REGISTRATION REPORT

Part B

Section 8

Environmental Fate

Detailed summary of the risk assessment

Product code: AG-F8-250 CS

Chemical active substance(s):

Flurochloridone, 250 g/L

Central Zone

Zonal Rapporteur Member State: Poland

CORE ASSESSMENT

(authorisation)

Sponsor: ADAMA Agan Ltd

Applicant: Country organisation/representative of ADAMA Agan Ltd. as reported in Part A

Submission date: January 2020

MS Finalisation date: October 2020 (initial Core Assessment)

March 2021 (final Core Assessment)

August 2021 (evaluation of additional data)

Version history

When	What
January 2020	dRR submitted by the Applicant
October 2020	Initial assessment by the zRMS The report in the dRR format has been prepared by the Applicant, therefore all comments, additional evaluations and conclusions of the zRMS are presented in grey commenting boxes. Minor changes are introduced directly in the text and highlighted in grey. Not agreed or not relevant information are ~~struck through and shaded for transparency~~.
March 2021	Final report (Core Assessment updated following the commenting period) Additional information/assessments included by the zRMS in the report in response to comments recieved from the cMS and the Applicant are highlighted in yellow.
July 2021	Update by the Applicant with additional lower application rate and pattern analysis for both rates in FOCUS surface water Step 3-4 only are highlighted in blue
August 2021	Evaluation of additional information by the zRMS. Additional evlauations, comments and corrections of the Applicants' text made by the zRMS are highlighted in green.

Table of Contents

8 Fate and behaviour in the environment (KCP 9)

zRMS comments:

The report in the dRR format has been prepared by the Applicant, therefore all comments, additional evaluations and conclusions of the zRMS are presented in grey commenting boxes. Minor changes are introduced directly in the text and highlighted in grey. Not agreed or not relevant information is struck through and shaded for transparency.

Although no comments in area of Section 8 were provided during the commenting period, new Step 4 simulations performed using VFSmod were submitted by the Applicant in order to further mitigate flurochloridone run-off in R scenarios. These new simulations were presented and evaluated by the zRMS in point 8.9 of this document.

After finalisation of the Core Assessment additional surface water modelling for the lower application rate has been provided by the Applicant. New information provided by the Applicant is highlighted in blue, while zRMS evaluation is highlighted in green in order to distinguish Applicants' text from zRMS assessment.

8.1 Critical GAP and overall conclusions

Table 8.1-1: Critical use pattern of the formulated product

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Use-No. *	Member state(s)	Crop and/or situation (crop destination / purpose of crop)	F, Fn, Fpn G, Gn, Gpn or I **	Pests or Group of pests controlled (additionally: developmental stages of the pest or pest group)	**Application**				**Application rate**			PHI (days)	Remarks: e.g. g safener/ synergist per ha	**Conclusion**
					Method / Kind	Timing / Growth stage of crop & season	Max. number a) per use b) per crop/ season	Min. interval between applications (days)	kg or L product/ha a) max. rate per appl. b) max. total rate per crop/season	g or kg as/ha a) max. rate per appl. b) max. total rate per crop/season	Water L/ha min/max			Groundwater
Zonal uses (field or outdoor uses, certain types of protected crops)														
1	PL	Potato (SOLTU)	F	broadleaved and grass weeds, pre-emergence	spray application	BBCH 00-09	1	n.a.	a) 1.5 - 2 L/ha b) 1.5 - 2 L/ha	a) 375 - 500 g/ha b) 375 - 500 g/ha	200 / 300	n.a.		A

* Use number(s) in accordance with the list of all intended GAPs in Part B, Section 0 should be given in column 1

** F: professional field use, Fn: non-professional field use, Fpn: professional and non-professional field use, G: professional greenhouse use, Gn: non-professional greenhouse use, Gpn: professional and non-professional greenhouse use, I: indoor application

Explanation for column 15 "Conclusion"

A	Safe use
R	Further refinement and/or risk mitigation measures required
C	To be confirmed by cMS
N	No safe use

Table 8.1-2: Assessed (critical) uses during approval of flurochloridone concerning the Section Environmental Fate

1	2	3	4	5	6	7	8	9	10	11	12	13	14
Use-No. *	Member state(s)	Crop and/or situation (crop destination / purpose of crop)	F, Fn, Fpn G, Gn, Gpn or I **	Pests or Group of pests controlled (additionally: developmental stages of the pest or pest group)	**Application**				**Application rate**			PHI (days)	Remarks: e.g. g safener/ synergist per ha
					Method / Kind	Timing / Growth stage of crop & season	Max. number a) per use b) per crop/ season	Min. interval between applications (days)	kg or L product/ha a) max. rate per appl. b) max. total rate per crop/season	g or kg as/ha a) max. rate per appl. b) max. total rate per crop/season	Water L/ha min/max		
1	N/S Europe ~~PL~~	Potato (SOLTU)	F	broadleaved and grass weeds, pre-emergence	spray application	BBCH 00-05 ~~BBCH 00-09~~	1	n.a.	a) 1.5 - 3 L/ha b) 1.5 - 3 L/ha ~~a) 1.5 - 2 L/ha b) 1.5 - 2 L/ha~~	a) 375 - 750 g/ha b) 375 - 750 g/ha ~~a) 375 - 500 g/ha b) 375 - 500 g/ha~~	200 / 400 ~~200 / 300~~	n.a.	

* Use number(s) in accordance with the list of all intended GAPs in Part B, Section 0 should be given in column 1

** F: professional field use, Fn: non-professional field use, Fpn: professional and non-professional field use, G: professional greenhouse use, Gn: non-professional greenhouse use, Gpn: professional and non-professional greenhouse use, I: indoor application

zRMS comments:

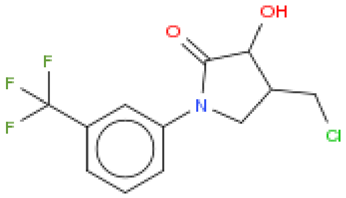
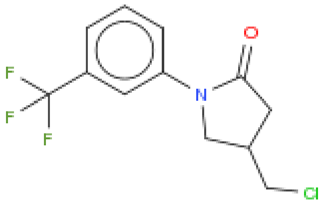
Table above has been amended in order to reflect GAP considered in the course of the EU review of flurochloridone provided in EFSA Journal 2010:8(12):1869

8.2 Metabolites considered in the assessment

The metabolites considered in the assessment are shown below. It was concluded during Annex I inclusion that the photolysis metabolite M8 did not need to be accounted for in the surface water exposure assessments (EFSA 2010, p. 10). Also, soil risk assessments were not considered necessary for the two soil metabolites (EFSA 2010, p. 12, 36).

The metabolites and the exposure assessments considered necessary (EFSA 2010) are listed in the table below. While these metabolite assessments are covered by the EU assessments, because the GAP for the intended use is a subset of the GAP at EU level, the assessments are updated using current guidance and models.

Table 8.2-1: Metabolites of flurochloridone potentially relevant for exposure assessment

Metabolite	Molar mass	Chemical structure	Maximum observed occurence in compartements	Exposue assessment required due to
R406639	293.7		Soil: 8.1% w/s system: 13.9%	PEC_{gw}: assessment with current guidance and models $PEC_{sw/sed}$: assessment with current guidance and models
R42819	277.7		Soil: 10.1% w/s system: 63.9%	PEC_{gw}: assessment with current guidance and models $PEC_{sw/sed}$: assessment with current guidance and models

zRMS comments:

Information regarding metabolites of flurochloridone is in line with EU agreed endpoints reported in EFSA Journal 2010;8(12):1869.

8.3 Rate of degradation in soil (KCP 9.1.1)

Studies on degradation in laboratory soil with the formulation were not available at Annex I inclusion (EFSA, 2010), since it was assumed that it is possible to extrapolate from data obtained with the active substance. Field dissipation studies with two different formulations are available that have been reviewed at Annex I inclusion. They have been re-evaluated according to current guidance (EFSA 2014) in a separate report (Finger and Ranke 2018) as shown in section 8.4.

8.3.1 Aerobic degradation in soil (KCP 9.1.1.1)

The aerobic degradation kinetics for flurochloridone and its two major soil metabolites where reviewed in detail in the European pesticide risk assessment peer review. For flurochloridone and R406639, geometric mean values were used as derived in the EFSA conclusion.

Table 8.3-1: Summary of aerobic degradation rates for flurochloridone - laboratory studies (EFSA 2010)

Soil name	Soil type	pH	t. °C	MWHC (%)	DT50 (d)	DT90 (d)	DT50 (d) 20°C pF2/10kPa	Kinetic model	Reference Evaluated on EU level
Richmond (two labels)	silt loam	6.1	20°C	41.6/45	24.4[a]/24[a]	306[a]/460[a]	58.013[b]	HS	Bowler (1998) yes
Keeton	sandy loam	7.7	28°C	40	38.5[a]	545.02[a]	180[c]	DFOP	Miaullis and Vispetto (1985) yes
Delco	silt loam	6.7	28°C	40	6.35[a]	51.46[a]	22.8[d]	FOMC	
Aurora	loam	7.4	28°C	40	6.7[a]	54.1[a]	33.252[d]	FOMC	
Geometric mean (n=4)							**53.0**		**yes**

[a] Best-fit kinetics was FOMC, DT90 in Richmond and Keeton soils extrapolated beyond study duration
[b] Obtained from the slower rate constant of the HS model
[c] Obtained from the slower rate constant of the DFOP model
[d] Obtained from the FOMC DT90 divided by 3.32

Table 8.3-2: Summary of aerobic degradation rates for R406639 - laboratory studies

Soil name	Soil type	pH	t.oC	MWHC %	DT50 (d)	ff	DT50 (d) 20°C pF2/10kPa	Chi2 (%)	Kinetic model	Reference Evaluated on EU level
Richmond (two labels)	silt loam	6.1	20°C	41.6/45	8.4/15.4	0.0833/0.1811	5.9/10.8	15.4/19	FOMC-SFO	Bowler (1998) yes
Keeton	sandy loam	7.7	28°C	40	131.2	0.0881	226.51	16.2	FOMC-SFO	Miaullis and Vispetto (1985) yes
Delco	silt loam	6.7	28°C	40	104	0.12883	153.2	5.4	FOMC-SFO	
Aurora	loam	7.4	28°C	40	60.5	0.071	123.42	11.6	FOMC-SFO	
Arithmetic mean (n=4)						**0.105**				**yes**
Geometric mean (n=4)							**77.4**			**yes**

A potential risk of contamination of groundwater with metabolite R42819 was identified in the European risk assessment review. Therefore, a new study was conducted (Walther 2013a). This study is summarised in Appendix A 2.1.

Table 8.3-3: Summary of aerobic degradation rates for R42819 - laboratory studies

Soil name	Soil type	pH	t.oC	MWHC %	DT50 (d)	ff	DT50 (d) 20°C pF2/10kPa	Chi2 (%)	Kinetic model	Reference Evaluated on EU level
Keeton	sandy loam	7.7	28°C	40	42.3	-	73[a]	16.2	FOMC-SFO	Miaullis and Vispetto (1985) yes
Delco	silt loam	6.7	28°C	40	8.7	-	12.81	5.4	FOMC-SFO	
Aurora	loam	7.4	28°C	40	262.8[b]	-	536.2	11.6	FOMC-SFO	
Mechtildshausen	loam	7.16	20°C	pF2	17.1	-[d]	17.1	5.41	SFO	Walther (2013a)[c] yes
Speyer 2.2	loamy sand	5.5	20°C	pF2	27.5	-[d]	27.5	3.79	SFO	
Fraunhofer 02-A	silt loam	6.84	20°C	pF2	18.2	-[d]	18.2	4.17	SFO	
Geometric mean for tier 1 (n=3)							**79.4**			
Geometric mean for tier 2 (n=6)							**40.3**			

[a] High uncertainty associated to the estimation according to EFSA (2010)
[b] Extrapolated beyond study duration
[c] New study evaluated as confirmatory data
[d] Not applicable as metabolite was dosed directly

zRMS comments:

Soil laboratory degradation data for flurochloridone and its metabolites are in line with EU agreed endpoints reported in EFSA Journal 2010;8(12):1869 (parent, metabolite R406639 and Tier 1 for metabolite R42819) and Addendum 2, B.8 on Confirmatory Data of July 2014 (Tier 2 values for metabolite R42819).

8.3.2 Anaerobic degradation in soil (KCP 9.1.1.1)

The breakdown of flurochloridone under anaerobic conditions was considered less extensive than under aerobic conditions. No further studies were performed.

zRMS comments:

Information on anaerobic soil degradation of flurochloridone is in line with EU agreed data reported in EFSA Journal 2010;8(12):1869.

8.4 Field studies (KCP 9.1.1.2)

8.4.1 Soil dissipation testing on a range of representative soils (KCP 9.1.1.2.1)

Trigger Endpoints

Field dissipation data for flurochloridone were evaluated during Annex I inclusion. The DT50 and DT90 values from the two studies found satisfactory on EU level are summarised in the table below. The kinetic evaluations were based on the FOMC model, which explains the large factor between DT50 and DT90.

Table 8.4-1: Summary of aerobic degradation rates for flurochloridone - field studies: Triggering endpoints

Soil type	Location	pH (H_2O)	Depth (cm)	DissT50 (d) actual	DT90 (d) actual	St. (χ^2)	Method of calculation	Evaluated on EU level
Sandy loam	Varendorf (DE)	5.7	0-10	31	234	58.6	FOMC	yes
Silty clay loam	Mechtersheim (DE)	7.5	0-10	26	181	17	FOMC	yes
Silty loam	Inzkofen (DE)	7.2	0-10	11	75	25.1	FOMC	yes
Sandy loam	Etzlberg (DE)	7.0	0-10	37	249	9.4	FOMC	yes
Silty clay	Grosseto (IT)	7.9	0-10	48	258	16.9	FOMC	yes
Sandy loam	Perugia (IT)	5.0	0-10	65	515	14	FOMC	yes
Loam	Dresano (IT)	5.6	0-10	62	205	23.7	FOMC	yes
Sandy loam	Mezzana Bigli (IT)	8.0	0-10	45	199	14.2	FOMC	yes
Maximum (n=8)				**65**	**515**			

zRMS comments:

Soil field degradation data for flurochloridone are in line with EU agreed values reported in EFSA Journal 2010;8(12):1869.

Modelling endpoints

No normalised endpoints for modelling were derived from the available field dissipation data at the time of Annex I inclusion. Meanwhile, the data has been evaluated according to current guidance by Finger and Ranke (2018).

~~**Report**~~	~~**Finger N. and Ranke J. (2018)**~~
~~**Title**~~	~~Kinetic evaluation of flurochloridone decline observed in eight legacy field dissipation trials in Europe using time-step normalisation~~
~~**Document No**~~	~~Report No ERA-1333A~~ ~~Agan Reference No. 90020995~~

~~The modelling endpoints obtained in this evaluation are given in the table below.~~

~~**Table 8.4-2: Summary of aerobic degradation rates for flurochloridone - field studies: Modelling endpoints**~~

~~Soil type~~	~~Location~~	~~pH (H_2O)~~	~~Formulation type~~	~~DT50 (d) 20°C, pF2~~	~~Fit, Kinetic~~	~~Reference Evaluated on EU level~~
~~Sandy loam~~	~~Varendorf (DE)~~	~~5.7~~	~~CS~~	~~39.85~~	~~SFO~~	~~Finger and Ranke (2018)~~ ~~no~~
~~Silty clay loam~~	~~Mechtersheim (DE)~~	~~7.5~~	~~CS~~	~~43.76~~	~~SFO~~	
~~Silty loam~~	~~Inzkofen (DE)~~	~~7.2~~	~~CS~~	~~41.51~~[a]	~~HS~~	
~~Sandy loam~~	~~Etzlberg (DE)~~	~~7.0~~	~~CS~~	~~39.1~~	~~SFO~~	
~~Silty clay~~	~~Grosseto (IT)~~	~~7.9~~	~~CS~~	~~64.9~~	~~SFO~~	
~~Sandy loam~~	~~Perugia (IT)~~	~~5.0~~	~~CS~~	~~207.1~~	~~SFO~~[b]	
~~Loam~~	~~Dresano (IT)~~	~~5.6~~	~~EC~~	~~22.18~~	~~SFO~~	
~~Sandy loam~~	~~Mezzana Bigli (IT)~~	~~8.0~~	~~EC~~	~~24.77~~	~~SFO~~	
~~**Geometric mean of all trials (n=8)**~~				~~**46.0**~~		
~~**Geometric mean trials with CS formulation (n=6)**~~				~~**58.0**~~		

[a] ~~calculated from k_{slow}~~
[b] ~~SFO with starting value for M0 set to 515.8~~

~~The overall geometric mean of the modelling DegT50 values is 46 days. However, as the values obtained~~

~~with the EC formulation are lower, it cannot be excluded that the CS formulation causes slower decline in the field. Therefore, in a conservative approach, the geometric mean DegT50 value of the trials performed with a CS formulation is proposed as an appropriate endpoint for modelling the fate of flurochloridone when applied as CS formulation.~~

zRMS comments:

The Applicant indicated that the soil field degradation data for flurochloridone reported in EFSA Journal 2010;8(12):1869 were not normalised and for this reason new kinetic evaluation using time-step normalisation has been provided in support of dossier for AG-F8-250 CS (Finger & Ranke, 2018). It should be, however, noted that according to conclusions of the CZSC from the meeting held in May 2014, kinetic evaluation is considered to be the new active substance data and as such should not be provided at the zonal level if not critical for the evaluation. Furthermore, the following is indicated in the Working Document of the Central Zone in area of Section 8:

[...] Note that according to the guidance document on the evaluation of new active substance data post approval (SANCO/10328/2004– rev 8, 24.01.2012) new active substance/metabolite data should not be considered unless they are necessary in order to show a safe use, they are needed as additional uses/crops are applied for authorisation, or they are "adverse" data. [...]

It should be also pointed out that the reason for kinetic re-evaluation of the EU agreed field studies in order to derive modelling endpoints is not fully clear, as at the EU level the groundwater and surface water modelling for flurochloridone were performed with consideration of DT_{50} derived from soil degradation studies performed under laboratory conditions and results of field studies were not considered for modelling purposes.

In addition to that in the text above the Applicant argues that the new geometric mean normalised field DT_{50} of 58 days derived from studies performed with CS formulation is longer than DT50 values derived from studies performed with EC formulation, which could indicate that degradation of the substance from CS formulation is slower and the new kinetic evaluation may be considered to be adverse data. The zRMS agrees that in fact, degradation of flurochloridone under field conditions was to some extent slower from CS formulation comparing to EC formulation, however the EU agreed DT_{50} of 53 days derived from laboratory studies is comparable to DT_{50} of 58 days derived under field conditions for CS formulation and evaluation and use of the new active substance data is therefore not justified. Taking this into account the zRMS is of the opinion that the groundwater and surface water exposure from the use of formulation AG-F8-250 CS may be reliably estimated based on the EU agreed DT_{50} of 53 days and the kinetic re-evaluation of the field dissipation studies was thus not validated as being not necessary.

8.4.2 Soil accumulation testing (KCP 9.1.1.2.2)

In the EU review it was established that soil accumulation and plateau concentration is not necessary for flurochloridone (EFSA 2010, p. 34).

zRMS comments:

Soil accumulation testing is not triggered for flurochloridone, in line with conclusions derived at the EU level and presented in EFSA Journal 2010;8(12):1869.

8.5 Mobility in soil (KCP 9.1.2)

Studies on mobility in soil with the formulation were not performed, since it is assumed that it is possible to extrapolate from data obtained with the active substance.

Table 8.5-1: Summary of soil adsorption/desorption for flurochloridone

Soil type	OC (%)	pH (-)	Kf (mL/g)	Kfoc (mL/g)	1/n (-)	Evaluated on EU level
Sandy loam	2.96	8.5	14	490	0.91	yes
Sand	0.58	5.1	6.5	1100	0.92	yes
Sandy loam	1.16	6.7	7.8	670	0.89	yes
Sandy clay loam	1.74	7.5	9.4	540	0.88	yes
Geometric mean (n=4)				**665**		
Arithmetic mean (n=4)				**700**	**0.9**	
pH-dependency				no		

For the two soil metabolites, EU sorption data are shown in the following tables. No Freundlich sorption data are available from the EU evaluation.

Table 8.5-2: Summary of soil adsorption/desorption for R406639

Soil type	OC (%)	pH (-)	Kd (mL/g)	Kdoc (mL/g)	1/n (-)	Evaluated on EU level
Loamy sand	2.3	5.6	10.5	463	-	yes
Loam	1.28	7.4	16.2	1265	-	yes
Clay loam	4.67	7.5	12.3	264	-	yes
Geometric mean (n=3)				**537**		
Arithmetic mean (n=3)				**664**	-	
pH-dependency				no		

A potential risk of contamination of groundwater with metabolite R42819 was identified in the European risk assessment review. Therefore, an additional study of sorption/desorption on soil was conducted with this metabolite (Walther 2013b) as summarised in Appendix A 2.2. These data are used in a refined groundwater risk assessment for this metabolite (tier 2). These data and a corresponding refined risk assessment have already been evaluated as confirmatory data, concluding that metabolite R42819 is not relevant for groundwater (European Commission, 2015, p. 5).

Table 8.5-3: Summary of soil adsorption/desorption for R42819

Soil type	OC (%)	pH ($CaCl_2$)	Kf (mL/g)	Kfoc (mL/g)	1/n (-)	Evaluated on EU level
Loamy sand	2.3	5.6	9.6[a]	415[a]	1[a]	yes
Loam	1.28	7.4	5.9[a]	463[a]	1[a]	yes
Clay loam	4.67	7.5	14.1[a]	302[a]	1[a]	yes
Mechthildshausen loam	1.19	7.5	1.81	152	0.77	yes[b]
Speyer 2.2 loamy sand	1.93	6.1	4.42	229	0.83	yes[b]
Fraunhofer 02-A silt loam	1.27	7.4	1.57	124	0.78	yes[b]
Geometric mean EU data (n=3)				**387**		
Geometric mean all soils (n=6) Tier 2				**251**		
Arithmetic mean EU data (n=3)				**393**	**1**	
Arithmetic mean all soils (n=6)				**281**	**0.90**	

[a]No Freundlich sorption data available, therefore 1/n is set to 1
[b]Evaluated as confirmatory data

zRMS comments:

Soil mobility data for flurochloridone and its metabolites are in line with EU agreed endpoints reported in EFSA Journal 2010;8(12):1869 (parent, metabolite R406639 and Tier 1 for metabolite R42819) and Addendum 2, B.8 on Confirmatory Data of July 2014 (Tier 2 values for metabolite R42819).

It is noted that the Applicant calculated geometric mean Kfoc values from individual EU agreed values. These values were checked by the zRMS and are confirmed to be correct. Arithmetic mean Kfoc values, as reported in the EFSA conclusion and the LoEP issued after evaluation of confirmatory data, has been inserted by the zRMS in the tables above.

8.5.1 Column leaching (KCP 9.1.2.1)

The mobility in soil of flurochloridone was evaluated during Annex I Inclusion. No additional studies have been performed.

zRMS comments:

At the EU level only aged residues leaching studies were evaluated and their results are reported in EFSA Journal 2010;8(12):1869. They are, however, not relevant for evlauation of AG-F8-250 CS, for which leaching potential has been addressed in groundwater modelling presented in point 8.8 of this report.

8.5.2 Lysimeter studies (KCP 9.1.2.2)

No lysimeter study was submitted during Annex I inclusion. No additional studies have been performed.

zRMS comments:

No lysimeter studies with flurochloridone were evaluated at the EU level.

8.5.3 Field leaching studies (KCP 9.1.2.3)

No such studies are required. The groundwater assessment is considered to be addressed fully by the FOCUS groundwater modelling.

zRMS comments:

No field leaching studies with flurochloridone were evaluated at the EU level.

8.6 Degradation in the water/sediment systems (KCP 9.2, KCP 9.2.1, KCP 9.2.2, KCP 9.2.3)

Studies on degradation in water/sediment systems with the formulation were not performed, since it is possible to extrapolate from data obtained with the active substance.

Flurochloridone is stable towards hydrolysis at pH 5, 7 and 9 (EFSA 2010, p. 37). It was concluded during Annex I inclusion that the photolysis metabolite M8 did not need to be accounted for in the surface water exposure assessments (EFSA 2010, p. 10).

Table 8.6-1: Summary of degradation in water/sediment of flurochloridone

Water/sediment system	Radiolabel	pH water/ sed.	DegT50 whole syst. (d)	DegT90 whole syst. (d)	Kinetic, Fit	Evaluated on EU level
Clay loam	Pyrrolidone	7.5	19.6	65.1	SFO	yes
Sand		5.5	10.3	34.0	SFO	yes
Clay loam	Phenyl	7.5	22.8	75.9	SFO	yes
Sand		5.5	9.2	30.5	SFO	yes
Geometric mean (n=4)			**14.3**			

Table 8.6-2: Summary of observed metabolites

R406639 Water/sediment system	Max. in water/sediment 13.9 %, geometric mean system DT50 52.3 days	Evaluated on EU level yes
R42819 Water/sediment system	Max. in water/sediment 63.9 %, geometric mean system DT50 261 days	Evaluated on EU level yes

zRMS comments:

Information on degradation of flurochloridone and its metabolites in water/sediment systems is in line with EU agreed data reported in EFSA Journal 2010;8(12): 1869.

8.7 Predicted Environmental Concentrations in soil (PEC_{soil}) (KCP 9.1.3)

8.7.1 Justification for new endpoints

No new endpoints are considered for PEC soil calculations. However, PEC soil values are recalculated for the current GAP (application of 500 g/ha to potatoes).

8.7.2 Active substance(s) and relevant metabolite(s)

The predicted environmental concentration in soil of AG-F8-250 CS and the active substance flurochloridone were calculated using equations proposed by the FOCUS soil persistence. The decline of flurochloridone concentrations in soil was estimated as established in the EU review, based on the FOMC model.

Table 8.7-1: Input parameters related to application for PEC_{soil} calculations

Use No.	1
Crop	Potatoes
Application rate	2 L AG-F8-250 EC per ha 500 g flurochloridone per ha
Number of applications	1 per year
Crop interception	0

The table below provides the substance specific data from the EFSA conclusion on flurochloridone that were used in the calculations.

Table 8.7-2: Input parameter for active substance(s) and relevant metabolite(s) for PEC_{soil} calculation

Parameter	Unit	Flurochloridone
Alpha	-	1.13
Beta	-	77.1

No long term maximum concentrations were derived, as no need for this was identified during Annex I inclusion.

Table 8.7-3: PEC_{soil} for flurochloridone on potatoes

Time		Actual [mg/kg dry weight]	Time weighted average [mg/kg dry weight]
Initial	0 h	0.67	-
Short term	24 h	0.66	0.66
	2 d	0.65	0.66
	4 d	0.63	0.65
Long term	7 d	0.60	0.63
	14 d	0.55	0.61
	21 d	0.51	0.58
	28 d	0.47	0.56
	42 d	0.41	0.52
	50 d	0.38	0.50
	100 d	0.26	0.41

For the assessment of secondary poisoning via earthworms, the 21 day time-weighted average concentration of 0.58 mg/kg dry weight for flurochloridone was converted to a wet weight concentration of 0.51 mg/L. Further, it was converted to a 21 day time-weighted average porewater concentration of 0.043 mg/L using the geometric mean flurochloridone K_{FOC} of 665 L/kg as K_{OC}. In these calculations, a dry bulk density of 1.5 kg/L, a volumetric water content of 20% and an organic carbon content of 2% w/w of the soil solids are assumed, as specified in the REACH guidance (R.16).

PEC_{soil} of metabolites

No metabolite PEC soil values are necessary according to the EU risk assessment (EFSA 2010, p. 12, 36).

zRMS comments:

The input parameters considered by the Applicant in soil exposure calculations is agreed by the zRMS. The application pattern was in line with the Central Zone GAP. As AG-F8-250 CS is intended to be applied on bare soil, crop interception of 0% was considered.

The soil exposure for flurochloridone was verified by the zRMS in independent calculations performed using ESCAPE ver. 2. The same PEC_{soil} values for one year were obtained, but with assumed degradation data ESCAPE predicted some accumulation of the substance in soil resulting with $PEC_{soil,accu}$ of 0.6936 mg a.s./kg dws after 10 years (20 cm tillage, see table below). In opinion of the zRMS, this value should be considered for purposes of the soil risk assessment as representing worst case. The worst case 21 d TWA PEC_{soil} of 0.6074 mg a.s./kg dws has been derived when accumulation was considered.

With regard to the pore-water concentration, with input parameters described above the ESCAPE program calculated initial $PEC_{porewater}$ to be 0.066 mg/L and 21 TWA $PEC_{porewater}$ of 0.0571 mg/L. As these values are higher than those calculated by the Applicant, they are considered to be more relevant for purposes of evaluation of the risk of secondary poisoning as representing worst case.

With regard to metabolites the zRMS agrees that no PEC_{soil} values are reported in EFSA Journal 2010;8(12):1869. No detailed explanation is provided but potentially these metabolites were considered to be not relevant as they were found below or just slightly above 10% of AR. However, current approach in determination of the relevant metabolites has changed and metabolites that are formed at 5% of AR at two consecutive samplings also trigger the exposure assessment. Information regarding distribution of radioactivity in the route and rate of degradation studies shows that metabolite R406639 was found at >5% AR at two consecutive samplings, while metabolite R42819 was found at 10.1% AR. Taking this into account it was decided by the zRMS to calculate the soil exposure to both metabolites using ESCAPE ver. 2 with consideration of the metabolites pseudo-application rates calculated from the rate of the parent corrected for the molar ratio and maximum occurrence.

Input parameters are presented in table below. It should be noted that in general, for soil exposure calculations the longest actual soil DT_{50} should be considered. However, for both metabolites the normalised laboratory DT_{50} values were much longer comparing to the actual values, which were derived in soils incubated at 28ºC. As at the time of application of AG-F8-250 CS the temperature will be significantly lower than 28ºC, it was decided by the zRMS to consider the normalised DT_{50} values as representing worst case and being more relevant for the conditions at application of the product.

Compound	Molar mass [g/mol]	Molar ratio	Maximum occurrence [%]	Application rate [g/ha]	DT_{50} [days]
Flurochloridone	312.1	-		500	-
R406639	293.7	0.941	8.1	38.1	226.5
R42819	277.7	0.890	10.1	44.9	536.2

Resulting PEC_{soil} values are reported in table below.

Compound	$PEC_{soil,ini}$ [mg/kg dws]	$PEC_{soil,plateau}$ [mg/kg dws]	$PEC_{soil,accu}$ [mg/kg dws]
Flurochloridone	0.6667	0.0269	0.6936
R406639	0.0062	0.0007	0.0069
R42819	0.0073	0.0030	0.0103

For the parent compound $PEC_{soil,accu}$ of 0.6936 mg a.s./kg dws is recommended for soil risk assessment, while for evaluation of the risk of secondary poisoning 21 TWA PEC_{soil} of 0.6074 mg a.s./kg dws, calculated with consideration of accumulation, should be considered. For the pore water approach, 21 TWA PEC of 0.0571 mg/L is relevant.

8.7.2.1 PEC_{soil} of AG-F8-250 CS

For the product AG-F8-250 CS, an initial PEC_{SOIL} of 2.96 mg product per kg dry soil was calculated, based on the application rate of 2 L product per ha and the density of AG-F8-250 CS of 1110 g/L.

zRMS comments:

PEC_{soil} value for the formulated product is agreed by the zRMS and may be used in the risk assessment for soil organisms.

8.8 Predicted Environmental Concentrations in groundwater (PEC_{gw}) (KCP 9.2.4)

8.8.1 Justification for new endpoints

~~No normalised endpoints for modelling were derived from the available field dissipation data at the time of Annex I inclusion. Meanwhile, the data has been evaluated according to current guidance by Finger and Ranke (2018). The resulting normalised modelling DegT50 values are shown in the table below.~~

~~**Table 8.8-1: Soil DegT50 values for flurochloridone derived from legacy field trials**~~

~~**Location**~~	~~**Formulation type**~~	~~**DegT50 [days]**~~
~~Varendorf~~	~~CS~~	~~39.85~~
~~Mechtersheim~~	~~CS~~	~~43.76~~
~~Inzkofen~~	~~CS~~	~~41.51~~
~~Etzlberg~~	~~CS~~	~~39.1~~
~~Grosseto~~	~~CS~~	~~64.9~~
~~Perugia~~	~~CS~~	~~207.1~~
~~Dresano~~	~~EC~~	~~22.19~~
~~Mezzana Bigli~~	~~EC~~	~~24.77~~
~~**Geometric mean of all trials (n=8)**~~		~~**46.0**~~
~~**Geometric mean of trials with CS formulation**~~		~~**58.0**~~

~~The overall geometric mean of the modelling DegT50 values is 46 days. However, as the values obtained with the EC formulation are lower, it cannot be excluded that the CS formulation causes slower decline in the field. Therefore, in a conservative approach, the geometric mean DegT50 value of the trials performed with a CS formulation is proposed as an appropriate endpoint for modelling the fate of flurochloridone when applied as CS formulation. For comparison, the EU endpoint was 53.0 days (EFSA, 2010, p. 32). Therefore, the normalised field DegT50 values for the CS formulation could be seen as adverse data and are therefore conservatively used in this groundwater assessment.~~

~~In addition, a potential risk of contamination of groundwater with metabolite R42819 was identified in the European risk assessment review. Therefore, two new studies, one on aerobic soil degradation and one on soil sorption were described in the respective sections above and were used at tier 2 in the groundwater modelling.~~

zRMS comments:

As already explained by the zRMS in point 8.4.1 of this report, the groundwater exposure to flurochloridone following application of AG-F8-250 CS may be sufficiently evaluated with consideration of the EU agreed soil DT_{50} of 53 days, derived from the laboratory degradation studies and for this reason kinetic re-evaluation of the EU agreed field dissipation data (i.e. new active substance data) was not validated as being not necessary. The text above was thus struck through. For detailed explanation, please refer to point 8.4.1 of this document.

8.8.2 Active substance flurochloridone and relevant metabolites (KCP 9.2.4.1)

Report	**Ranke J. (2018a)**
Title	FOCUS groundwater calculations for flurochloridone and its soil metabolites following application of AG-F8-250 CS in Poland
Document No	Report No jrwb-127 Agan Reference No. 000100956

Table 8.8-2: Input parameters related to application for PEC_{gw} calculations

Use No.	1
Crop	Potatoes
Application rate	500 g/ha flurochloridone
Number of applications	1
Relative application date	7 days pre-emergence
Crop interception	0%
Frequency of application	annual
Models used for calculation	FOCUS PEARL v4.4.4, FOCUS PELMO v5.5.3, FOCUS MACRO v5.5.4

Table 8.8-3: Input parameters related to flurochloridone for PEC_{gw} calculations

Parameter	Value	Unit	Remark	Value in accordance to EU endpoint Reference
Molecular weight	312.1	g/mol		yes
Saturated vapour pressure	$2.7 \cdot 10^{-4}$	Pa	25 °C	yes
Water solubility	21.9	mg/L	20°C, pH7	yes
$DT_{50,soil}$	58	days	Geometric mean of normalised DegT50 values from field dissipation studies conducted with CS formulation	53 days used in EU evaluation
Formation fraction	0.105	-	To R406639	yes
Formation fraction	0.895	-	To R42819	yes
K_{foc}	665	L/kg	Geometric mean, n=4	Calculated from EU endpoints
K_{fom}	385.5	L/kg	Calculated from K_{foc}	Calculated from EU endpoints
Freundlich Exponent 1/n	0.9	-	Arithmetic mean, n=4	yes
Plant Uptake	0	-	Conservative default value	0.5 used in EU evaluation

Table 8.8-4: Input parameters related to R406639 for PEC_{gw} calculations

Parameter	Value	Unit	Remark	Value in accordance to EU endpoint Reference
Molecular weight	293.7	g/mol		yes
Saturated vapour pressure	$2.97 \cdot 10^{-6}$	Pa	25 °C	yes
Water solubility	848.9	mg/L	25 °C	yes
$DT_{50,soil}$	77.4	days	Geometric mean, n=3	yes
K_{foc}	537	L/kg	Geometric mean, n=3	Calculated from EU endpoints
K_{fom}	311	L/kg	Calculated from K_{foc}	Calculated from EU endpoints
Freundlich Exponent 1/n	1	-		yes
Plant Uptake	0	-	Conservative default value	yes

Table 8.8-5: Input parameters related to R42819 for PEC_{gw} calculations at tier 1

Parameter	Value	Unit	Remark	Value in accordance to EU endpoint Reference
Molecular weight	277.7	g/mol		yes
Saturated vapour pressure	$1.6 \cdot 10^{-3}$	Pa	25 °C	yes
Water solubility	50.97	mg/L	25 °C	yes
$DT_{50,soil}$	79.4	days	Geometric mean, n=3	yes
K_{foc}	387	L/kg	Geometric mean, n=3	Calculated from EU endpoints
K_{fom}	224.5	L/kg	Calculated from K_{foc}	Calculated from EU endpoints
Freundlich Exponent 1/n	1	-		yes
Plant Uptake	0	-	Conservative default value	yes

Table 8.8-6: Refined input parameters related to R42819 for PEC_{gw} calculations at tier 2

Parameter	Value	Unit	Remark	Value in accordance to EU endpoint
$DT_{50,soil}$	40.3	days	Geometric mean including new data, n=6	yes (Confirmatory data) ~~no~~
K_{foc}	251	L/kg	Geometric mean including new data, n=6	
K_{fom}	146	L/kg	Calculated from K_{foc}	
Freundlich Exponent 1/n	0.90	-	Including three linear values with 1/n assumed as 1, arithmetic mean, n=6	

Table 8.8-7: PEC_{gw} for flurochloridone and metabolites in potatoes at tier 1

Model	Scenario	80th Percentile PEC_{gw} at 1 m Soil Depth (µg/L)		
		flurochloridone	**R406639**	**R42819**
PELMO	Châteaudun	< 0.001	0.002	**0.105**
	Hamburg	< 0.001	0.010	**0.395**
	Jokioinen	< 0.001	0.001	0.082
	Kremsmünster	< 0.001	0.010	**0.374**
	Okehampton	< 0.001	0.018	**0.565**
	Piacenza	< 0.001	0.014	**0.450**
	Porto	< 0.001	0.009	**0.337**
	Sevilla	< 0.001	< 0.001	0.002
	Thiva	< 0.001	< 0.001	0.032
PEARL	Châteaudun	< 0.001	< 0.001	**0.174**
	Hamburg	< 0.001	0.001	**0.569**
	Jokioinen	< 0.001	< 0.001	0.099
	Kremsmünster	< 0.001	< 0.001	**0.438**
	Okehampton	< 0.001	0.001	**<u>0.611</u>**
	Piacenza	< 0.001	0.001	**0.509**
	Porto	< 0.001	< 0.001	**0.211**
	Sevilla	< 0.001	< 0.001	0.005
	Thiva	< 0.001	< 0.001	0.053
MACRO	Châteaudun	< 0.001	0.005	**0.181**

Values in **bold** exceed the threshold concentration of 0.1 µg/L; maximum PEC_{gw} is additionally <u>underlined</u>

Table 8.8-8: PEC$_{gw}$ for flurochloridone and metabolites in potatoes at tier 2

Model	Scenario	80th Percentile PEC$_{gw}$ at 1 m Soil Depth (µg/L)		
		flurochloridone	R406639	R42819
PELMO	Châteaudun	< 0.001	0.002	< 0.001
	Hamburg	< 0.001	0.010	0.001
	Jokioinen	< 0.001	0.001	< 0.001
	Kremsmünster	< 0.001	0.010	0.001
	Okehampton	< 0.001	0.018	0.003
	Piacenza	< 0.001	0.014	0.003
	Porto	< 0.001	0.009	0.001
	Sevilla	< 0.001	< 0.001	< 0.001
	Thiva	< 0.001	< 0.001	< 0.001
PEARL	Châteaudun	< 0.001	< 0.001	< 0.001
	Hamburg	< 0.001	0.001	< 0.001
	Jokioinen	< 0.001	< 0.001	< 0.001
	Kremsmünster	< 0.001	< 0.001	< 0.001
	Okehampton	< 0.001	0.001	< 0.001
	Piacenza	< 0.001	0.001	< 0.001
	Porto	< 0.001	< 0.001	< 0.001
	Sevilla	< 0.001	< 0.001	< 0.001
	Thiva	< 0.001	< 0.001	< 0.001
MACRO	Châteaudun	< 0.001	0.005	< 0.001

Predicted environmental concentrations in groundwater for flurochloridone were below 0.001 µg/L. For metabolite R406639, they were below 0.02 µg/L. At tier 1, predicted environmental concentrations in groundwater for R42819 were below 0.7 µg/L. At tier 2, they were below 0.005 µg/L.

zRMS comments:

Application pattern

The application pattern assumed by the Applicant in simulations is in line with the Central Zone GAP presented in Table 8.1-1. Relative application dates set to 7 days before emergence are agreed.

Input parameters

Input parameters presented in Tables 8.8-3 to 8.8-5 are in general in line with endpoints agreed in the course of the initial EU review of flurochloridone (Tier 1 parameters for all compounds) or during evaluation of the confirmatory data in 2014 (Tier 2 values for metabolite R42819). Nevertheless there are some exceptions discussed below:

- For flurochloridone geometric mean DT_{50} of 58 days derived from the kinetic re-evaluation of the EU agreed soil field dissipation trials performed with CS formulation was used by the Applicant. However, the new geometric mean field DT_{50} of 58 days is considered to be not sufficiently different from the geometric mean laboratory DT_{50} of 53 days agreed at the EU level for groundwater modelling, to justify the use of new active substance data at the zonal level. Taking this into account, the kinetic re-evaluation of the EU agreed soil field dissipation trials was not validated by the zRMS as being not necessary. For more details regarding the zRMS approach, please refer to point 8.4.1 of this report. Nevertheless, the zRMS is of the opinion that consideration of DT_{50} of 58 days had no significant impact on the results of the groundwater modelling, especially for the active compound, for which this value represented slightly worst case comparing to the EU agreed endpoint. In order to check the impact of the DT_{50} on leaching potential for metabolites, additional modelling has been performed by the zRMS (see below).
- For all compounds the geometric mean Kfoc values were considered instead of the EU agreed arithmetic mean values. This deviation is agreed by the zRMS as the geometric mean Kfoc are lower than the arithmetic mean values and represent thus worst case in terms of the leaching potential. Moreover, consideration of the geometric mean Kfoc is in line with current EFSA recommendations. The geometric mean values were calculated from the individual Kfoc values reported in the LoEP or in Addendum 2, B.8 on Confirmatory Data of July 2014 and are confirmed by the zRMS to be correct.

For all compounds PUF values of 0 was assumed, in line with current recommendations of the FOCUS groundwater guidance document (2014).

As already mentioned above, in order to check the impact of the longer DT_{50} for the parent on leaching potential of metabolites, additional groundwater modelling has been performed by the zRMS. These additional simulations were based on fully EU agreed input parameters, including arithmetic mean Kfoc values for all compounds and geometric mean laboratory soil DT_{50} of 53 days for the parent. Although at the EU level for flurochloridone PUF of 0.5 was assumed, in zRMS calculations PUF of 0 was considered for all compounds, as being in line with current FOCUS recommendations.

As expected, no impact on the parent PEC_{gw} was noted and values calculated by the zRMS using all modelling programs were <0.001 µg/L in all scenarios.
With regard to metabolites, slightly lower PEC_{gw} were obtained by the zRMS at Tier 1 (both metabolites) and Tier 2 (metabolite R42819), which most probably was the result of consideration of arithmetic mean Kfoc, which is higher than geometric mean Kfoc, considered by the Applicant.

Overall, based on the results of the groundwater modelling performed by the Applicant and the zRMS, no unacceptable leaching of flurochloridone and its metabolites is expected when AG-F8-250 CS is used according to the Central Zone GAP.

Please note that additional groundwater modelling may be required by the concerned Member States that do not accept simulations performed according to FOCUS recommendations.

8.9 Predicted Environmental Concentrations in surface water (PEC_{SW}) (KCP 9.2.5)

8.9.1 Justification for new endpoints

No normalised endpoints for modelling were derived from the available field dissipation data at the time of Annex I inclusion. Meanwhile, the data has been evaluated according to current guidance by Finger and Ranke (2018). Please see the groundwater modelling section for details.

PEC values for sediment are only given for Step 1, where total system DT_{50} values are used as input parameters for aquatic sediment systems. At Steps 2, 3 and 4, only PEC surface water values are used in the ecotoxicological assessment. Therefore, the default value of 1000 days was only used for the water compartment, and the total system DT_{50} values were used for the sediment compartment. As this is conservative for PEC surface water modelling, it was not necessary to also do the modelling with reversed DT_{50} values as recommended in the FOCUS guidance.

8.9.2 Active substance(s), relevant metabolite(s) and the formulation (KCP 9.2.5)

Report	**Ranke J. (2018b)**
Title	FOCUS Step 3-4 surface water calculations for flurochloridone following application of AG-F8-250 CS in Poland
Document No	Report No jrwb-128 Agan Reference No. 000100957

Report	**Weber D. and Jarvis T. (2020)**
Title	Predicted environmental concentrations in surface water after pre-emergence application of flurochloridone to potatoes in the European Union - FOCUS Step 3-4 calculations
Document No	Report No 2000626.SW0-6397 Agan Reference No. XXXXXX

Report	**Weber D. and Jarvis T. (2021)**
Title	Predicted environmental concentrations in surface water after pre-emergence application of flurochloridone to potatoes in the European Union - FOCUS Step 3-4 calculations
Document No	Report No 2000626.SW0-1750 Agan Reference No. XXXXXX

Table 8.9-1: Input parameters related to application for $PEC_{SW/SED}$ calculations

Plant protection product	AG-F8-250 CS
Use No.	1
Crop	Potatoes
Application rate	500 g/ha flurochloridone 375 g/ha flurochloridone (Parent Step 3-4 only)
Number of applications	1
Application window	Mar-May (Step 2) 30 days starting 14 days pre-emergence (Step 3)
Application method	Ground spray
CAM (Chemical application method)	2
Models used for calculation	FOCUS SWASH v5.3, FOCUS SPIN 2.2/3.3, FOCUS PRZM v4.3.1, FOCUS MACRO v5.5.4, FOCUS TOXWA v5.5.3, EVA 3, rev 2e/h

Table 8.9-2: FOCUS Step 3 Scenario related input parameters for $PEC_{sw/sed}$ calculations for the application of flurochloridone to potatoes

Scenario	Crop cycle	Emergence date	Application window	Application date
D3	1st	10 May	26 April – 26 May	4 May 1992
D4	1st	22 May	8 May – 7 June	17 May 1985
D6	1st	10 April	27 March – 26 April	2 April 1986
	2nd	5 August	22 July – 21 August	25 July 1986
R1	1st	5 May	21 April – 21 May	26 April 1984
R2	1st	15 Mar	1 March – 31 March	1 March 1977
R3	1st	10 Apr	27 March – 26 April	28 March 1980

Table 8.9-3: Input parameters related to active substance flurochloridone

Parameter	Value	Unit	Remark	Value in accordance to EU endpoint Reference
Molecular weight	312.1	g/mol		yes
Saturated vapour pressure	2.7×10^{-4} 1.4×10^{-4}	Pa	25 °C 20 °C (converted from 2.7×10^{-4} at 25°C (EVA3 2h))	yes no
Water solubility	21.9	mg/L	20°C, pH7	yes
$DT_{50,soil}$	58	days	Geometric mean of normalised DegT50 values from field dissipation studies conducted with CS formulation	53 days used in EU evaluation
K_{foc}	664.5	L/kg	Geometric mean, n=4	Calculated from EU endpoints
K_{fom}	385.5	L/kg	Calculated from K_{foc}	Calculated from EU endpoints
Freundlich Exponent 1/n	0.9	-	Arithmetic mean, n=4	yes
Plant Uptake	0	-	Conservative default value	0.5 used in EU evaluation
$DT_{50,whole\ system}$	14.3	days	Geometric mean, n=4	yes
$DT_{50,water}$	1000	days	Default value, used for PECsw	yes
$DT_{50,sed}$	14.3	days	Total system value, used for PECsw	yes

Table 8.9-4: Input parameters related to metabolite R406639

Parameter	Value	Unit	Remark	Value in accordance to EU endpoint Reference
Molecular weight	293.7	g/mol		yes
Water solubility	848.9	mg/L	EPIWEB 4.0	yes
$DT_{50,soil}$	77.4	days	Geometric mean, n=4	yes
K_{foc}	537	L/kg	Geometric mean of Koc values, n=3	Calculated from EU endpoints
$DT_{50,whole\ system}$	52.3	days	Geometric mean, n=3	yes
$DT_{50,water}$	1000	days	Default value, used for PECsw at Step 2	yes
$DT_{50,sed}$	52.3	days	Total system value, used for PECsw at Step 2	yes
Maximum occurrence in soil	8.1	%		yes
Maximum occurrence in water/sediment systems	13.9	%		yes

Table 8.9-5: Input parameters related to metabolite R42819

Parameter	Value	Unit	Remark	Value in accordance to EU endpoint Reference
Molecular weight	277.7	g/mol		yes
Water solubility	50.97	mg/L	EPIWEB 4.0	yes
$DT_{50,soil}$	79.4	days	Geometric mean, n=3	yes
K_{foc}	387	L/kg	Geometric mean of Koc values, n=3	Calculated from EU endpoints
$DT_{50,whole\ system}$	261	days	Geometric mean, n=4, extrapolated	yes
$DT_{50,water}$	1000	days	Default value, used for PECsw at Step 2	yes
$DT_{50,sed}$	261	days	Total system value, used for PECsw at Step 2	yes
Maximum occurrence in soil	10.1	%		yes
Maximum occurrence in water/sediment systems	63.9	%		yes

$PEC_{sw/sed}$

Table 8.9-6: FOCUS Step 1 PEC_{sw} and PEC_{sed} for flurochloridone and its metabolites following application to potatoes (500 g/ha)

Substance	Maximum PEC_{sw} [µg/L]	Maximum PEC_{sed} [µg/kg]
Flurochloridone	92.94	587.46
R406639	20.71	108.41
R42819	75.00	286.05

Table 8.9-7: FOCUS Step 2 PEC_{sw} for flurochloridone and its metabolites following application to potatoes (500 g/ha)

Substance	Region	Maximum PEC_{sw} [µg/L]
Flurochloridone	Northern Europe	19.60
	Southern Europe	36.44
R406639	Northern Europe	4.25
	Southern Europe	8.10
R42819	Northern Europe	15.76
	Southern Europe	29.59

FOCUS Step 3 and 4

Surface water PEC values at Steps 3 and 4 are shown in the table below. Maximum time weighted average concentrations for a 7 day window (7 d TWA values) are included for ecotoxicological assessment.

Table 8.9-8: Step 3 and Step 4 PEC_{sw} values for flurochloridone following application to potatoes (500 g/ha)

Scenario		PECsw [µg/L]					
		Step 3		Step 4 (drift buffer + vegetated filter strip)			
				10 m vegetated buffer		20 m vegetated buffer	
		Maximum	7 d TWA	Maximum	7 d TWA	Maximum	7 d TWA
D3	ditch	2.621 (sd)	0.428	0.455 (sd)	0.086	0.237 (sd)	0.045
D4	pond	0.763 (dr)	0.759	0.761 (dr)	0.758	0.760 (dr)	0.756
	stream	2.169 (sd)	0.545	0.857 (dr)	0.545	0.857 (dr)	0.545
D6	ditch	2.598 (sd)	0.185	0.457 (sd)	0.172	0.329 (sd)	0.172
D6 2nd	ditch	2.641 (sd)	1.245	2.049 (dr)	0.777	2.049 (dr)	0.777
R1	pond	0.400 (ro)	0.379	0.183 (ro)	0.174	0.099 (ro)	0.094
	stream	3.812 (ro)	0.456	1.726 (ro)	0.204	0.902 (ro)	0.106
R2	stream	2.398 (sd)	0.484	0.964 (ro)	0.218	0.505 (ro)	0.114
R3	stream	8.001 (ro)	0.696	3.649 (ro)	0.320	1.914 (ro)	0.168

(sd): drift entry; (dr): drainage entry; (ro): run-off entry

Table 8.9-9: Step 4 PEC_{sw} values for flurochloridone following application to potatoes, vfsmod (500 g/ha)

Scenario		PECsw [µg/L] Step 4			
		10 m vegetated buffer +vfsmod		20 m vegetated buffer +vfsmod	
		Maximum	7 d TWA	Maximum	7 d TWA
D3	ditch	0.455 (sd)	0.086	0.237 (sd)	0.045
D4	pond	0.761 (dr)	0.758	0.760 (dr)	0.756
	stream	0.857 (dr)	0.545	0.857 (dr)	0.545
D6	ditch	0.457 (sd)	0.172	0.329 (dr)	0.172
D6 2nd	ditch	2.049 (dr)	0.777	2.049 (dr)	0.777
R1	pond	0.076 (ro)	0.072	0.050 (ro)	0.047
	stream	0.417 (sd)	0.013	0.218 (sd)	0.007
R2	stream	0.550 (sd)	0.008	0.287 (sd)	0.004
R3	stream	0.932 (ro)	0.134	0.303 (sd)	0.015

(sd): spray drift entry; (dr): drainage entry; (ro): run-off entry

At Step 3, the maximum predicted concentrations in surface water for the drainage scenarios of around 2.6 µg/L occurs in the D6 ditch scenario after application to the second crop cycle of potatoes. With the exception of the D4 pond scenario, where the maximum PEC is related to drainage, these maximum PEC values are caused by drift entry. When applying up to 20 m drift mitigation, drainage entry becomes relevant also for the D4 stream scenario and for the D6 ditch scenario. In the run-off scenarios at Step 3, the highest maximum PEC values of up to 8.0 µg/L are obtained in the run-off scenario R3. The application of run-off mitigation in the form of a vegetated filter strip according to the values proposed in the FOCUS Landscape and Mitigation report leads to a reduction of these maximum PEC values to around 1.9 µg/L, occurring in the R3 stream scenario.
Further, Step 3-4 calculations were re-calculated by Weber and Jarvis (2020), adding new Step 4 calculations for 500g/ha using vegetated filter strips (vfs) of 10 m and 20 m with VFSmod, resulting in a maximum run-off PEC value of 0.932 and 0.303 µg/L for 10 and 20 m, respectively. For the re-calculation, the vapor pressure was converted to 1.4×10^{-4} at 20°C from 2.7×10^{-4} at 25°C, using the German EVA3 tool (version 2h). All other input parameters were identical with the original calculations. No significant change in the PEC values is expected.

Additionally, a complete new set of Step 3-4 calculations were simulated using an application rate of 375 g/ha (Weber and Jarvis, 2021). The same approach and input parameters as in Weber and Jarvis (2020) were used, including 10 and 20 m VFSmod.

Table 8.9-10: Step 3 and Step 4 PEC_{sw} values for flurochloridone following application to potatoes (375 g/ha)

Scenario		PECsw [µg/L] Step 3		Step 4			
				10 m vegetated buffer		20 m vegetated buffer	
		Maximum	7 d TWA	Maximum	7 d TWA	Maximum	7 d TWA
D3	ditch	1.965 (sd)	0.321	0.342 (sd)	0.065	0.178 (sd)	0.034
D4	pond	0.548 (dr)	0.546	0.547 (dr)	0.545	0.546 (dr)	0.544
	stream	1.627 (sd)	0.398	0.635 (dr)	0.398	0.635 (dr)	0.398
D6	ditch	1.948 (sd)	0.139	0.343 (sd)	0.127	0.251 (dr)	0.127
D6 2nd	ditch	1.980 (sd)	0.932	1.487 (dr)	0.545	1.487 (dr)	0.545
R1	pond	0.297 (ro)	0.282	0.137 (ro)	0.130	0.074 (ro)	0.070
	stream	2.813 (ro)	0.337	1.274 (ro)	0.151	0.666 (ro)	0.079
R2	stream	1.798 (sd)	0.354	0.703 (ro)	0.159	0.368 (ro)	0.083
R3	stream	5.831 (ro)	0.513	2.659 (ro)	0.235	1.395 (ro)	0.124

(sd): spray drift entry; (dr): drainage entry; (ro): run-off entry

Table 8.9-11: Step 4 PEC_{sw} values for flurochloridone following application to potatoes, vfsmod (375 g/ha)

Scenario		PECsw [µg/L]			
		Step 4			
		10 m vegetated buffer +vfsmod		20 m vegetated buffer +vfsmod	
		Maximum	7 d TWA	Maximum	7 d TWA
D3	ditch	0.342 (sd)	0.065	0.178 (sd)	0.034
D4	pond	0.547 (dr)	0.545	0.546 (dr)	0.544
	stream	0.635 (dr)	0.398	0.635 (dr)	0.398
D6	ditch	0.343 (sd)	0.127	0.251 (dr)	0.127
D6 2nd	ditch	1.487 (dr)	0.545	1.487 (dr)	0.545
R1	pond	0.058 (ro)	0.054	0.037 (ro)	0.035
	stream	0.313 (sd)	0.009	0.164 (sd)	0.005
R2	stream	0.412 (sd)	0.006	0.215 (sd)	0.003
R3	stream	0.686 (ro)	0.099	0.227 (sd)	0.011

(sd): spray drift entry; (dr): drainage entry; (ro): run-off entry

At Step 3, the maximum predicted concentrations in surface water for the drainage scenarios of around 1.98 µg/L occurs in the D6 ditch scenario after application to the second crop cycle of potatoes. Except for the D4 pond scenario, where the maximum PEC is related to drainage, these maximum PEC values are caused by drift entry. When applying up to 20 m drift mitigation, drainage entry becomes relevant also for the D4 stream scenario and for the D6 ditch scenario. In the run-off scenarios at Step 3, the highest maximum PEC values of up to 5.831 µg/L are obtained in the run-off scenario R3. The application of run-off mitigation in the form of a vegetated filter strip according to the values proposed in the FOCUS Landscape and Mitigation report leads to a reduction of these maximum PEC values to around 1.395 µg/L, occurring in the R3 stream scenario.

Further, vegetated filter strips (vfs) of 10 m and 20 m with VFSmod were calculated, resulting in a maximum run-off PEC value of 0.686 and 0.227 µg/L for 10 and 20 m, respectively.

Exposure pattern analysis

A brief pattern analysis was done with a threshold level of 0.1 µg/L to identify relevant key characteristics of the exposure profiles for the Step 4 simulations, using 10 and 20 m vegetated filter strips with VFSmod.

Table 8.9-12: Overview of pattern analysis for 10 m db+vfsmod (500 g/ha)

Type	Substance	Crop	Scenario	No events	Max PECsw [µg/L]	Max duration [d]	Min interval [d]	AUC total [µg/L×h]
Step 4	FCL	Potatoes	D3 Ditch	1	0.455	1.75	-	13
Step 4	FCL	Potatoes	D4 Pond	2	0.761	146.167	200.666	1895
Step 4	FCL	Potatoes	D4 Stream	3	0.857	34.084	12.458	398
Step 4	FCL	Potatoes	D6 Ditch	4	0.457	5.417	0.792	46
Step 4	FCL	Potatoes	D6 Ditch 2nd	8	2.049	14.75	3.875	513
Step 4	FCL	Potatoes	R1 Stream	1	0.417	0.25	-	2
Step 4	FCL	Potatoes	R2 Stream	1	0.550	0.125	-	1
Step 4	FCL	Potatoes	R3 Stream	2	0.932	1.25	22.209	27

Table 8.9-13: Details of single events for 10 m db+vfsmod (500 g/ha)

Scenario	Event no.	Max. PECsw [µg/L]	Event start [d]	Event end [d]	Event duration [d]	Event AUC [µg/L×h]	Interval to event [d]
D3 Ditch	1	0.455	124.375	126.125	1.75	13.1	-
D4 Pond	1	0.101	137	138.167	1.167	2.8	-
D4 Pond	2	0.761	338.833	485	146.167	1891.6	200.666
D4 Stream	1	0.498	136.375	136.458	0.083	0.9	-
D4 Stream	2	0.857	337.208	371.292	34.084	325.8	200.75
D4 Stream	3	0.266	383.75	398.75	15	71.2	12.458
D6 Ditch	1	0.119	6.542	7.25	0.708	1.9	-
D6 Ditch	2	0.457	91.375	92.167	0.792	5.7	84.125
D6 Ditch	3	0.329	301.458	306.875	5.417	23.5	209.291
D6 Ditch	4	0.211	307.667	311.625	3.958	14.8	0.792
D6 Ditch 2nd	1	0.725	6.375	12.375	6	40.6	-
D6 Ditch 2nd	2	0.312	26.458	33.542	7.084	38.1	14.083
D6 Ditch 2nd	3	0.606	37.417	51.25	13.833	71.4	3.875
D6 Ditch 2nd	4	0.476	205.375	210.875	5.5	40.0	154.125
D6 Ditch 2nd	5	2.049	301.458	316.208	14.75	216.1	90.583
D6 Ditch 2nd	6	0.462	350.958	365.25	14.292	77.3	34.75
D6 Ditch 2nd	7	0.492	382.875	386.375	3.5	18.0	17.625
D6 Ditch 2nd	8	0.226	412.708	416.083	3.375	11.9	26.333
R1 Stream	1	0.417	56.375	56.625	0.25	2.0	-
R2 Stream	1	0.550	0.375	0.5	0.125	1.3	-
R3 Stream	1	0.581	27.375	27.833	0.458	4.6	-
R3 Stream	2	0.932	50.042	51.292	1.25	22.0	22.209

Table 8.9-14: Overview of pattern analysis for 20 m db+vfsmod (500 g/ha)

Type	Substance	Crop	Scenario	No events	Max PECsw [µg/L]	Max duration [d]	Min interval [d]	AUC total [µg/L×h]
Step 4	FCL	Potatoes	D3 Ditch	1	0.237	1.375	-	6.3
Step 4	FCL	Potatoes	D4 Pond	1	0.760	146.125	-	1888.3
Step 4	FCL	Potatoes	D4 Stream	3	0.857	34.084	12.458	397.4
Step 4	FCL	Potatoes	D6 Ditch	4	0.329	5.417	0.792	42.8
Step 4	FCL	Potatoes	D6 Ditch 2nd	8	2.049	14.75	3.875	492.4
Step 4	FCL	Potatoes	R1 Stream	1	0.218	0.208	-	1.0
Step 4	FCL	Potatoes	R2 Stream	1	0.287	0.125	-	0.7
Step 4	FCL	Potatoes	R3 Stream	1	0.303	0.375	-	2.2

Table 8.9-15: Details of single events for 20 m db+vfsmod (500 g/ha)

Scenario	Event no.	Max. PECsw [µg/L]	Event start [d]	Event end [d]	Event duration [d]	Event AUC [µg/L×h]	Interval to event [d]
D3 Ditch	1	0.237	124.375	125.75	1.375	6.3	-
D4 Pond	1	0.760	338.875	485	146.125	1887.9	-
D4 Stream	1	0.263	136.375	136.458	0.083	0.5	-
D4 Stream	2	0.857	337.208	371.292	34.084	325.8	200.75
D4 Stream	3	0.266	383.75	398.75	15	71.2	12.458
D6 Ditch	1	0.119	6.542	7.25	0.708	1.9	-
D6 Ditch	2	0.240	91.375	91.958	0.583	2.7	84.125
D6 Ditch	3	0.329	301.458	306.875	5.417	23.5	209.5
D6 Ditch	4	0.211	307.667	311.625	3.958	14.8	0.792
D6 Ditch 2nd	1	0.725	6.375	12.375	6	40.6	-
D6 Ditch 2nd	2	0.312	26.458	33.542	7.084	38.1	14.083
D6 Ditch 2nd	3	0.606	37.417	51.25	13.833	71.4	3.875
D6 Ditch 2nd	4	0.254	205.375	209.417	4.042	18.9	154.125
D6 Ditch 2nd	5	2.049	301.458	316.208	14.75	216.1	92.041
D6 Ditch 2nd	6	0.462	350.958	365.25	14.292	77.3	34.75
D6 Ditch 2nd	7	0.492	382.875	386.375	3.5	18.0	17.625
D6 Ditch 2nd	8	0.226	412.708	416.083	3.375	11.9	26.333
R1 Stream	1	0.218	56.375	56.583	0.208	1.0	-
R2 Stream	1	0.287	0.375	0.5	0.125	0.7	-
R3 Stream	1	0.303	27.375	27.75	0.375	2.2	-

Table 8.9-16: Overview of pattern analysis for 10 m db+vfsmod (375 g/ha)

Type	Substance	Crop	Scenario	No events	Max PECsw [µg/L]	Max duration [d]	Min interval [d]	AUC total [µg/L×h]
Step 4	FCL	Potatoes	D3 Ditch	1	0.342	1.583	-	10
Step 4	FCL	Potatoes	D4 Pond	1	0.547	145.75	-	1368
Step 4	FCL	Potatoes	D4 Stream	3	0.635	32.125	14.334	280
Step 4	FCL	Potatoes	D6 Ditch	3	0.342	3.375	2.875	26
Step 4	FCL	Potatoes	D6 Ditch 2nd	10	1.487	12.583	0.417	356
Step 4	FCL	Potatoes	R1 Stream	1	0.313	0.25	-	2
Step 4	FCL	Potatoes	R2 Stream	1	0.412	0.125	-	1
Step 4	FCL	Potatoes	R3 Stream	2	0.686	1.208	22.25	19

Table 8.9-17: Details of single events for 10 m db+vfsmod (375 g/ha)

Scenario	Event no.	Max. PECsw [µg/L]	Event start [d]	Event end [d]	Event duration [d]	Event AUC [µg/L×h]	Interval to event [d]
D3 Ditch	1	0.342	124.375	125.958	1.583	9.6	-
D4 Pond	1	0.547	339.25	485	145.75	1367.6	-
D4 Stream	1	0.373	136.375	136.458	0.083	0.7	-
D4 Stream	2	0.635	337.333	369.458	32.125	229.3	200.875
D4 Stream	3	0.207	383.792	396.25	12.458	49.5	14.334
D6 Ditch	1	0.342	91.375	92.083	0.708	4.1	-
D6 Ditch	2	0.251	301.5	304.875	3.375	13.1	209.417
D6 Ditch	3	0.159	307.75	310.708	2.958	9.2	2.875
D6 Ditch 2nd	1	0.542	6.417	10.792	4.375	25.0	-
D6 Ditch 2nd	2	0.235	26.5	32.625	6.125	26.9	15.708
D6 Ditch 2nd	3	0.460	37.5	50.083	12.583	52.0	4.875
D6 Ditch 2nd	4	0.358	205.375	210.167	4.792	28.6	155.292
D6 Ditch 2nd	5	1.487	301.458	307.208	5.75	76.7	91.291
D6 Ditch 2nd	6	0.862	307.625	315.583	7.958	75.1	0.417
D6 Ditch 2nd	7	0.181	351.042	354.958	3.916	14.0	35.459
D6 Ditch 2nd	8	0.354	355.708	363.958	8.25	40.8	0.75
D6 Ditch 2nd	9	0.368	382.875	385.333	2.458	11.4	18.917
D6 Ditch 2nd	10	0.168	412.75	414.458	1.708	5.5	27.417
R1 Stream	1	0.313	56.375	56.625	0.25	1.5	-
R2 Stream	1	0.412	0.375	0.5	0.125	1.0	-
R3 Stream	1	0.436	27.375	27.792	0.417	3.3	-
R3 Stream	2	0.686	50.042	51.25	1.208	16.1	22.25

Table 8.9-18: Overview of pattern analysis for 20 m db+vfsmod (375 g/ha)

Type	Substance	Crop	Scenario	No events	Max PECsw [µg/L]	Max duration [d]	Min interval [d]	AUC total [µg/L×h]
Step 4	FCL	Potatoes	D3 Ditch	1	0.177	1.167	-	4.3
Step 4	FCL	Potatoes	D4 Pond	1	0.546	145.708	-	1365.0
Step 4	FCL	Potatoes	D4 Stream	3	0.635	32.125	14.334	279.2
Step 4	FCL	Potatoes	D6 Ditch	3	0.251	3.375	2.875	24.1
Step 4	FCL	Potatoes	D6 Ditch 2nd	10	1.487	12.583	0.417	339.7
Step 4	FCL	Potatoes	R1 Stream	1	0.164	0.167	-	0.6
Step 4	FCL	Potatoes	R2 Stream	1	0.215	0.083	-	0.4
Step 4	FCL	Potatoes	R3 Stream	1	0.227	0.333	-	1.6

Table 8.9-19: Details of single events for 20 m db+vfsmod (375 g/ha)

Scenario	Event no.	Max. PECsw [µg/L]	Event start [d]	Event end [d]	Event duration [d]	Event AUC [µg/L×h]	Interval to event [d]
D3 Ditch	1	0.177	124.375	125.542	1.167	4.3	-
D4 Pond	1	0.546	339.292	485	145.708	1364.8	-
D4 Stream	1	0.197	136.375	136.458	0.083	0.4	-
D4 Stream	2	0.635	337.333	369.458	32.125	229.3	200.875
D4 Stream	3	0.207	383.792	396.25	12.458	49.5	14.334
D6 Ditch	1	0.180	91.375	91.875	0.5	1.8	-
D6 Ditch	2	0.251	301.5	304.875	3.375	13.1	209.625
D6 Ditch	3	0.159	307.75	310.708	2.958	9.2	2.875
D6 Ditch 2nd	1	0.542	6.417	10.792	4.375	25.0	-
D6 Ditch 2nd	2	0.235	26.5	32.625	6.125	26.9	15.708
D6 Ditch 2nd	3	0.460	37.5	50.083	12.583	52.0	4.875
D6 Ditch 2nd	4	0.189	205.375	208.625	3.25	12.4	155.292
D6 Ditch 2nd	5	1.487	301.458	307.208	5.75	76.7	92.833
D6 Ditch 2nd	6	0.862	307.625	315.583	7.958	75.1	0.417
D6 Ditch 2nd	7	0.181	351.042	354.958	3.916	14.0	35.459
D6 Ditch 2nd	8	0.354	355.708	363.958	8.25	40.8	0.75
D6 Ditch 2nd	9	0.368	382.875	385.333	2.458	11.4	18.917
D6 Ditch 2nd	10	0.168	412.75	414.458	1.708	5.5	27.417
R1 Stream	1	0.164	56.375	56.542	0.167	0.6	-
R2 Stream	1	0.215	0.375	0.458	0.083	0.4	-
R3 Stream	1	0.227443	27.375	27.708	0.333	1.58	-

zRMS comments:

Application pattern

The application pattern assumed by the Applic ant in simulations is in line with the Central Zone GAP presented in Table 8.1-1. The application windows indicated in Table 8.9-1 (Step 1-2) and Table 8.9-2 (Step 3) are agreed by the zRMS.

Input parameters

Input parameters presented in Tables 8.9-3 to 8.9-5 are in general in line with endpoints agreed in the course of the EU review of flurochloridone and reported in EFSA Journal 2010;8(12):1869. Nevertheless there are some exceptions discussed below:

- For flurochloridone geometric mean DT_{50} of 58 days derived from the kinetic re-evaluation of the EU agreed soil field dissipation trials performed with CS formulation was used by the Applicant. However, the new geometric mean field DT_{50} of 58 days is considered to be not sufficiently different from the geometric mean laboratory DT_{50} of 53 days agreed at the EU level for surface water modelling, to justify the use of new active substance data at the zonal level. Taking this into account, the kinetic re-evaluation of the EU agreed soil field dissipation trials was not validated by the zRMS as being not necessary. For more details regarding the zRMS approach, please refer to point 8.4.1 of this report. Nevertheless, the zRMS is of the opinion that consideration of DT_{50} of 58 days represents worst case and is thus agreed.
- For all compounds the geometric mean Kfoc values were considered instead of the EU agreed arithmetic mean values. This deviation is agreed by the zRMS as the geometric mean Kfoc are lower than the arithmetic mean values and represent thus worst case in terms of the leaching potential. Moreover, consideration of the geometric mean Kfoc is in line with current EFSA recommendations. The geometric mean values were calculated from the individual Kfoc values reported in the LoEP and are confirmed by the zRMS to be correct.
- At the EU level additional simulations were performed for the parent with consideration of the sediment DT_{50} set to 1000 d, as representing worst case for this compartment. Nevertheless, in the LoEP the endpoints for sediment dwelling organisms are reported as mg/L with no endpoints relevant for the exposure via sediment. For this reason the worst case calculations for sediment are deemed not necessary as not being used in the aquatic RA.

Step 3 simulations for flurochloridone were performed with consideration of PUF of 0, in line with current FOCUS recommendations.

Analysis of the information presented in the modelling report demonstrated that most probably the 4 d TWA PEC_{sw} values are reported in Table 8.9-8 instead of 7 d TWA PEC_{sw}. This could be confirmed only for D3 scenario for which the TOXSWA summary files were provided, while they were not available for remaining scenarios. The surface water exposure estimations were independently validated by the zRMS and confirmed that TWA PEC_{sw} values reported in Table 8.9-8 are relevant for 4 d, while for 7 d these values are lower. It is, however, noted that for purposes of evaluation of the risk of secondary poisoning the maximum Step 1 PEC_{sw} was considered in area of Section 9 and TWA PEC_{sw} were not used at all. Taking this into account Table 9.8-9 was not corrected and reported TWA values are struck through as not necessary for the risk assessment.

Overall, the surface water exposure presented in Tables 8.9-6 to 8.9-8 may be used in the aquatic risk assessment.

During the commenting period the Applicant submitted additional surface water modelling by Weber & Jarvis (2020, Rep. No 2000626.SW0-6397) performed at Step 4 using VFSmod in order to further mitigate flurochloridone run-off in R scenarios, which is acceptable in Poland. Input parameters and application data already agreed by the zRMS were used and may be found in Tables 8.9-1 to 8.9-3 above. The input by volatilisation and deposition was quantified using EVA 3, similarly as in the initial modelling summarised above (Ranke, 2018b, Ref. No 000100957).

Obtained results were independently validated by the zRMS using the same parameters with exception of Q10, which was manually set to 2.2, while the Applicant considered Q10 of 2.58. Manual change of Q10 is recommended by the Working Document of the Central Zone in area of Section 8[1] for active compounds for which the degradation data were normalised using Q10 of 2.2.

[1] Working Document of the Central Zone in the Authorisation of Plant Protection Products, Section 8, Environmental Fate and Behaviour, Version 1, rev. 1, June 2018

Results obtained by the zRMS were slightly lower than these provided in the modelling report, which was due to different Q10 used – consideration of Q10 of 2.2 results in lower PEC values. Overall, the new modelling provided by the Applicant was well performed and is considered acceptable. Below results copied from the modelling report are presented and may be used for purposes of the aquatic risk assessment. Please note that Step 3 PEC_{sw} values are the same as reported in Table 8.9-8 above and are reported for completeness only.

Step 3 and Step 4 PEC_{sw} values for flurochloridone following application to potatoes (VFSmod used to mitigate run-off in R scenarios)

Scenario		PECsw [µg/L]		
		Step 3	Step 4	
			10 m (db + VFSmod)	20 m (db + VFSmod)
		Maximum	Maximum	Maximum
D3	ditch	2.621 (sd)	0.455 (sd)	0.237 (sd)
D4	pond	0.763 (dr)	0.761 (dr)	0.760 (dr)
	stream	2.169 (sd)	0.857 (dr)	0.857 (dr)
D6	ditch	2.598 (sd)	0.457 (sd)	0.329 (sd)
D6 2nd	ditch	2.641 (sd)	2.049 (dr)	2.049 (dr)
R1	pond	0.400 (ro)	0.076 (ro)	0.050 (ro)
	stream	3.812 (ro)	0.417 (ro)	0.218 (ro)
R2	stream	2.398 (sd)	0.550 (ro)	0.287 (ro)
R3	stream	8.001 (ro)	0.932 (ro)	0.303 (ro)

(sd): drift entry; (dr): drainage entry; (ro): run-off entry; db: drift buffer

Comments on additional surface water modelling (31.08.2021):

After finalisation of the zonal assessment of AG-F8250 CS in March 2021, additional surface water modelling has been provided by the Applicant for the lower application rate of 375 g a.s./ha (see 8.1-1 in point 8.1 of this document).

The input parameters used for these additional simulations were the same as for the higher rate and were already agreed by the zRMS. It is noted that the saturated vapour pressure was converted to 1.4×10^{-4} at 20°C from 2.7×10^{-4} at 25°C using EVA3 tool (version 2).

At Step 4 simulations were performed with VFSmod with consideration of vegetated filter strips of 10 and 20 m.

The Applicants' calculations were independently validated by the zRMS. Obtained results were insignificantly lower comparing to these presented in the report of Weber & Jarvis (2021, Rep. No 2000626.SW0-1750). In additional modelling performed by the zRMS the same input parameters were used with exception of Q10, which was manually set to 2.2, while the Applicant considered Q10 of 2.58. Manual change of Q10 is recommended by the Working Document of the Central Zone in area of Section 8[2] for active compounds for which the degradation data were normalised using Q10 of 2.2. Therefore PECsw values calculated by the zRMS values were lower. Overall, the new modelling provided by the Applicant was well performed and is considered acceptable.

Exposure pattern analysis was performed for Step 4 simulations using 10 and 20 m vegetated filter strips with VFSmod, with a threshold level of 0.1 µg/L for both application rates of 500 and 375 g a.s./ha. The independent calculations performed by the zRMS confirm obtained results, being in good agreement with values calculated by the Applicant.
Overall, the surface water exposure presented in Tables 8.9-6 to 8.9-19 may be used in the aquatic risk assessment.

Please note that additional surface water modelling may be required by the concerned Member States that do not accept simulations performed according to FOCUS recommendations. It should be also kept in mind that some MS may not accept calculations performed using VFSmod.

[2] Working Document of the Central Zone in the Authorisation of Plant Protection Products, Section 8, Environmental Fate and Behaviour, Version 1, rev. 1, June 2018

8.9.2.1 PEC_{sw} of AG-F8-250 CS

The surface water risk assessment of the product AG-F8-250 CS is considered to be covered by the assessment of the active substance and its metabolites at Steps 1-4 (please refer to Part B9 for details).

zRMS comments:

Evaluation performed in area of Section 9 demonstrated that the formulated product is not more toxic than the active substance and for this reason no separate risk assessment for the formulation was deemed necessary. In consequence, calculation of formulation PEC_{sw} was not required.

8.10 Fate and behaviour in air (KCP 9.3, KCP 9.3.1)

Table 8.10-1 Summary of atmospheric degradation and behaviour

Compound	flurochloridone
Vapour pressure [Pa]	2.7×10^{-4} (25°C)
Direct photolysis in air	No data
Photochemical oxidative degradation in air	DT_{50}: 6.4 h, Atkinson method OH (12h) concentration assumed = 1.5×10^{6} OH/cm^{3}
Volatilisation	from plant surfaces: 6.3% loss after 24 h from soil: 6.5% loss after 24 h
Metabolites	No volatiles other than CO_2 were identified in the environmental studies

The vapour pressure at 20 °C of the active substance flurochloridone is > 10^{-4} Pa. Hence the active substance flurochloridone is regarded as semivolatile (volatilisation from soil and plant surfaces). Therefore exposure of adjacent surface waters and terrestrial ecosystems by the active substance flurochloridone due to volatilization with subsequent deposition is considered in the PEC surface water calculations above.
The photochemical oxidative degradation in air was estimated to be 6.4 hours and therefore, significant long-range transport and accumulation in the stratosphere is deemed unlikely (see FOCUS working group report: Pesticides in Air: Considerations for exposure assessment, SANCO/10553/2006, June 2008).

zRMS comments:

Provided above information is in line with EU agreed data reported in EFSA Journal (2010);8(12):1869.

Due to the vapour pressure above trigger of 10^{-5} Pa, flurochloridone may be considered as semi-volatile and respective studies on volatilisation from soil and plant surfaces were performed at the EU level demonstrating low potential for volatilisation.
In addition to that, with air DT_{50} being only 6.4 hours (i.e. clearly below the trigger of 2 days), flurochloridone is not expected to be the subject to the long- or short-range transport.

Taking this into account the contamination of the atmosphere from the intended uses of AG-F8-250 CS is considered to be negligible.

Appendix 1 Lists of data considered in support of the evaluation

List of data submitted by the applicant and relied on

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Owner
KCP 9.2.4	Ranke J.	2018a	FOCUS groundwater calculations for flurochloridone and its soil metabolites following application of AG-F8-250 CS in Poland Report No jrwb-127 Agan Reference No. 000100956 GLP: not applicable Unpublished	N	ADM
KCP 9.2.5/01	Ranke J.	2018b	FOCUS Step 3-4 surface water calculations for flurochloridone following application of AG-F8-250 CS in Poland Report No jrwb-128 Agan Reference No. 000100957 GLP: not applicable Unpublished	N	ADM
KCP 9.2.5 / 02	Weber D. and Jarvis T.	2020	Predicted environmental concentrations in surface water after pre-emergence application of flurochloridone to potatoes in the European Union - FOCUS Step 3-4 calculations Report No.: 2000626.SW0-6397 Agan Reference No. XXXXXX GLP: not applicable Unpublished	N	ADM
KCP 9.2.5 / 03	Weber D. and Jarvis T.	2021	Predicted environmental concentrations in surface water after pre-emergence application of flurochloridone to potatoes in the European Union - FOCUS Step 3-4 calculations Report No.: 2000626.SW0-1750 Agan Reference No. XXXXXX GLP: not applicable Unpublished	N	ADM

List of data submitted or referred to by the applicant and relied on, but already evaluated at EU peer review

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Owner	Remarks
KCP 9.1.1.1	Walther D.	2013a	Metabolite R42819: Degradation rate in three soils incubated under aerobic conditions Harlan Laboratories Report D45332 Agan Reference No. 90015009 GLP Unpublished	N	ADM	Evaluated in 2014 as part of Confirmatory Data (see Addendum 2, B.8 of July 2014)
KCP 9.1.2	Walther D.	2013b	Metabolite R42819: Adsorption/desorption on soil Harlan Laboratories Report D45331 Agan Reference No. 90015008 GLP Unpublished	N	ADM	Evaluated in 2014 as part of Confirmatory Data (see Addendum 2, B.8 of July 2014)

List of data submitted by the applicant and not relied on

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Owner	Reason for rejection
KCP 9.1.1.2.1	Finger N. and Ranke J.	2018	Kinetic evaluation of flurochloridone decline observed in eight legacy field dissipation trials in Europe using time-step normalisation Report No ERA-1333A Agan Reference No. 90020995	N	ADM	Kinetic re-evaluation of the EU agreed field dissipation trials was not required for the exposure estimation

List of data relied on and not submitted by the applicant but necessary for evaluation

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Owner
There were no studies relied on and not submitted by the Applicant.					

Appendix 2 Detailed evaluation of the new Annex II studies

A 2.1 Walther (2013a): Metabolite R42819: Degradation rate in three soils incubated under aerobic conditions

The following study was already evaluated at EU level in the course of the evaluation of confirmatory data and was considered acceptable.

Comments of zRMS:	The study has been already evaluated at the EU level as a part of confirmatory data and considered acceptable. For details of the evaluation, please refer to Addendum 2, B.8 on Confirmatory Data of July 2014. The summary below is struck through as being not necessary.

Reference:	KCP 9.1.1.1
Report	Metabolite R42819: Degradation rate in three soils incubated under aerobic conditions Walther D. 2013 Harlan Laboratories Report D45332 Agan Reference No. 90015009
Guideline(s):	OECD 307
Deviations:	No
GLP:	Yes
Acceptability:	Agreed at the EU level (see Addendum 2, B.8 on Confirmatory Data of July 2014)

~~**Executive Summary**~~

~~The rate of decline of R42819, a soil metabolite of Flurochloridone, was investigated in three field soils under aerobic conditions.~~

~~Fresh soil samples (100 g dry weight) were transferred to 1 liter glass metabolism flasks. The samples were treated with R42819 at a target rate of 0.1 mg/per kg soil dry weight. This rate corresponds to an application of the parent substance flurochloridone at a field rate of 75 kg/ha, assuming a complete conversion to R42819 and even distribution in the top 5 cm of soil at a bulk density of 1.5 g/cm^3. The flasks were placed at 20 ± 2 °C in the dark and continuously ventilated with moistened air. The soil moisture was maintained at moisture levels corresponding to pF 2.0-2.5.~~

~~Duplicate flasks were sampled immediately after treatment (time 0) and at multiple time points up to 112 days. The soil was extracted with acetonitrile/water (4:1, v/v). The extracts were diluted and analyzed by LC-MS to determine the concentration of R42819.~~

~~The analytical method was shown to be specific, accurate and reproducible. Mean recoveries from fortified soils were 102.2% for soil I, 99.6% for soil II and 101.7 % for soil III, confirming method validity and analyte stability during sample work-up and analysis.~~

~~The mean amounts of R42819 recovered from treated soil at time 0 were 98.2 – 98.6% for soils I-III. Thereafter, the recovery decreased progressively to 5.5% (soil I), 9.4% (soil II) and 4.1% (soil III) by day 112 at the end of the study.~~

~~The rates of decline of R42819 in the three soils were determined in accordance with FOCUS Guidance using the kinetic evaluation software KinGUII®. Single first order kinetics (SFO) gave an adequate fit of the experimental data. Goodness of fit of the SFO model and derived DT50 and DT90 values are given below:~~

~~**Table A 1: Summary of results**~~

~~SFO Parameters~~	~~Soil I~~	~~Soil II~~	~~Soil III~~
~~DT_{50} (days)~~	~~17.1~~	~~27.5~~	~~18.2~~
~~DT_{90} (days)~~	~~56.9~~	~~91.2~~	~~60.3~~
~~Chi^2Err%~~	~~5.41~~	~~3.79~~	~~4.17~~
~~r^2~~	~~0.9899~~	~~0.9921~~	~~0.9932~~

The DT_{50} and DT_{90} values appeared to correlate with the clay content of the soils. DT values were shorter in the clay rich soils I (18% clay) and III (16% clay) than in the sandy soil II (7.3% clay).

I. MATERIALS AND METHODS

A. MATERIALS

1. Test material Metabolite R42819
(4-(chloromethyl)-1-(3-(trifluoromethyl)phenyl)pyrrolidin-2-one)

Description Not stated
Batch # HHHL-001-00-1
Purity 96.1%
Stability of test material Stability not stated. The test material was stored at -20 °C. Expiry date: 09 Jan 2013

2. Soils The following soils were used in the study:

Table A 2: Description of soils used in the study

Soil description	Soil I	Soil II	Soil III
Name	Mechtildshausen	Speyer 2.2	Fraunhofer 02-A
Batch	6/12	F2.2 2512	06/12
pH (0.01 M $CaCl_2$)	7.16	5.5	6.84
Organic carbon [%; g/100 g soil]	1.14	1.77	1.18
Maximum water holding capacity [g water/100g soil]			
at pF 1.0	43.17	7.3	15.86
at pF 2.0	27.67	13.8	71.69
at pF 2.5	23.67	78.9	12.45
Cation exchange capacity [mmol/100 g soil]	14.75	10.1	15.49
Carbonate ($CaCO_3$) (%)	<0.30	<0.30	<0.30
Nitrogen content (%)	0.12	0.17	0.13
Organic matter (%)	1.97	3.05	2.03
C/N ratio			
Particle size distribution according to USDA [%]			
Soil type (USDA)	Loam	Loamy sand	Silt loam
Clay < 0.002 mm	18.32	7.3	15.86
Silt: 0.002-0.050 mm	44.45	13.8	71.69
Sand: >0.050 mm	37.23	78.9	12.45
Biomass (mg org.C/100 g dry soil)			
Start of incubation	36.9	26.4	25.6
End of incubation	19.3	17.6	26.9

Soil preparation Sampling sites were not exposed to pesticides or fertilizers for at least 4 years prior to sampling. Soil samples were taken from the top 20 cm layer after removal of the vegetation. The soils were sieved through a 2-mm screen and stored at 4 °C. Prior to the study, the soils were acclimated to room temperature for several days. Storage and acclimation did not exceed three months from soil sampling in the field.

Soil moisture was determined in triplicate soil aliquots based on weight loss after drying in a halogen dryer. Moisture was adjusted by air-drying and/or adding purified water. The soil was sub-sampled in aliquots of 100 g (dry weight) in 1 liter glass metabolism flasks at moisture levels allowing handling without clumping. After mixing the test item with the soil, the moisture level was raised as/if needed to reach final water contents in the range of pF 2.0 - 2.5, suitable for microbial activity without causing clumps that would limit aeration.

B. STUDY DESIGN AND METHODS

1. In-life dates 08.06.2012 to 20.12.2012

2. Experimental conditions

The target rate of R42819 (metabolite of Flurochloridone) was 0.1 mg per kg dry soil (0.01 mg/metabolism flask). This rate corresponded to an application of Flurochloridone at a field rate of 75 kg a.i./ha, assuming a complete conversion to R42819 and even distribution in the top 5 cm of soil at a bulk density of 1.5 g/cm^3.
An aliquot of 0.4 mL application solution was spread drop-wise on the soil sample in each metabolism flask. Control flasks (used for fortification and biomass determination) were treated with the same volume of solvent but without test item. Treated flasks were swirled to mix the test item into the soil. Additionally, aliquots of the application solution were dispensed in solvent for verification of the applied amount by LC-MS. Applied amounts derived from LC-MS analysis averaged 10.5 µg/application aliquot, confirming the expected amount of 10.0 µg. The expected amount (10.0 µg) was taken as the 100% applied amount for calculation of recoveries.
The soil was incubated in aliquots of 100 g (on a dry weight basis) in 1 liter glass metabolism flasks (≈ 10.6 cm inner diameter). The flasks were kept in the dark at 20 ± 2 °C and continuously ventilated with moistened air.
-Water losses were kept to a minimum by circulating moistened air at a minimum flow rate required for bubble formation in the water bottle used for moistening the incoming air. Soil moisture was adjusted periodically to pF 2.0-2.5 by weighing the metabolism flasks and adding the amounts of water that may have evaporated.

3. Sampling and measurements

Duplicate flasks were sampled immediately after treatment (time 0) and after 3, 7, 14, 28, 56 and 112 days of incubation.
The soil was extracted three times with acetonitrile/water (4:1, v/v). The amount of solvent used per extraction was about 1 mL per g soil. Extractions at ambient temperature were performed on a shaker at about 250 rpm for 30 minutes. Beginning with day 3 samples, ambient extractions were followed by Soxhlet extraction with acetonitrile/water (4:1, v/v) for 4 hours using 3 mL solvent per g soil.
Extracts were separated from soil by centrifugation. The extracts of each soil sample were pooled and the pools were adjusted to specific volumes (e.g. 300 mL for ambient extracts and 540 mL or 560 mL for ambient and Soxhlet extracts).
Aliquots of 200 µL pooled extracts were mixed with 800 µL 0.1% formic acid in water for LC-MS analyes, except for day 112 samples which were diluted by mixing 500 µL extract with 500 µL 0.1% formic acid in water. Measured concentrations of R42819 were expressed in percent of the applied amount and µg parent equivalents/kg dry soil.
All samples were either analyzed on the day of sampling or kept at 4 °C for short term storage (e.g. overnight) or -20 °C for prolonged storage.
Control flasks with untreated soil were used for determination of the microbial biomass at the start and end of incubation. Untreated soil was also used for fortification with metabolite R42819 in order to monitor accuracy and repeatability of the analytical method.

4. Analytics

The analytical method consisted of LC (liquid chromatography) coupled with MS/MS (tandem mass spectrometric detection).
HPLC conditions: column: Inertsil ODS-3 (GL Sciences); 2.1 mm x 33 mm; particle size 3 µm; eluent A: water/ methanol/ formic acid (95:5:0.1 v/v/v) 5mM ammonium formate; eluent B: water/ methanol/ formic acid (5:95:0.1 v/v/v) 5mM ammonium formate; gradient: 0 min 50% A/50% B, 1.5 min 0% A/100% B, 2.0 min 0% A/100% B, 2.1 min 100% A/0% B, 2.4 min 100% A/0% B, 2.5-4.0 min 50%

~~A/50% B; flow rate 300 µL/min; injection volume: 5 µL; retention time of the test item: 1.5 min (typical value)~~

~~MS conditions: Mass spectrometer API4000; ionisation mode: ESI; gases: nebulizer and heater gas: air, curtain and collision gas: nitrogen; ion source: heater gas temperature: 550 °C, spray voltage: 5500 V; scan mode: multiple reaction monitoring; ion polarity: positive $[M+H]^+$; precursor ion: m/z 278.0; product ion: m/z 258.1; collision energy: 32 eV; dwell time: 300 ms.~~

~~The LOQ was defined as the lowest fortification level with recoveries ranging from 70% to 110%. This criterion was met at a fortification level of 10 µg/kg.~~

~~The LOD was derived from the lowest calibration point (0.1 ng/mL). It was found to be 2.7 µg/kg for soils I-III corresponding to 2.7% of the applied amount.~~

~~II. RESULTS AND DISCUSSION~~

~~A. RECOVERY OF R42819 FROM TREATED SOIL~~

~~The mean amounts of R42819 recovered from treated soil at time 0 were 98.2 - 98.6% for soils I-III. Thereafter, the recovery decreased progressively to 5.5% (soil I), 9.4% (soil II) and 4.1% (soil III) by day 112 at the end of the study.~~

~~Table A 3: Recovered amounts of R42819 from Soils I-III following incubation up to 112 days~~

~~Soil~~	~~Recovered R42819 in % of applied at time points up to 112 days~~						
	~~0 d~~	~~3 d~~	~~7 d~~	~~14 d~~	~~28 d~~	~~56 d~~	~~112 d~~
~~Soil I~~	~~98.6~~	~~95.4~~	~~78.1~~	~~61.6~~	~~28.9~~	~~11.0~~	~~5.5~~
	~~97.8~~	~~96.7~~	~~75.1~~	~~60.2~~	~~28.1~~	~~11.4~~	~~5.5~~
~~Mean~~	~~98.2~~	~~96.0~~	~~76.6~~	~~60.9~~	~~28.5~~	~~11.2~~	~~5.5~~
~~Soil II~~	~~99.4~~	~~95.3~~	~~83.6~~	~~75.6~~	~~46.7~~	~~23.8~~	~~9.7~~
	~~97.8~~	~~96.2~~	~~83.8~~	~~75.6~~	~~45.4~~	~~22.9~~	~~9.2~~
~~Mean~~	~~98.6~~	~~95.8~~	~~83.7~~	~~75.6~~	~~46.0~~	~~23.4~~	~~9.4~~
~~Soil III~~	~~98.1~~	~~92.9~~	~~79.2~~	~~64.3~~	~~30.8~~	~~8.4*~~	~~4.5*~~
	~~98.2~~	~~94.4~~	~~78.4~~	~~62.1~~	~~34.6~~	~~9.4*~~	~~3.8*~~
~~Mean~~	~~98.1~~	~~93.6~~	~~78.8~~	~~63.2~~	~~32.7~~	~~8.9*~~	~~4.1~~

~~* Values <LOQ and >LOD; therefore used for modeling kinetics~~

~~B. RATE OF DECLINE OF R42819~~

~~Rates of decline of R42819 in soils I-III were determined in accordance with FOCUS Guidance using the kinetic evaluation software KinGUI®. Single first order kinetics (SFO) gave an adequate fit of the experimental data. Goodness of fit of the SFO model and derived DT_{50} and DT_{90} values are given below:~~

~~Table A 4: Summary of results~~

~~SFO Parameters~~	~~Soil I~~	~~Soil II~~	~~Soil III~~
~~DT_{50} (days)~~	~~17.1~~	~~27.5~~	~~18.2~~
~~DT_{90} (days)~~	~~56.9~~	~~91.2~~	~~60.3~~
~~Chi^2Err%~~	~~5.41~~	~~3.79~~	~~4.17~~
~~r^2~~	~~0.9899~~	~~0.9921~~	~~0.9932~~

~~The DT_{50} and DT_{90} values appeared to correlate with the clay content of the soils. DT values were shorter in the clay rich soils I (18% clay) and III (16% clay) than in the sandy soil II (7.3% clay).~~

~~III. CONCLUSION~~

~~The rate of decline of R42819 was investigated in three agricultural soils under aerobic conditions at 20 ± 2 °C in the dark. Single first order kinetics (SFO) gave an adequate fit of the experimental data. The DT_{50} and DT_{90} values appeared to correlate with the clay content of the soils. DT values were shorter in the clay rich soils I (18% clay) and III (16% clay) than in the sandy soil II (7.3% clay). The DT_{50} values were 17.1 days for Soil I, 27.5 days for Soil II and 18.2 days for Soil III.~~

A 2.2 Walther (2013b): Metabolite R42819: Adsorption/Desorption on soil

The following study was already evaluated at EU level in the course of the evaluation of confirmatory data and was considered acceptable.

Comments of zRMS:	The study has been already evaluated at the EU level as a part of confirmatory data and considered acceptable. For details of the evaluation, please refer to Addendum 2, B.8 on Confirmatory Data of July 2014. The summary below is struck through as being not necessary.

Reference:	KCP 9.1.2
Report	Metabolite R42819: Degradation rate in three soils incubated under aerobic conditions Walther D., 2013 Harlan Laboratories Report D45332 Agan Reference No. 90015009
Guideline(s):	OECD 307
Deviations:	No
GLP:	Yes
Acceptability:	Agreed at the EU level (see Addendum 2, B.8 on Confirmatory Data of July 2014)

~~**Executive Summary**~~

~~The sorption behaviour of Metabolite R42819 was investigated by studying its distribution between soil and an aqueous phase according to the batch equilibrium method described in OECD Guideline No. 106. Three agriculture soils were used in the study. The soils represented a range of properties important for adsorption, i.e. organic carbon content, clay content, texture and the pH value.~~
~~Preliminary investigations indicated that the study could be performed in Teflon tubes at the soil-solution ratio 5/25 g/mL.~~
~~Adsorption kinetics were determined for the soil-solution ratio 5/25 g/mL (soils I-III) an initial test item concentration of 0.18 mg/L and adsorption intervals of 2, 5, 24 and 48 hours. Adsorption to soils I-III reached 33.9-62.8% of the applied amount at the adsorption equilibrium that was reached after 24 hours of adsorption. Corresponding K_d values were 2.6-8.6 mL/g and the K_{oc} values were 206-481 mL/g.~~
~~Desorption kinetics were determined for the soil-solution ratio 5/25 g/mL (soils I-III), an initial test item concentration of 0.18 mg/L and desorption intervals of 2, 5 and 24 hours, following 24 hours of adsorption. Desorption from soils I-III reached 28-50.5% of the adsorbed amounts. The corresponding K_{des} values were 5.0-13.3 mL/g and the K_{oc} values were 392-675 mL/g.~~
~~The total amount of test item recovered from the test system (supernatant and soil extract) amounted to 104-109% of the applied amount. These values were slightly excessive but within acceptable range (< 110%).~~
~~The Freundlich adsorption/desorption isotherms were based on five test item concentrations in the range of 0.02 and 2 mg/L.~~

~~**Table A 5: Summary of results**~~

~~Parameter~~	~~Soil I (Sandy loam)~~	~~Soil II (Silt loam)~~	~~Soil III (Sandy clay loam)~~
~~K_F~~	~~1.812~~	~~4.418~~	~~1.569~~
~~K_{FOC}~~	~~152~~	~~229~~	~~124~~
~~1/n~~	~~0.77~~	~~0.83~~	~~0.78~~
~~r^2~~	~~0.9974~~	~~0.9997~~	~~0.9961~~
~~$K_{des,F}$~~	~~0.943~~	~~3.663~~	~~0.620~~
~~$K_{des,FOC}$~~	~~79.284~~	~~189.791~~	~~48.848~~
~~1/n~~	~~0.644~~	~~0.774~~	~~0.635~~
~~r^2~~	~~0.994~~	~~1.000~~	~~0.989~~

~~The Freundlich adsorption coefficients K_F were in the range of 1.569 – 4.418 for soils I-III. The corresponding K_{FOC} coefficients were 124 – 229. The 1/n values were 0.77 – 0.83, indicating nonlinear adsorption behavior.~~
~~The Freundlich desorption coefficients $K_{des,F}$ were in the range of 0.620 –3 .663 for soils I-III. The low $K_{des,F}$ indicate reversibility of the adsorption. The 1/n values were 0.635 to 0.774.~~
~~A certain degree of correlation was noticed between the adsorption coefficients K_F and the organic carbon content (R^2 = 0.97), clay content (R^2 = 0.95) and soil pH (R^2 = 0.98). Since the correlation is based only on three soils, it may not predict sorption behavior in a larger array of soils.~~

~~I. MATERIALS AND METHODS~~

~~A. MATERIALS~~

~~1. Test material~~ ~~Metabolite R42819~~
~~(4-(chloromethyl)-1-(3-(trifluoromethyl)phenyl)pyrrolidin-2-one)~~

~~Description~~ ~~Not stated~~
~~Batch #~~ ~~HHHL-001-00-1~~
~~Purity~~ ~~96.1%~~
~~Stability of test material~~ ~~Stability not stated. The test material was stored at -20 °C. Expiry date: 09 Jan 2013~~

~~2. Soils~~ ~~The following soils were used in the study:~~

~~Table A 6: Description of soils used in the study~~

~~Soil description~~	~~Soil I~~	~~Soil II~~	~~Soil III~~
~~Name~~	~~Mechtildshausen~~	~~Speyer 2.2~~	~~Fraunhofer 02-A~~
~~Batch~~	~~6/11~~	~~F2.2 0911~~	~~01/12~~
~~pH (0.01 M $CaCl_2$)~~	~~7.01~~	~~5.5~~	~~6.92~~
~~Organic carbon [%; g/100 g soil]~~	~~1.19~~	~~1.93~~	~~1.27~~
~~Maximum water holding capacity [g water/100g soil]~~			
~~at pF 1.0~~	~~49.62~~	~~48.43~~	~~56.98~~
~~at pF 2.0~~	~~29.46~~	~~22.03~~	~~37.34~~
~~at pF 2.5~~	~~21.45~~	~~13.63~~	~~24.39~~
~~Cation exchange capacity [mmol/100 g soil]~~	~~12.33~~	~~10.0~~	~~13.53~~
~~Carbonate ($CaCO_3$) (%)~~	~~0.60~~	~~0.60~~	~~0.6~~
~~Nitrogen content (%)~~	~~0.11~~	~~0.17~~	~~0.14~~
~~Organic matter (%)~~	~~2.05~~	~~3.33~~	~~2.19~~
~~C/N ratio~~	~~10.8~~	~~11.4~~	~~9.07~~
~~Particle size distribution according to USDA [%]~~			
~~Soil type (USDA)~~	~~Loam~~	~~Loamy sand~~	~~Silt loam~~
~~Clay < 0.002 mm~~	~~17.82~~	~~6.6~~	~~16.02~~
~~Silt: 0.002-0.050 mm~~	~~44.35~~	~~12.1~~	~~70.82~~
~~Sand: 0.050-2.0 mm~~	~~37.83~~	~~81.3~~	~~13.16~~

~~Soil preparation~~ ~~Soil samples were taken from the top 20 cm layer after removal of the vegetation. The soils were sieved to 2 mm and air-dried at room temperature. All soils were used in non-sterilised form. The residual soil moisture was determined by drying three soil aliquots in an infrared drier until there was no significant change in weight.~~

~~B. STUDY DESIGN AND METHODS~~

~~1. In-life dates~~ ~~08.06.2012 to 23.08.2012~~

~~2. Experimental conditions~~

Test conditions

Preliminary investigations indicated that the study could be performed in Teflon tubes (40 mL capacity) at the soil-solution ratio 5/25 g/mL.
Pre-equilibration of the soil was performed by shaking the soil for at least overnight in about 90% of the final volume of 0.01 M $CaCl_2$ solution. The volume was adjusted with 0.01 M $CaCl_2$ after the application to reach specific soil-solution ratios.
Test tubes were shaken horizontally at about 140 rpm at 20 ± 2 °C in the dark. The agitation kept the soil in suspension. Soil suspensions were centrifuged at forces capable of removing particles larger than 0.2 µm from the solution (e.g. 3500 rpm/min for 30 min). The amount of test item in the supernatant was determined by LC-MS and subtracted from the applied amount to determine the adsorbed amount (i.e. indirect method).
Adsorption/desorption kinetics were performed at the soil-solution ratio 5/25 g/mL. A material balance was determined at the adsorption equilibrium to determine the recovery of the test item from the test system. Control tubes (i.e. without soil) were used to measure test item stability and applied amounts. Blank tubes (i.e. without test item) were used to detect potential background signals. All experiments including controls and blanks were performed in duplicates.
Solutions were prepared in appropriate solvents and at concentrations below the limits of solubility. Solutions were briefly sonicated after their preparation and before further use. Short term storage (e.g. overnight) was at approximately 5 °C whereas prolonged storage was at -20 °C.
The soil-solution system was treated by applying specific aliquots of application solution A or B to the surface of the supernatant for targeting rates in the range of 0.05 to 5 ug/tube. Actual amounts applied were determined by LC-MS in the controls solutions. Application details and applied amounts are given below:

Table A 7: Application of the test item

Test	Application solution[a]	Application aliquot (µL)	Target rate (µg/tube)	Actual rate determined in application controls (µg/tube)
Screening	A	200	5	4.45
Advanced	A	20	0.5	0.41
		60	1.5	1.23
	B	100	5	4.61
		300	15	14.51
		1000	50	48.38

a Application solution A: prepared by dissolving 2.6 mg test item in 1.25 mL acetone and adding 0.01 M $CaCl_2$ to a final volume of 100 mL 12.5% acetone in 0.01M $CaCl_2$, resulting in a concentration of 25 µg/mL, corrected for purity of 96.1%.
Application solution B: prepared by dissolving 2.6 mg test item in 1.25 mL acetone and 2.5% acetone in 0.01M $CaCl_2$ to a final volume of 50 mL, resulting in a concentration of 50 µg/mL.

Diluted solutions were prepared of all experimental samples prior to LC-MS analysis. Samples were diluted with water/acetonitrile/formic acid (84/16/0.1; v/v). Samples from Screening Tests were diluted 5-fold whereas samples from the Advanced Test were diluted 2-fold (1.0 and 1.5µg/tube), 5-fold (5.0 µg/tube), 10-fold (15 µg/tube) or 20-fold (50 µg/tube).

Preliminary tests

Test item stability, applied amounts and adsorption to the surface of test vessels were investigated by determining the recovery of the test item from 0.01 M CaCl2 solutions contained in glass and Teflon tubes (without soil).

Background signals were assessed in blank tubes (without test item) to ensure that the test system was free of contamination.

A soil-solution ratio of 5/25 g/mL was shown to be adequate for studying the sorption behavior of the test item.

Screening tests

pH Measurements

The pH of the aqueous phase was measured before and after contact with the soils, in the latter case after 24 hours agitation at the soil-solution ratio 5/25 g/mL.

Adsorption Kinetics and Coefficients

Adsorption kinetics were determined for the soil-solution ratio 5/25 g/mL (soils I-III), an initial test item concentration of 0.18 mg/L and adsorption intervals of 2, 5, 24 and 48 hours.
Adsorption coefficients K_d and K_{oc} were calculated based on test item distribution between soil and supernatant at the adsorption equilibrium. The time point for the equilibrium was defined by the interval at which the adsorption reached a plateau.

Material Balance

The material balance at the adsorption equilibrium was determined for the soil-solution ratio 5/25 g/mL (soils I-III) and an initial test item concentration of 0.18 mg/L.
The balance was composed of the amount of test item in supernatant and extract. The pore water and its test item content were included with the extract. The soil was extracted three times with acetonitrile/water (4/1; v/v). The extracts for each soil were pooled for LC-MS analysis.

Desorption Kinetics and Coefficients

Desorption kinetics were determined for the soil-solution ratio 5/25 g/mL (soils I-III), an initial test item concentration of 0.18 mg/L and desorption intervals of 2, 5 and 24 hours, following 24 hours of adsorption.
After the adsorption phase, the tubes were centrifuged, the supernatant removed and replaced with the same volume of 0.01 M $CaCl_2$. The tubes were then agitated for the desorption intervals. The pore water from the adsorption phase (incl. test item content) was determined gravimetrically and deducted from the desorption supernatant.
Desorption coefficients $K_{des,F}$ and $K_{des,\ FOC}$ were calculated based on test item distribution between soil and supernatant at the desorption equilibrium. The time point for the equilibrium was defined by the interval at which desorption reached a plateau.

Advanced test

The Freundlich adsorption/desorption isotherms were determined to assess the effect of test item concentration on sorption. The tests were performed at the soil-solution ratio 5/25 g/mL (soils I-III) five test item concentrations in the range of 0.02 to 2 mg/L and 24 hours of adsorption followed by 24 hours of desorption.

3. Analytics

All samples were analyzed by LC-MS. Potential matrix effects were determined by comparing the LC-MS signal of the analyte in spiked experimental samples with the signal emitted by the analyte in control solutions (0.01 M $CaCl_2$).
HPLC conditions: column: Inertsil ODS-3 (GL Sciences); 2.1 mm x 33 mm; particle size 3 µm; eluent A: water/ methanol/ formic acid (95:5:0.1 v/v/v) 5mM ammonium formate; eluent B: water/ methanol/ formic acid (5:95:0.1 v/v/v) 5mM ammonium formate; gradient: 0 min 50% A/50% B, 1.5 min 0% A/100% B, 2.0 min 0% A/100% B, 2.1 min 100% A/0% B, 2.4 min 100% A/0% B, 2.5-4.0 min 50% A/50% B; flow rate 300 µL/min; injection volume: 5 µL; retention time of the test item: 1.5 min (typical value)

MS conditions: Mass spectrometer API4000; ionisation mode: ESI; gases: nebulizer and heater gas: air, curtain and collision gas: nitrogen; ion source: heater gas temperature: 550 °C, spray voltage: 5500 V; scan mode: multiple reaction monitoring; ion polarity: positive $[M+H]^+$; precursor ion: m/z 278.0; product ion: m/z 258.1; collision energy: 32 eV; dwell time: 300 ms.
The LOQ of the analyte was derived from the lowest calibration point (0.5 ng/mL). The LOQ values were found to be 2.5 µg/L (= 1.25% of applied) for the analyte in the $CaCl_2$ solution and in the soil extract.

II. RESULTS AND DISCUSSION

A. PRELIMINARY TESTS

The test item was fully recoverable from the aqueous phase (soil-free controls) in glass (mean recovery 99.2%) and Teflon vessels (mean recovery 99.4%). Furthermore, the blanks (soil solution samples without test item) were free of analyte, confirming that the test system was uncontaminated. The soil-solution ratio 5/25 g/mL was found to be suitable for investigating the sorption behavior of R42819.

B. SCREENING TESTS

pH in the aqueous phase

The pH in the aqueous phase without soil was 6.9. After 24 hours agitation at the soil-solution ratio 5/25 g/mL the pH was 5.83-7.3 for soils I-III.

Adsorption Kinetics and Coefficients

Adsorption kinetics were determined for the soil-solution ratio 5/25 g/mL (soils I-III), an initial test item concentration of 0.18 mg/L and adsorption intervals of 2, 5, 24 and 48 hours. Adsorption to soils I-III reached 33.9-62.8% of the applied amount at the adsorption equilibrium, after 24 hours of adsorption. Corresponding K_d values were 2.6-8.6 mL/g and the K_{oc} values were 206-481 mL/g.

Table A 8: Screening Test: Distribution of Metabolite R42819 and Adsorption Coefficients

Soil	USDA soil type	Soil-solution ratio (g/mL)	Mean adsorption after 24hours (%)	Mean m(ads)s (µg)	Mean m(ads)aq (µg)	Mean $K_{d,ads}$ (mL/g)	Mean K_d ratio (mL/g)	Mean K_{oc} (mL/g)
Soil I Mechtildshausen	Loam	5:25	53.0	2.36	2.09	5.73	1.13	481
Soil II Speyer 2.2	Loamy sand	5:25	62.8	2.80	1.65	8.56	1.69	444
Soil III Fraunhofer 02-A	Silt loam	5:25	33.9	1.51	2.94	2.62	0.51	206

Mean: Mean of duplicate sampling
m(ads)s: Mass of the test item adsorbed on the soil at adsorption equilibrium
m(ads)aq: Mass of the test item in the aqueous solution at the adsorption equilibrium
K_d: Adsorption coefficient
K_{oc}: Adsorption coefficient normalised to the organic carbon content of the soil

Material Balance

The total amount of test item recovered from the test system (supernatant and soil extract) amounted to 104-109% of the applied amount. These values were slightly excessive but within the acceptable range (< 110%).

Desorption Kinetics and Coefficients

Desorption kinetics were determined for the soil-solution ratio 5/25 g/mL (soils I-III), an initial test item concentration of 0.18 mg/L and desorption intervals of 2, 5 and 24 hours, following 24 hours of adsorption. Desorption from soils I-III reached 28-50.5% of the adsorbed amounts. The corresponding K_{des} values were 5.0-13.3 mL/g and the K_{oc} values were 392-675 mL/g.

Table A 9: Screening Test: Distribution of Metabolite R42819 and Desorption Coefficients

Soil	USDA soil type	Soil-solution ratio (g/mL)	Mean desorption after 24hours (%)	Mean m(des)s (µg)	Mean m(des)aq (µg)	Mean K_{des} (mL/g)	Mean $K_{oc,des}$ (mL/g)
Soil I Mechtildshausen	Loam	5:25	42.8	1.23	0.92	6.79	571
Soil II Speyer 2.2	Loamy sand	5:25	28.0	2.14	0.83	13.03	675
Soil III Fraunhofer 02-A	Silt loam	5:25	50.5	0.95	0.97	4.98	392

Mean: Mean of duplicate sampling
m(des)s: Mass of the test item remaining adsorbed at desorption equilibrium
m(des)aq: Mass of the test item in the aqueous solution at the desorption equilibrium
K_d: Desorption coefficient
K_{oc}: Desorption coefficient normalised to the organic carbon content of the soil

C. ADVANCED TEST

Adsorption Isotherms

The Freundlich adsorption isotherms were based on five test item concentrations in the range of 0.02 to 2 mg/L and the soil-solution ratio 5/25 g/mL (soils I-III).
The Freundlich adsorption parameters K_F, K_{FOC} and 1/n were given below:

Table A 10: Freundlich adsorption parameters

Parameter	Soil I (Sandy loam)	Soil II (Silt loam)	Soil III (Sandy clay loam)
Log (K_F)	0.258	0.645	0.196
K_F	1.812	4.418	1.569
K_{FOC}	152	229	124
K_{Fom}	88	133	72
1/n	0.77	0.83	0.78
r^2	0.9974	0.9997	0.9961

K_F Freundlich adsorption constant
K_{FOC} Freundlich adsorption constant related to soil organic carbon content
K_{FOM} Freundlich adsorption constant related to soil organic matter content
1/n Freundlich exponent
r^2 Coefficient of determination

The Freundlich adsorption coefficients K_F were in the range of 1.569-4.418 for soils I-III The corresponding K_{FOC} coefficients were 124-229. The 1/n values were 0.77-0.83, indicating nonlinear adsorption behaviour in soils I-III.
A certain degree of correlation was noticed between the adsorption coefficients K_F and the organic carbon content (r^2 = 0.97), clay content (r^2 = 0.95) and soil pH (r^2 = 0.98). Since the correlation is based only on three soils, it may not predict sorption behavior in a larger array of soils.

Desorption Isotherms

The Freundlich desorption isotherms were determined for five test item concentrations in the range of 0.02 to 2 mg/L and the soil-solution ratio 5/25 g/mL (soils I-III) after 24 hours desorption following 24 hours adsorption.
Desorption in soils I and III at the highest application rate of the advanced test was excluded from the calculation of the Freundlich desoprtion parameters. The reason was the near complete desorption, leading to high system variability.

The Freundlich adsorption parameters K_F, K_{FOC} and 1/n are given below:

Table A 11: Freundlich desorption parameters

Parameter	Soil I (Sandy loam)	Soil II (Silt loam)	Soil III (Sandy clay loam)
Log ($K_{des,F}$)	-0.025	0.564	-0.207
$K_{des,F}$	0.943	3.663	0.620
$K_{des,FOC}$	79.284	189.791	48.848
$K_{des,Fom}$	45.988	110.087	28.334
1/n	0.644	0.774	0.635
r^2	0.994	1.000	0.989

$K_{des,F}$ Freundlich desorption constant
$K_{des,FOC}$ Freundlich desorption constant related to soil organic carbon content
$K_{des,FOM}$ Freundlich desorption constant related to soil organic matter content
1/n Freundlich exponent
r^2 Coefficient of determination

The Freundlich desorption coefficients $K_{des,F}$ were in the range of 0.620-3.663 for soils I-III. The low $K_{des,F}$ indicate the reversibility of the adsorption. The 1/n values were 0.635 to 0.774 for soils I-III.

III. CONCLUSION

The sorption behaviour of metabolite R42819 was investigated by studying its distribution between soil and an aqueous phase according to the batch equilibrium method described in OECD Guideline No. 106. Three agriculture soils were used in the study. The soils represented a range of properties important for adsorption, i.e. organic carbon content, clay content, texture and the pH value.
The Freundlich adsorption/desorption isotherms were determined for three test item concentrations in the range of 0.02 to 0.2 mg/L at the soil-solution ratio 5/25 g/mL (soils I-III).
The Freundlich adsorption coefficients K_F were in the range of 1.569 – 4.418 for soils I-III The corresponding K_{FOC} coefficients were 124-229. The 1/n values were 0.77 – 0.83, indicating nonlinear adsorption behavior in soils I-III.
The Freundlich desorption coefficients $K_{des,F}$ were in the range of 0.620 – 3.663 for soils I-III. The low $K_{des,F}$ indicate the reversibility of the adsorption. The 1/n values were 0.635 to 0.774 for soils I-III.
A certain degree of correlation was noticed between the adsorption coefficients K_F and the organic carbon content (r^2 = 0.97), clay content (r^2 = 0.95) and soil pH (r^2 = 0.98). Since the correlation is based only on three soils, it may not predict sorption behavior in a larger array of soils.