given in Table 9.2.5- 18 and Table 9.2.5- 19.

Table 9.2.5- 17: Overview of FOCUS Step 3 assessments

Run IDs (DGR / PMT)	GAP group name (DGR)	Assessment name (PMT)	FOCUS crop (crop group)
DGR I PMT I	Winter oilseed rape	Seed treatment	Oil seed rape, winter (arable crops)

GAP group name winter oilseed rape, assessment name Seed treatment

Table 9.2.5- 18: Summarised FOCUS Step 3 application data (PAT settings)

Assessment name	Scenario	Application window used in modelling
Seed treatment	D2 Ditch/Stream	01-Sep - 01-Oct
	D3 Ditch	19-Aug - 18-Sep
	D4 Pond/Stream	20-Aug - 19-Sep
	D5 Pond/Stream	06-Sep - 06-Oct
	R1 Pond/Stream	21-Aug - 20-Sep
	R3 Stream	21-Sep - 21-Oct

Table 9.2.5- 19: Full FOCUS Step 3 application data

Run IDs	DGR I / PMT I
GAP group name (DGR)	Winter oilseed rape
Assessment name (PMT)	Seed treatment
FOCUS model crop (crop group)	Oil seed rape, winter (arable crops)
Use pattern	0.012 kg a.s./ha
Appl. method (Run-off CAM, depth inc.)	Soil incorp. (8 - incorp soil at one depth, 3 cm)
PAT start date (relative to crop event or absolute)	14 days before emergence
PAT window range	30 days for all scenarios (min = 30 days)

Drainage scenarios	PAT start/end date (Julian day)	Application date	Runoff scenarios	PAT start/end date (Julian day)	Application date
D2 Ditch/Stream	01-Sep/01-Oct (244/274)	03-Sep	R1 Pond/Stream	21-Aug/20-Sep (233/263)	21-Aug
D3 Ditch	19-Aug/18-Sep (231/261)	18-Aug	R3 Stream	21-Sep/21-Oct (264/294)	23-Sep
D4 Pond/Stream	20-Aug/19-Sep (232/262)	27-Aug			
D5 Pond/Stream	06-Sep/06-Oct (249/279)	07-Sep			

Steps 1-2 calculations were performed according to formulas implemented in FOCUS STEPS 1+2 version 3.2.

Step 3 calculations were performed using the FOCUS SWASH 5.3 suite, including
- FOCUS PRZM 4.3.1
- FOCUS MACRO 5.5.4
- FOCUS TOXSWA 5.5.3

Standard procedures and settings were used for Steps 1-2 and 3 assessments.

Substance related parameters which have been used for fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657188) and M-03 (AE 0608000) and whose derivation is described in detail in the core modelling document KCP 9.2.5/01 have been used in the calculations at FOCUS SW Steps 1-2 level are summarised in Table 9.2.5- 20 and at Step 3/4 level in Table 9.2.5- 21.

Table 9.2.5- 20: Substance parameters used at FOCUS Steps 1-2 level

Parameter	Unit	Fluopicolide	M-01 (AE C653711)	M-02 (AE C657188)	M-03 (AE 0608000)
Molar mass	(g/mol)	383.59	190.03	225.56	399.58
Water solubility	(mg/L)	2.8	1830	9721	10
Koc	(mL/g)	267.7	24.1	5.7	106.9
Degradation					
Soil	(days)	182	146	1.6	17.9
Total system	(days)	1000	1000	1000	1.9
Water	(days)	1000	1000	1000	1.9
Sediment	(days)	1000	1000	1000	1000
Max occurrence					
Water / sediment	(%)	100	20.3	8.2	0.001
Soil	(%)	100	48	16.4	10.6

Table 9.2.5- 21: Substance parameters used for fluopicolide and its metabolite M-03 (AE 0608000) at Step 3/4 level

Parameter	Unit	Parent	Metabolite
Substance		Fluopicolide	M-03 (AE 0608000)
SWASH code		FLC	M03
General			
Molar mass	(g/mol)	383.59	399.58
Water solubility (temp.)	(mg/L)	2.8 (20 °C)	10 (20 °C)
Vapour pressure (temp.)	(Pa)	3.03E-07 (20 °C)	0 (20 °C)
Crop processes			
Coefficient for uptake by plant (TSCF)	(-)	0.5	0
Wash-off factor	(1/m)	50	50
Sorption			
K_{OC}	(mL/g)	267.74	106.89
K_{OM}	(mL/g)	155.3	62
Freundlich exponent ($^1/_n$)	(-)	0.888	0.971
Transformation			
DT50 in soil	(days)	182	17.9
temperature	(°C)	20	20
moisture content (pF)	(log(cm))	2	2
formation fraction in soil	(-)	-	0.53
DT50 in water	(days)	1000	1.9
temperature	(°C)	20	20
formation fraction in water	(-)	-	-
DT50 in sediment	(days)	1000	1000
temperature	(°C)	20	20
formation fraction in sediment	(-)	-	-
DT50 on canopy	(days)	10	10
Exponent for the effect of moisture			
PRZM and TOXSWA (Walker exp.)	(-)	0.7	0.7
MACRO (calibrated value)	(-)	0.49	0.49
Effect of temperature			
TOXSWA (molar activation energy)	(kJ/mol)	65.4	65.4
MACRO (effect of temperature)	(1/K)	0.0948	0.0948
PRZM (Q_{10})	(-)	2.58	2.58

II. Results and Discussion

The PEC values were calculated for fluopicolide and its metabolites M-01 (AE C653711), M-02 (AE C657188) and M-03 (AE 0608000) according to the equations implemented in the "STEPS 1-2 in FOCUS" calculator Table 9.2.5- 22 to Table 9.2.5- 25.

Parent substance fluopicolide

Winter oilseed rape - Seed treatment – 1 × 12g a.s./ha (DGR I / PMT I)

Table 9.2.5- 22: FOCUS Steps 1-2 PECsw and PECsed for fluopicolide, GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC_{sw} (µg/L)*	Dominant entry route	7d-$PEC_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 1	-	2.95	RunOff	2.94	7.89
Step 2					
Northern Europe	Oct. - Feb.(Autumn)	1.45 *	RunOff	1.45	3.89 *
Southern Europe	Oct. - Feb.(Autumn)	1.16 *	RunOff	1.16	3.11 *

* Single applications are marked.
** TWA interval as required by ecotox

Metabolite M-01 (AE C653711)

Winter oilseed rape - Seed treatment – 1 × 12g a.s./ha (DGR I / PMT I)

Table 9.2.5- 23: FOCUS Steps 1-2 PECsw and PECsed for M-01 (AE C653711), GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC_{sw} (µg/L)*	Dominant entry route	7d-$PEC_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 1	-	1.31	-	1.31	0.316
Step 2					
Northern Europe	Oct. - Feb.(Autumn)	0.644 *	-	0.643	0.155 *
Southern Europe	Oct. - Feb.(Autumn)	0.515 *	-	0.514	0.124 *

* Single applications are marked.
** TWA interval as required by ecotox

Metabolite M-02 (AE C657188)

Winter oilseed rape - Seed treatment – 1 × 12g a.s./ha (DGR I / PMT I)

Table 9.2.5- 24: FOCUS Steps 1-2 PECsw and PECsed for M-02 (AE C657188), GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC_{sw} (µg/L)*	Dominant entry route	7d-$PEC_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 1	-	0.574	-	0.573	0.033
Step 2					
Northern Europe	Oct. - Feb.(Autumn)	0.128 *	-	0.128	0.007 *
Southern Europe	Oct. - Feb.(Autumn)	0.103 *	-	0.102	0.006 *

* Single applications are marked.
** TWA interval as required by ecotox

Metabolite M-03 (AE 0608000)

Winter oilseed rape - Seed treatment – 1 × 12g a.s./ha (DGR I / PMT I)

Table 9.2.5- 25: FOCUS Steps 1-2 PECsw and PECsed for M-03 (AE 0608000), GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC_{sw} (µg/L)*	Dominant entry route	7d-$PEC_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 1	-	0.387	-	0.140	0.413
Step 2					
Northern Europe	Oct. - Feb.(Autumn)	0.166 *	-	0.065	0.177 *
Southern Europe	Oct. - Feb.(Autumn)	0.133 *	-	0.052	0.142 *

* Single applications are marked.
** TWA interval as required by ecotox

Step 3 calculations were conducted for fluopicolide and its metabolite M-03 (AE 0608000) employing the models of the FOCUS SW suite. Reported values represent loadings *via* all relevant entry routes are shown in Table 9.2.5- 26 and Table 9.2.5- 27.

Parent substance fluopicolide

Winter oilseed rape - Seed treatment - 0.012 kg a.s./ha (DGR I / PMT I)

Table 9.2.5- 26: FOCUS Step 3 PECsw and PECsed for fluopicolide, GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC_{sw} (µg/L)*	Dominant entry route	7d-$PEC_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 3					

D2	Ditch	<0.001	*	Drainage	<0.001	0.006 *
D2	Stream	<0.001	*	Drainage	<0.001	0.003 *
D3	Ditch	<0.001	*	Drainage	<0.001	<0.001 *
D4	Pond	0.002	*	Drainage	0.002	0.011 *
D4	Stream	0.004	*	Drainage	0.003	0.004 *
D5	Pond	0.002	*	Drainage	0.002	0.018 *
D5	Stream	0.003	*	Drainage	0.001	0.004 *
R1	Pond	<0.001	*	RunOff	<0.001	0.001 *
R1	Stream	<0.001	*	RunOff	<0.001	<0.001 *
R3	Stream	<0.001	*	RunOff	<0.001	<0.001 *

* Single applications are marked.
** TWA interval as required by ecotox

Metabolite M-03 (AE 0608000)

Winter oilseed rape - Seed treatment - 0.042 kg a.s./ha (DGR I / PMT I)

Table 9.2.5- 27: FOCUS Step 3 PECsw and PECsed for M-03 (AE 0608000), GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC$_{sw}$ (µg/L)*	Dominant entry route	7d-PEC$_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 3					
D2	Ditch	0.001 *	-	<0.001	0.002 *
D2	Stream	<0.001 *	-	<0.001	0.001 *
D3	Ditch	<0.001 *	-	<0.001	<0.001 *
D4	Pond	0.002 *	-	0.002	0.002 *
D4	Stream	0.004 *	-	0.003	0.004 *
D5	Pond	<0.001 *	-	<0.001	<0.001 *
D5	Stream	0.001 *	-	<0.001	<0.001 *
R1	Pond	<0.001 *	-	<0.001	<0.001 *
R1	Stream	<0.001 *	-	<0.001	<0.001 *
R3	Stream	<0.001 *	-	<0.001	<0.001 *

* Single applications are marked.
** TWA interval as required by ecotox

III. Conclusion

Predicted environmental concentrations of the fungicide fluopicolide and its metabolites in surface water (PECsw) and sediment (PECsed) were calculated for the use in winter oilseed rape in Europe, employing the tiered FOCUS Surface Water (SW) approach (FOCUS 2001, 2015). All relevant entry routes of a compound into surface water (principally a combination of spray drift and runoff/erosion or drain flow) were considered.

Assessment and conclusion by applicant:

The risk assessment report was conducted according to FOCUS (2001,2015) and is considered valid to assess predicted environmental concentrations in surface water (PEC_{SW}) and sediment (PECsed) for fluopicolide and its metabolites in oil seed rape (winter).

PEC_{sw} for fluoxastrobin

Data Point:	KCP 9.2.5/03
Report Author:	[redacted]
Report Year:	2020
Report Title:	Fluoxastrobin (FXA): PECsw,sed FOCUS EUR - Use in winter oilseed rape in Europe
Report No:	EnSa-20-0400
Document No:	M-687158-01-1
Guideline(s) followed in study:	FOCUS 2015 Generic guidance for FOCUS Surface Water Scenarios Version 14 May 2015
Deviations from current test guideline:	None
Previous evaluation:	No, not previously submitted
GLP/Officially recognised testing facilities:	No, not conducted under GLP/Officially recognised testing facilities
Acceptability/Reliability:	Yes

Executive Summary

Predicted environmental concentrations of the fungicide fluoxastrobin in surface water (PECsw) and sediment (PECsed) were calculated for the use in Europe, employing the tiered FOCUS Surface Water (SW) approach (FOCUS 2001, 2015). All relevant entry routes of a compound into surface water (principally a combination of spray drift and runoff/erosion or drain flow) were considered in these calculations.

The uses of fluoxastrobin in winter oilseed rape were assessed according to the Good Agricultural Practice (GAP) in Europe.

I. Materials and Methods

Intended GAPs for the use of fluoxastrobin in Europe were analysed and consolidated according to regulatory and modelling requirements. As a result, one or more uses may be covered by a single modelling GAP row (DGR). The translation of the regulatory GAP for modelling purposes is shown in Table 9.2.5-28.

Table 9.2.5-28: GAP translation for modelling purposes

GAP group ID	GAP group name (DGR) and use IDs	Covered crop(s)	Growth stage	Max. apps	Interval (days)	Rate (kg a.s./ha)
DGR I	winter oilseed rape	winter oilseed rape	BBCH 00	1	-	1 × 0.009

The implementation of the modelling GAP (Table 9.2.5-28) at Steps 1-2 level is shown in Table 9.2.5-29. One or more calculations (modelling tasks, PMT) are necessary to fully cover the use assessed. The number and name of the respective DGR is provided for easier reference.

Table 9.2.5- 29: FOCUS Steps 1-2 specific data for the GAPs assessed

Run IDs (DGR / PMT)	GAP group name (DGR)	Assessment name (PMT)	FOCUS crop (crop group)	Season	Crop cover
DGR I PMT I	winter oilseed rape	Seed treatment	oil seed rape, winter (arable crops)	autumn (Oct. - Feb.)	no interception

This section provides the implementation of the modelling GAP (Table 9.2.5-28) at Step 3 level. Also, here one or more calculations (modelling tasks, PMT) are necessary to fully cover the use assessed. The number and name of the respective DGR is provided for easier reference.

Please note that PMTs at Steps 1-2 and Step 3 do not necessarily fully correspond to each other due to inherent differences in the models.

The application dates for this assessment were set with the help of the tool AppDate (Klein 2018), which proposes dates for specific crop stages (given as BBCH code) based on the crop development as defined in the FOCUS model scenarios for groundwater and surface water.

The summary of all Step 3 PMTs is provided in Table 9.2.5- 30. The detailed information on individual uses is given in Table 9.2.5- 31 and Table 9.2.5- 32.

Table 9.2.5- 30: Overview of FOCUS Step 3 assessments

Run IDs (DGR / PMT)	GAP group name (DGR)	Assessment name (PMT)	FOCUS crop (crop group)
DGR I PMT I	Winter oilseed rape	Seed treatment	Oil seed rape, winter (arable crops)

GAP group name winter oilseed rape, assessment name Seed treatment

Table 9.2.5- 31: Summarised FOCUS Step 3 application data (PAT settings)

Assessment name	Scenario	Application window used in modelling
Seed treatment	D2 Ditch/Stream D3 Ditch D4 Pond/Stream D5 Pond/Stream R1 Pond/Stream R3 Stream	01-Sep - 01-Oct 19-Aug - 18-Sep 20-Aug - 19-Sep 06-Sep - 06-Oct 21-Aug - 20-Sep 21-Sep - 21-Oct

Table 9.2.5- 32: Full FOCUS Step 3 application data

Run IDs	DGR I / PMT I
GAP group name (DGR)	Winter oilseed rape
Assessment name (PMT)	Seed treatment
FOCUS model crop (crop group)	Oil seed rape, winter (arable crops)
Use pattern	0.009 kg a.s./ha
Appl. method (Run-off CAM, depth inc.)	Soil incorp. (8 - incorp soil at one depth, 3 cm)
PAT start date (relative to crop event or absolute)	14 days before emergence
PAT window range	30 days for all scenarios (min = 30 days)

Drainage scenarios	PAT start/end date (Julian day)	Application date	Runoff scenarios	PAT start/end date (Julian day)	Application date
D2 Ditch/Stream	01-Sep/01-Oct (244/274)	03-Sep	R1 Pond/Stream	21-Aug/20-Sep (233/263)	21-Aug
D3 Ditch	19-Aug/18-Sep (231/261)	18-Aug	R3 Stream	21-Sep/21-Oct (264/294)	23-Sep
D4 Pond/Stream	20-Aug/19-Sep (232/262)	27-Aug			
D5 Pond/Stream	06-Sep/06-Oct (249/279)	07-Sep			

Step 1-2 calculations were performed according to formulas implemented in FOCUS STEPS 1+2 version 3.2.

Step 3 calculations were performed using the FOCUS SWASH 5.3 suite, including

FOCUS PRZM 4.3.1
FOCUS MACRO 5.5.4
FOCUS TOXSWA 5.5.3

Standard procedures and settings were used for Steps 1-2 and 3 assessments.

Substance related parameters which have been used for fluoxastrobin have been taken from the EFSA LoEP [EFSA Scientific report 102, 12 June 2007]. The parameters used in the calculations at FOCUS SW Steps 1-2 level are summarised in Table 9.2.5- 33 and at Step 3/4 level in Table 9.2.5- 34.

Table 9.2.5- 33: Substance parameters used at FOCUS Steps 1-2 level

Parameter	Unit	Fluoxastrobin
Molar mass	(g/mol)	458.8
Water solubility	(mg/L)	2.29
Koc	(mL/g)	752
Degradation		
Soil	(days)	39.1
Total system	(days)	182
Water	(days)	182
Sediment	(days)	1000
Max occurrence		
Water / sediment	(%)	100
Soil	(%)	100

Table 9.2.5- 34: Substance input parameters at Steps 3/4 level

Parameter	Unit	Parent
Substance		Fluoxastrobin
SWASH code		FXA
General		
Molar mass	(g/mol)	458.8
Water solubility (temp.)	(mg/L)	2.29 (20 °C)
Vapour pressure (temp.)	(Pa)	0 (20 °C)
Crop processes		
Coefficient for uptake by plant (TSCF)	(-)	0
Wash-off factor	(1/m)	50
Sorption		
K_{OC}	(mL/g)	751.66
K_{OM}	(mL/g)	436
Freundlich exponent ($^1/_n$)	(-)	0.86
Transformation		
DT50 in soil	(days)	39.1
temperature	(°C)	20
moisture content (pF)	(log(cm))	2
formation fraction in soil	(-)	-
DT50 in water	(days)	182
temperature	(°C)	20
formation fraction in water	(-)	-
DT50 in sediment	(days)	1000
temperature	(°C)	20
formation fraction in sediment	(-)	-
DT50 on canopy	(days)	10
Exponent for the effect of moisture		
PRZM and TOXSWA (Walker exp.)	(-)	0.7
MACRO (calibrated value)	(-)	0.49
Effect of temperature		
TOXSWA (molar activation energy)	(kJ/mol)	65.4
MACRO (effect of temperature)	(1/K)	0.0948
PRZM (Q_{10})	(-)	2.58

II. Results and Discussion

The PEC values were calculated for fluoxastrobin according to the equations implemented in the "STEPS 1-2 in FOCUS" calculator are shown in Table 9.2.5- 35.

Winter oilseed rape - Seed treatment – 1 × 9 g a.s./ha (DGR I / PMT I)

Table 9.2.5- 35: FOCUS Steps 1-2 PECsw and PECsed for fluoxastrobin, GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC_{sw} (µg/L)*	Dominant entry route	7d-$PEC_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 1		1.58	RunOff	1.52	11.5
Step 2					
Northern Europe	Oct. - Feb.(Autumn)	0.747 *	Erosion	0.732	5.55 *
Southern Europe	Oct. - Feb.(Autumn)	0.607 *	Erosion	0.594	4.50 *

* Single applications are marked.
** TWA interval as required by ecotox

Step 3 calculations were conducted for fluoxastrobin a employing the models of the FOCUS SW suite. Reported values represent loadings *via* all relevant entry routes are shown in Table 9.2.5- 36.

Winter oilseed rape - Seed treatment - 0.009 kg a.s./ha (DGR I / PMT I)

Table 9.2.5- 36: FOCUS Step 3 PECsw and PECsed for fluoxastrobin, GAP group name winter oilseed rape, assessment name Seed treatment (DGR I / PMT I)

Scenario FOCUS	Waterbody	Max PEC_{sw} (µg/L)*	Dominant entry route	7d-$PEC_{sw,twa}$ (µg/L)**	Max PECsed (µg/kg)*
Step 3					
D2	Ditch	<0.001 *	Drainage	<0.001	<0.001 *
D2	Stream	<0.001 *	Drainage	<0.001	<0.001 *
D3	Ditch	<0.001 *	Drainage	<0.001	<0.001 *
D4	Pond	<0.001 *	Drainage	<0.001	<0.001 *
D4	Stream	<0.001 *	Drainage	<0.001	<0.001 *
D5	Pond	<0.001 *	Drainage	<0.001	<0.001 *
D5	Stream	<0.001 *	Drainage	<0.001	<0.001 *
R1	Pond	<0.001 *	RunOff	<0.001	<0.001 *
R1	Stream	<0.001 *	RunOff	<0.001	<0.001 *
R3	Stream	<0.001 *	RunOff	<0.001	<0.001 *

* Single applications are marked

** TWA interval as required by ecotox

III. Conclusion

Predicted environmental concentrations of the fungicide fluoxastrobin in surface water (PECsw) and sediment (PECsed) were calculated for the use in winter oilseed rape in Europe, employing the tiered FOCUS Surface Water (SW) approach (FOCUS 2001, 2015). All relevant entry routes of a compound into surface water (principally a combination of spray drift and runoff/erosion or drain flow) were considered.

Assessment and conclusion by applicant:

The risk assessment report was conducted according to FOCUS (2001,2015) and is considered valid to assess predicted environmental concentrations in surface water (PEC_{SW}) and sediment (PECsed) for fluoxastrobin in oil seed rape (winter).

CP 9.3 Fate and behaviour in air

For information on the fate and behaviour in air please refer to Document MCA, Section 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 Document MCA, Sections 7.3.1 and 7.3.2.

CP 9.4 Estimation of concentrations for other routes of exposure

There are no other routes of exposure if the product is used according to good agricultural practice. Therefore no further estimations are considered necessary.