Bayer CropScience

Document Title

Summary of the fate and behaviour in the environment

Flurtamone + Diflufenican SC 350

Data Requirements

EU Regulation 1107/2009 & EU Regulation 284/2013

Document MCP

Section 9: Fate and behaviour in the environment

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

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Version history

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

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CP Section 9 - Fate and behaviour in the environment

Introduction

Flurtamone is a herbicide which was included into Annex I of Directive 91/414 /EEC on 25th September 2003 by Commission Directive 2003/84/EC for entry into force on 1st Jan 2004.

The representative formulation for the renewal of flurtamone within the EU is 'Flurtamone + Diflufenican SC 350' and contains two herbicidal compounds that act by blocking carotenoid synthesis by inhibition of phytoene desaturase. This dossier contains a summary of studies that were either submitted and reviewed during the inclusion in Annex I process (thus are included in the baseline dossier) or were not previously submitted or are new studies. New or not previously submitted studies have an individual study summary in MCA section 7. This section 9 contains all the exposure calculations and study summaries of the exposure modelling studies for Predicted Environmental Concentrations in Soil, Surface water and Ground water. These values are then used for risk assessments in Chapter 10.

Furtamone + Diflufenican SC 350 is a suspension concentrate (SC) formulation that is used on cereals against broad-leaved weeds. It is applied either pre-emergence (BBCH 00-09) or post-emergence (BBCH10-29) in a single application. It is applied at 0.5 L/ha, giving application rates of 125 g/ha for flurtamone and 50 g/ha for diflufenican. It is not a slow-release formulation and so the fate of both flurtamone and diflufenican can be assumed to be the same as that reported for the active substances. The impact of formulation additives on long-term processes such as degradation and distribution is negligible.

Table 9-1 Intended application pattern

Crop	Timing of Application	Number of applications	Maximum Label Rate	Maximum application rate, individual treatment [g a.s./ha]	
	BBCH		[L/ha]	FLT	DFF
Winter and spring cereals	00 - 29	1	0.5	125	50

It is proposed that the relevant residue in the environment (soil, groundwater, surface water and air) be defined as the parent substances, flurtamone and diflufenican. All relevant data concerning the fate and behaviour of the compounds in the environment, except PEC_{Soil}, PEC_{GW}, PEC_{SW} and PEC_{Sed} are summarized within the respective dossiers under MCA Section 7. The key endpoints for soil, water and air are summarized here.

Flurtamone is a compound that was originally developed by the Chevron Chemical Company. It was purchased by Rhône-Poulenc Agriculture, which later merged with a division of Schering Agrochemicals to form Aventis CropScience. Aventis CropScience was purchased by Bayer to form part of Bayer CropScience, the current owner of flurtamone. As a result of this sequence, flurtamone and many of its metabolites have a number of different codes associated with them.

The original code number for flurtamone was RE 40885 and for its metabolites the codes were also RE followed by a five-digit number. In some reports there is a hyphen between the RE and the digits (eg RE-40885). When the molecule was owned by Rhône-Poulenc the compounds were given new (RPA) codes. In addition, metabolites not previously identified were detected and these were given RPA codes. When Aventis CropScience was formed the compounds were given another set (AE) of

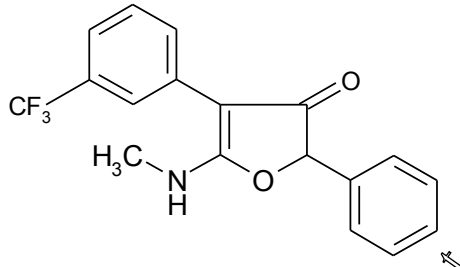
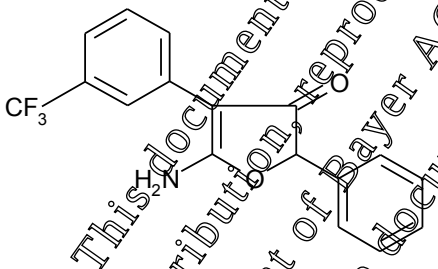
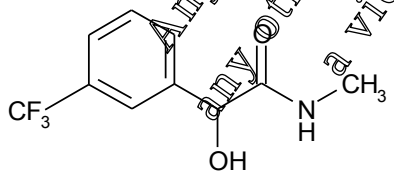
codes. The AE codes continued to be used by Bayer CropScience except where studies conducted since the molecules' acquisition have resulted in additional metabolites (for which there was no AE code existing). More recently Bayer CropScience codes (BCS) have also been used. The key codes and standardized names for for flurtamone and its environmental degradates/metabolites are summarized in the table below.

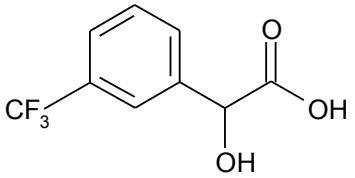
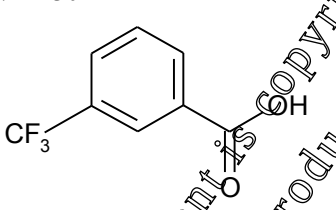
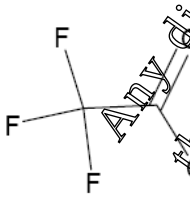
Summary of fate and behaviour in the environment

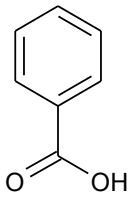
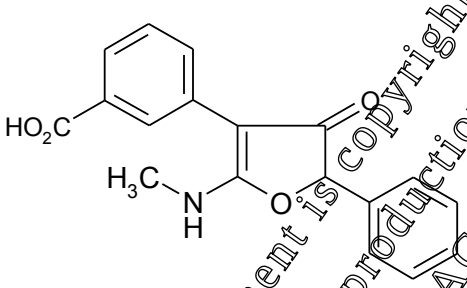
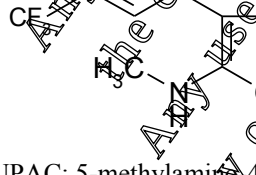
Flurtamone is extensively and quickly mineralized and the pathway in soil is fairly simple. As a result there are only two major aerobic soil metabolites and one major soil photolysis degradate with three minor ones having been detected (and these are so short-lived that they do not reach trigger concentrations). In aqueous photolysis there is only a single degradate that can be classified as major. In water-sediment systems the degradation/dissipation is again rapid with significant mineralization and only one intermediate metabolite is detected at concentrations that define it as major. Some of the soil metabolites are seen as minor metabolites in water-sediment studies. As a consequence there are only eight environmental metabolites/degradates (of which only five are major) listed in the table overleaf.

In the following summaries the metabolite number and name is used in the text except for the parent compound for which the name alone is used. Where appropriate the abbreviated names for the metabolites trifluoromethylbenzoic acid (M04 TFMBA) and trifluoroacetate (M05 TFA) are used.

Table 9-2 **Flurtamone and its metabolites (including Aventis and/or BCS [a], Chevron [b] and Rhone-Poulenc [c] codes)**

No.	Name, Structure IUPAC name CAS name, CAS number (if known)	Molecular formula molar mass Other names / codes	Occurrence Major/Minor Compartment(s)
AS	FLURTAMONE  Name IUPAC: 5-Methylamino-2-phenyl-4-(3-trifluoromethylphenyl)-3(2H)-furanone Name CAS: 3(2H)-Furanone, 5-(methylamino)-2-phenyl-4-[3-(trifluoromethyl)phenyl]-, (±)- CAS No.: 96525-23-4	$C_{18}H_{14}F_3NO_2$ 333.3 g mol^{-1} [a] AE B107587 [a] BCS-AD26195 [b] RE 40885 [c] RPA 590513 (also 201948 and 304563) Report name: flurtamone	Active substance
M01	SM1/PM5/AM8  Name IUPAC: 5-amino-2-phenyl-4-(3-trifluoromethylphenyl)-3(2H)-furanone Name CAS: 3(2H)-Furanone, 5-amino-2-phenyl-4-[3-(trifluoromethyl)phenyl]-, (±)- CAS No.: 96525-22-3	$C_{17}H_{12}F_3NO_2$ 319.3 g mol^{-1} [a] AE B107584 [a] BCS-AC85393 [b] RE 39748 [c] RPA 202450 aka desmethyl flurtamone Report name: flurtamone-desmethyl	Minor in soil (Aerobic soil – 'trace') Cereals, Sunflower Rat, Hen
M02	SM2/PM8/AM23  Name IUPAC: 2-Hydroxy-N-methyl-2-(3-trifluoromethylphenyl)acetamide Name CAS: Benzeneacetamide, a-hydroxy-N-methyl-3-(trifluoromethyl)-CAS No.: 143236-54-8	$C_{10}H_{10}F_3NO_2$ 233.2 g mol^{-1} [a] AE 0540067 [a] BCS-AX71147 [b] RE 53285 [c] RPA 591119 aka N-methyl-3-trifluoro methyl mandelamide Report name:flurtamone-trifluoromethyl-N-methyl-mandelamide	Minor in soil/aquatic Aerobic soil – max. 4% Soil photolysis – max. 1.4% Water / sediment total – max. 3.5% Cereals, Sunflower Rat, Goat

No.	Name, Structure IUPAC name CAS name, CAS number (if known)	Molecular formula molar mass Other names / codes	Occurrence Major/Minor Compartment(s)
M03	SM3/PM10/AM27  Name IUPAC: 2-hydroxy-2-(3-trifluoromethylphenyl)acetic acid Name CAS: Benzeneacetic acid, a-hydroxy-3-(trifluoromethyl)- CAS No.: 349-10-0	$C_9H_7F_3O_3$ 220.2 g mol^{-1} [a] AE 0592368 [a] BCS-AX85463 [b] RE 54588 [c] RPA 406510 aka 3-trifluoromethyl mandelic acid Report name: flurtamone-trifluoromethyl-mandelic acid	Minor in soil : Soil photolysis – max. 0.2% irradiated, 0.3% in dark controls Cereals, Sunflower Rat, Hen, Goat
M04	SM4/PM11/AM30  Name IUPAC: 3-Trifluoromethylbenzoic acid Name CAS: Benzoic acid, 3-(trifluoromethyl)- CAS No.: 454-92-2 Sodium salt: Name IUPAC: sodium 3-(trifluoromethyl)benzoate CAS No.: 69226-41-1	$C_8H_5F_3O_2$ 190.1 g mol^{-1} [a] AE C518919 [a] BCS-AA22670 [a] BCS-CX97256 (sodium salt) [b] RE 54488 [c] RPA 025905 Common abbreviation: TFMBA Report name: TFMBA	**Major in soil** **Aerobic soil – max. 24.7%** Soil photolysis – max. 3.8% Water/sediment total – max. 4.1% Cereals, Sunflower Rat, Hen, Goat
M05	SM5/PM12/  Name IUPAC: Trifluoroacetic acid Sodium trifluoroacetate Name CAS: Trifluoroacetic acid Sodium trifluoroacetate CAS No.: 76-05-1 (acid) 2923-18-4 (sodium salt)	$C_2HF_3O_2$ 114.0 g mol^{-1} [a] AE C502988 (acid) [a] BCS-AL85845 (acid) [b] none given [c] RPA 017503 (acid) [a] AE1046319 (sodium salt) [a] BCS-AZ56567 (sodium salt) Common abbreviation: TFA (or TFAA) Report name: Trifluoroacetic acid or trifluoroacetate	**Major in soil** **Aerobic soil – max. 9.8%** **Confined rotational crops**

No.	Name, Structure IUPAC name CAS name, CAS number (if known)	Molecular formula molar mass Other names / codes	Occurrence Major/Minor Compartment(s)
M06	SM6  Name IUPAC: Benzoic acid Name CAS: Benzoic acid CAS No.: 65-85-0	$C_7H_6O_2$ 122.1 g mol^{-1} [a] BCS-AG74706 [b] none given [c] RPA435491 Report name: Benzoic acid	**Major in soil:** **Soil photolysis – max 7.2%**
M07	AQM1  Name IUPAC: 3-(2-Methylamino-4-oxo-5-phenyl-4,5-dihydrofuran-3-yl)benzoic acid Name CAS: Benzoic acid, 3-(4,5-dihydro-2-(methylamino)-4-oxo-5-phenyl-3-furanyl]- CAS No.: 148681-60-1	$C_{18}H_{15}NO_4$ 309.3 g mol^{-1} [a] AE 1083976 [a] BCS-BA29451 [b] none given [c] RPA 203507 Report name: flurtamone-carboxylic acid	**Major in Aqueous photolysis – max. 33.5%**
M08	AQM2  Name IUPAC: 5-methylamino-4-(3-trifluoromethylphenyl)-3(2H)-furanone Name CAS: 3(2H)-Furanone, 5-(methylamino)-4-[3-(trifluoromethyl)phenyl]- CAS No.: 96525-53-0	$C_{12}H_{10}F_3NO_2$ 257.2 g mol^{-1} [a] AE 2093305 [a] BCS-BT61400 [b] none given [c] RPA 591120 Report name: flurtamone-desphenyl	**Major in Aquatic** Water – max. 7.8% Sediment – max.3.6% **Total max. 10.7%**

CP 9.1 - Fate and behaviour in soil

Aerobic Degradation. The original aerobic degradation study in soil ([redacted] and [redacted], 1993, M-158234-01-1 and [redacted], [redacted] and [redacted] 1994, M-158348-01-1) demonstrated that flurtamone is degraded via biological processes, with 24 to 40 % mineralization after 100 days and 32 % non-extractable residues. Two metabolites were observed: M04 TFMBA (3-trifluoromethyl-benzoic acid, AE C518919) which was detected as a major metabolite at 8.3 to 10.8 % and M05 TFA (trifluoracetate, BCS-AZ56567) which was observed at a maximum of 9.8%. This study used only two agricultural soils, compound labelled in only one ring and an invalid experimental study design. New studies to remedy these deficiencies have been conducted and are fully summarized in MCA Section 7 (along with a pilot study not previously available). The results from the new studies are summarized below.

In a non-guideline non-GLP pilot study ([redacted] 1991, M-249325-02-1) the route of degradation of flurtamone was investigated in a US sandy loam soil. The soil was incubated in the dark, at a moisture content equivalent to 75% of field capacity (⅓ bar) under aerobic conditions at 25 °C, after treatment with radiolabelled flurtamone. Experiments were separately performed with compound uniformly labelled in either the phenyl or trifluoromethyl phenyl rings or labelled at the 5-position of the furanone ring. Treatment rates were equivalent to the very high rates of between 6 and 7.5 kg/ha. Single samples were taken after 0, 15, 28 and 42 days of incubation.

Flurtamone was extensively degraded with up to 22% of the radioactivity detected as $^{14}CO_2$, indicating the potential for rapid mineralization of the phenyl and furanone rings of flurtamone. Mineralization of the trifluoromethylphenyl ring was somewhat slower with 6% detected as $^{14}CO_2$ after 42 days. Two metabolites were observed: M04 TFMBAwhich was detected as a major metabolite in excess of 20% and M02 3-trifluoromethyl-N-methyl-mandelamide (AE 0540067) which was observed at a maximum of 4%.

GLP-compliant studies conducted to current guidelines were performed with both phenyl and trifluoromethyl phenyl ring-labelled compound in the same soils at a similar time in the same facility. ([redacted] and [redacted], 2012a M-442030-01-1 and 2012b M-440226-01-1). Each study used four European soils at 55% of the maximum water holding capacity and incubated at 20°C. In each case the compound was applied at a rate equivalent to 375 g/ha.

The study with trifluoromethyl-phenyl-ring-labelled compound showed that, besides the test item, two major transformation products were detected in the extracts. M04 TFMBA accounted for up to 12.1, 15.5, 4.8 and 24.7% of AR and the amounts of M05 TFA reached up to 4.6, 5.5, 4.9 and 4.9% of AR at the end of the study in soils. Furthermore, three minor degradation products reaching up to 3.1% of AR were characterized according to their separation distances in TLC. The sum of the non-characterized minor transformation products did not exceed 2.5% of AR.

The amount of formed $^{14}CO_2$ increased steadily during the entire study period. At the end of the study, 87 days after application, between 51.1 and 55.1% of AR was quantified as carbon dioxide. No significant amounts of volatile organic compounds were detected. At the end of the incubation period the recovered radioactivity in the extracts had decreased to 11.7 - 13.1% of AR. Non-extractable ^{14}C-residues increased from 0.8, 1.3, 1.1 and 1.2% of AR at DAT-0 to maximum amounts of 36.0, 34.8, 41.8 and 36.6% of AR at DAT-36 or DAT-59 and declined already slightly to 33.6, 32.9, 37.2 and 33.9% of AR at DAT-87.

The study with unsubstituted phenyl ring-labelled compound showed that, besides the test item, four minor degradation products were detected in the extracts and characterized according to their retention times in HPLC. The maximum amount of a single transformation product was 2.0% of AR. In addition, several very minor metabolites were detected. Their sum did not exceed 4% of AR.

The amount of formed $^{14}CO_2$ increased steadily during the entire study period. At the end of the study, 59 days after application, between 57.4 and 64.0% of AR was quantified as carbon dioxide. No significant amounts of volatile organic compounds were detected in the polyurethane foam of the trap attachments. At the end of the incubation period the recovered radioactivity in the extracts had decreased to 4.9 - 7.1% of AR. Non-extractable ^{14}C-residues increased from 0.7, 1.1, 0.9 and 0.8% of AR at DAT-0 to maximum amounts of 33.6, 32.2, 37.5 and 38.4% of AR at DAT-35 and had declined to 31.0, 31.8, 33.4 and 34.9% of AR by the end of the study at DAT-59.

These studies confirmed that flurtamone is rapidly degraded with a high level of mineralization and the formation of just two significant metabolites (M04 TFMBA and M05 TFA).

Anaerobic Degradation. The anaerobic study ([redacted] and [redacted] C M, 1999, M-183875-01-1) originally submitted, was conducted to the old EU guideline, in which treatment was made to an already anaerobic system. No significant degradation of flurtamone was observed. A new study, designed to meet current guidelines was conducted and is fully summarized in MCA Section 7, along with a pilot study not previously available.

In a non-guideline non-GLP pilot study ([redacted] 1991, M-249275-02-1) the route of degradation of [^{14}C]-flurtamone, uniformly labelled in the trifluoromethylphenyl ring was investigated under anaerobic conditions in a US sandy loam soil (USDA classification). The application rate was not stated. Treated soil samples were incubated in the dark under aerobic conditions for 30 days, at a moisture content equivalent to 75% of field capacity (⅓ bar) at 25 ºC. After 30 days air was displaced from the sealed flasks by the introduction of nitrogen. All flasks were incubated in the dark at 25 °C and anaerobic conditions were maintained by connection of each flask to a low pressure nitrogen supply. The flasks were incubated under anaerobic conditions for a further 42 days (92 days in total).

The soil samples were extracted. The extracts were concentrated and examined by HPLC. Only parent and M04 TFMBA were detected and it was concluded that no unique metabolites were formed under anaerobic conditions.

In a new modern GLP-compliant guideline study ([redacted] and [redacted] 2012a, M-440634-01-1), the route and rate of degradation of the herbicide flurtamone was investigated in one European soil under flooded anaerobic conditions following an aerobic incubation phase. Flurtamone was applied to soil at a nominal rate of 100 µg/100 g soil (dry matter). Assuming a homogeneous distribution in 2.5 cm topsoil layer, this rate was equivalent to 375 g/ha Duplicate test systems were analyzed after 0 and 14 days of aerobic incubation. Further samples were taken directly after water logging (day 14) and 17, 21, 29, 35, 48, 77, 104 and 134 days after treatment , corresponding to 0, 3, 7, 15, 21, 34, 63, 90 and 120 days after soil flooding . Soil and water layers were separated by decanting to allow for separate analysis of the phases with the water being analyzed directly.

Within the aerobic phase of the study, the amount of the test item flurtamone in the entire test systems decreased rapidly from 93.9% to 25.4% of the AR (mean values). During the following anaerobic incubation period (i.e. flooded state) a slight decrease was observed. At the end of the study flurtamone accounted for 23.4% of the AR. The amounts of the transformation product M04 TFMBA in the entire system increased from 0.7% of the AR at DAT-0 to 23.2% of the AR during the aerobic incubation period and further to 32.3% of the AR towards study termination (mean values). The amounts of M04 TFA increased up to 1.6% of AR during the aerobic incubation period and remained at this low level during the anaerobic incubation period until study termination.

The total unidentified radioactivity in the entire systems reached values not higher than 6.1% of the AR. Maximum levels of individual unidentified minor transformation products in the entire system were not higher than 3.4% of the AR.

In the aerobic incubation phase, non-extractable radioactivity (NER) in soil increased from 13 to 25.1% of the AR (mean values). NER then varied between 23.4 and 26.5% of the AR until the end of the anaerobic (flooded) incubation period (mean values). During the aerobic phase, the maximum amount of $^{14}CO_2$ was 11.2% of the AR. Formation of other volatile radioactivity was insignificant (< 0.1% of the AR) in the aerobic and anaerobic incubation phase.

In soil under anaerobic conditions flurtamone is essentially stable. Its main aerobic soil metabolites M04 TFMBA and M05 TFA are also stable under the same conditions. As a result no new metabolites (i.e. additional to those identified in aerobic soil studies) are formed.

Soil Photolysis. In the original soil photolysis study ([redacted] and [redacted] 1993, M-162193-01-1) the degradation rate of flurtamone was slightly enhanced in the presence of light. M04 TFMBA and M05 TFA, known soil metabolites, were detected in minor quantities at maximum occurrence of 3.8% and 1.4%, respectively. No unique photodegradation products were detected. This study was conducted with compound labelled in one ring only so a new study ([redacted] N. & [redacted]. 2012c, M-443626-01-1) was carried out with the label in a different ring. This is fully summarized in MCA Section 7 and the results are presented below.

The phototransformation of [phenyl-UL-^{14}C]-flurtamone was studied on a European silt loam soil at 20±1°C and a soil moisture of about 55% of the maximum water holding capacity. Flurtamone was applied at a nominal rate corresponding to the maximum single field use rate. The soil samples were continuously exposed to artificial irradiation (xenon lamp with < 290 nm cut-off filter, 643 W m^{-2}). In addition, dark controls were set up. Samples were taken in duplicate after 0, 0.25, 1, 2, 3, 5 and 6 days of incubation.

In the irradiated test systems, the amount of flurtamone decreased from an average of 100.2% AR at DAT-0 to 38.6% AR towards the end of the study (DAT-6). One major (< 5% AR at consecutive time-points) transformation product was detected and identified as M06 benzoic acid. It reached a maximum amount of 7.2% AR at DAT-5. In addition, up to 12 minor transformation products were characterized according to their retention times. Each individual one accounted for ≤ 3.2% AR. $^{14}CO_2$ formation increased up to 17.6% AR towards the end of the study. Organic volatile formation was negligible (≤ 0.1% AR).

In the extracts of the dark test systems, flurtamone decreased from an average of 100.2% AR at DAT-0 to 86.2% AR towards the end of the incubation period (DAT-6). In addition, up to 13 minor transformation products were characterized according to their retention times. Each individual one

accounted for ≤ 1.1% AR. $^{14}CO_2$ formation increased up to 3.2% AR towards the end of the study. Organic volatile formation was negligible (≤ 0.1% AR).

Phototransformation on soil can contribute to the degradation of flurtamone under outdoor conditions. Besides carbon dioxide, benzoic acid was found as a major product in the irradiated samples but not in the dark controls where it was rapidly degraded. Benzoic acid is discussed in a position paper that is summarized below.

Report:	**KCP-9.1 /01; [redacted] P. 2013**
Title:	An Assessment of the Environmental Impact of the Photodegradate of Flurtamone: Benzoic Acid
Organisation:	[redacted]
Report No.:	Battelle Report VC/12/006A Bayer CropScience Document **M-453572-02-1**
Publication:	unpublished
Dates of experimental work:	Not applicable
Guidelines:	**Not relevant.**
Deviations:	Not relevant
GLP/GEP	**No**

Executive Summary

This position paper discussed the likely relevance to the environment of the generation of benzoic acid as a degradate (M06) of flurtamone in a soil photolysis study. The available data on the fate and ecotoxicology of benzoic acid was reviewed. Benzoic acid is a naturally occurring substance that is known to be readily biodegradable under both aerobic and anaerobic conditions. It is rapidly degraded in soil under aerobic and anaerobic conditions and in groundwater. When formed from flurtamone under aerobic conditions it will degrade (by mineralization). If anaerobic conditions occur after it has been formed it will still degrade by mineralization. Benzoic acid has low toxicity to vertebrates and aquatic organisms and is not therefore of ecotoxicological concern.

It was concluded that benzoic acid produced by photodegradation of flurtamone is not a compound of concern for the environment.

Material and Methods

A new study on the photolysis of flurtamone on a soil surface was conducted with the compound radiolabelled in the unsubstituted phenyl ring. Previous studies had used flurtamone that was radiolabelled in the trifluoromethylphenyl ring. In the new study benzoic acid was identified as a degradate (M06) and was found at > 5% of applied radioactivity at consecutive time-points. It was, therefore, a new significant metabolite. It is likely that it was a very minor metabolite in the aerobic soil study conducted on [phenyl-UL-^{14}C]-flurtamone and so its identification was not required in that study. In the soil photolysis study the concentration of M06 benzoic acid increased (to 7.2% AR) up to the penultimate time-point and then decreased at the final time-point (to 5.8% AR).

The available data on the presence and fate of benzoic acid in the environment and its ecoxicity were reviewed. Benzoic acid is found in the soil and occurs naturally free and bound as benzoic acid esters in many plant and animal species and so is found naturally in many foodstuffs (berries, milk, potatoes

honey and many others). It is also used as a preservative in food (and therefore some processed foods contain artificially elevated concentrations) and drink and in cosmetics.

At most environmental pHs benzoic acid (pKa 4.2) will be in the form of a benzoate. Benzoic acid is a compound that is itself listed on Annex I. The review report stated it is a substance naturally occurring in soil where it can be readily biodegraded. In addition the report shows that rapid and almost complete mineralization occurs in lake water samples and in sewage samples. Sodium benzoate is the reference substance required by the OECD aerobic mineralization in surface water guideline.

An assessment produced under the auspices of the World Health Authority also reported that standardized tests on ready or inherent biodegradation showed benzoic acid to be readily biodegraded. Easy degradation of benzoic acid was also observed in different non-standardized experiments using sewage sludge as inoculum. It was found to be degraded by adapted anaerobic sewage sludge at 86-93% after 14 days by aerobic activated sludge (adapted) at 95% after 5-20 days and by unadapted aerobic activated sludge at 61-69% after 2-3 days with a preceding lagtime of 8-20 h. The use of a synthetic sewage inoculated with laboratory bacterial cultures led to complete degradation of benzoic acid after 14 days under anaerobic conditions.

Rapid mineralization has been shown to occur in groundwater and subsurface soil samples. In groundwater, a half-life of 41 h has been found for benzoic acid under aerobic condition. Half-lives of 7.3 h and 18.2 h, respectively, have been observed for aerobic and anaerobic degradation of benzoic acid metabolized to $^{14}CO_2$ in subsurface soils.

The assessment concluded that the available data indicate that benzoic acid has only a low toxicity potential in the terrestrial environment. From its physical/chemical properties, benzoic acid emitted to water and soil is not expected to volatilize to the atmosphere or to adsorb to sediment or soil particles. From the results of numerous removal experiments, the main elimination pathway for both chemicals should be biotic mineralization.

Benzoic acid is considered of low toxicity to vertebrates and aquatic organisms. The oral and dermal toxicity in rats resulted in a LD50 > 2000 mg/kg bw and dermal toxicity in rabbits was LD50 > 5000 mg/kg bw. Acute studies on fish (*Oncorhynchus mykiss*), aquatic invertebrates (*Daphnia magna*) and algae (*Pseudokirchneriella subcapitata*) revealed NOECs of 120 mg/L for fish, 55 mg/L for *Daphnia* and 7.5 mg/L (EbC50 = 33 mg/L) for algae. A risk to these organisms can therefore be excluded.

Discussion

The photolysis of flurtamone on a soil surface produced small quantities of benzoic acid (never reaching 10% AR but reaching > 5% AR at consecutive time-points). Benzoic acid is a naturally occurring substance that is known to be readily biodegradable under both aerobic and anaerobic conditions. It is rapidly degraded in soil under aerobic and anaerobic conditions and in groundwater. When formed from flurtamone under aerobic conditions it will degrade (by mineralization). If anaerobic conditions occur after it has been formed it will still degrade by mineralization. Benzoic acid has low toxicity to vertebrates and aquatic organisms and is not therefore of ecotoxicological concern.

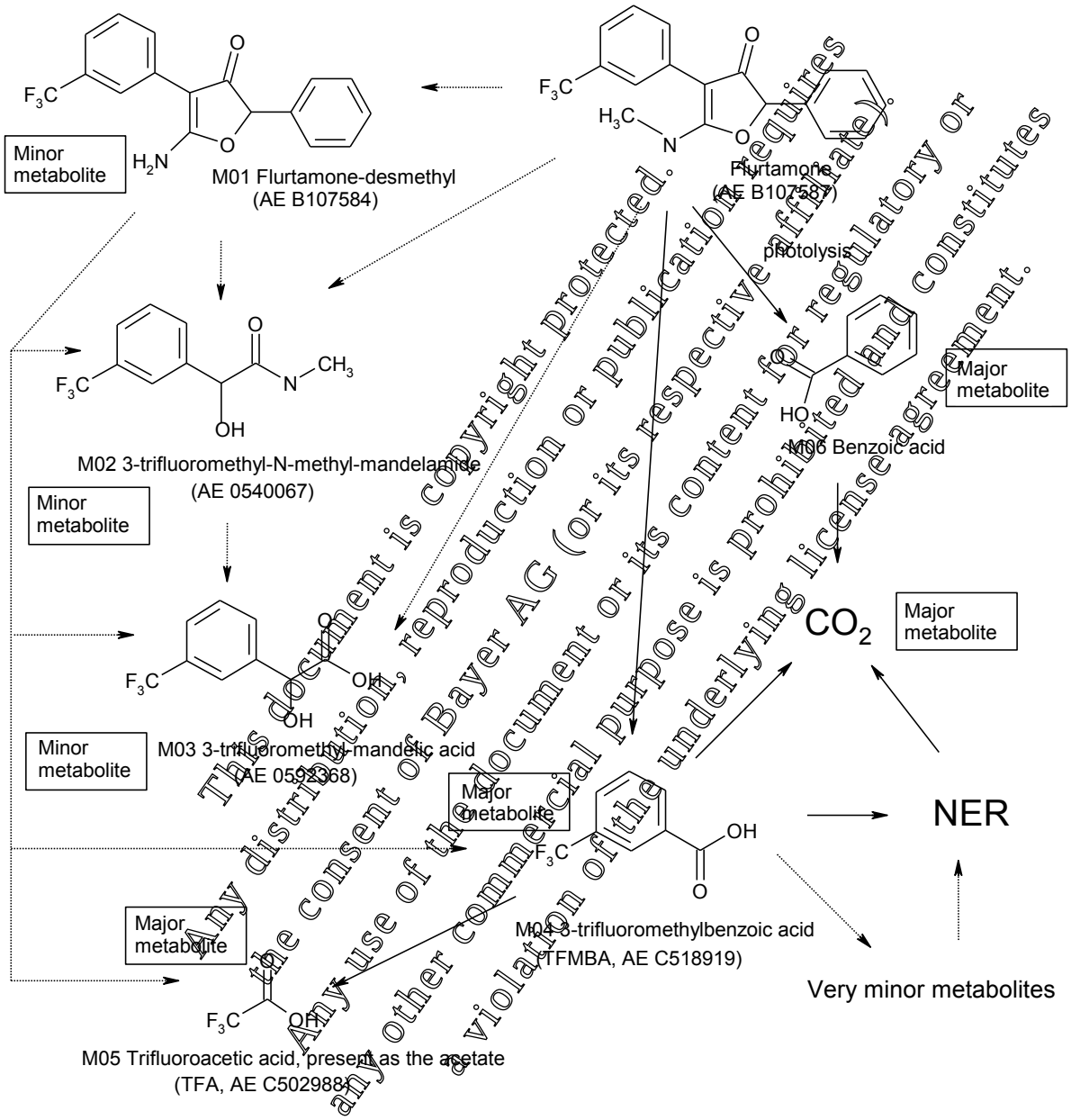
Conclusions

Benzoic acid produced by photodegradation of flurtamone is not a compound of concern for the environment.

Summary of route of degradation of in soil

A metabolic pathway for the degradation of flurtamone in soil is shown below.

Figure 9.1-1 Proposed metabolic pathway of flurtamone in soil



CP 9.1.1 - Rate of degradation in soil

CP 9.1.1.1 - Laboratory studies

Aerobic degradation of the active substance. The original aerobic soil study ([redacted] and [redacted], 1993, M-158234-01-1 and [redacted], [redacted] and [redacted] 1994, M-158348-01-1) conducted to EPA guidelines used two agricultural soils and an artificial soil. The agricultural soils gave non-normalized half-lives of 48.3 and 59.0 days for flurtamone, calculated according to current recommendations. The normalized values are 47.8 and 41.3 days. This original study had a number of unusual aspects which may have affected the rate of degradation. These are discussed in a position paper summarized in MCA Section 7 and below. With a study of dubious quality in only two agricultural soils and with compound labelled in only one ring it was necessary to conduct studies in more soils and with labels in more than one ring. These studies were commissioned and are also fully summarized in MCA Section 7, along with the pilot study, not previously available.

The position paper ([redacted] 2013, M-460121-01-1) reviewed the old flurtamone aerobic soil degradation study of Burr & Austin with addendum by Burr, Newby & Austin, (plus an interim report that was not audited that gave further details of the study). The soil samples were treated at a rate equivalent to 325 g ha^{-1} using flurtamone labelled in the trifluromethylphenyl ring. The incubations conditions were those required by US EPA, namely a moisture content of 1/3 bar moisture holding capacity and a temperature of 22°C. The duration of the study also conformed to US EPA recommendations with samples being taken for analysis at intervals up to a year (366 days).

The study used only two agricultural soils, the third soil being an artificial soil (later discontinued). The study design was experimental. Instead of individual flasks, each with its own set of traps, the soil samples were placed on petri dishes and these were stacked on aluminium stands. The stands were housed in vertical glass towers which were placed in a temperature-controlled room. Moistened air was passed into the towers and after passage through the tower it was drawn through ethylene glycol and potassium hydroxide traps. This design was quickly abandoned, deemed invalid andnever used again .

The unusual study set-up may have caused, or at least contributed to, a number of other defects in the study. There was significant variability between replicate samples and a loss of mass balance at later time-points. Some soil samples were frozen prior to analysis.

The behaviour of the artificial soil was very different from that of the agricultural soil and it was agreed that the rate of degradation was excluded from modelling. Given the major differences in the conduct of the study from a standard study (and current guidelines) and the very different results obtained in comparison to those obtained from modern, guideline studies it was concluded that, in addition to the artificial soil already excluded from risk assessment, the clay loam and sandy loam soil should be also excluded.

In a non-GLP, non-guideline pilot study ([redacted] B.V. 1991, M-249325-02-1) the rate of degradation of [^{14}C]-flurtamone was investigated in one soil under aerobic conditions at 25°C and at a rate of 8 to 10 ppm, equivalent to the very high application rate of 6 to 7.5 kg/ha. Flurtamone degraded at a rapid rate in soil with a reported DT_{50} value of 28 days (SFO kinetics).

In modern aerobic soil studies ([redacted] N. & [redacted] M. 2012a M-442039-01-1 and 2012b M-440226-01-1) the experiments with [trifluoromethylphenyl-UL-^{14}C]-flurtamone gave half-lives of

flurtamone, calculated by the best fit kinetics according to FOCUS for trigger evaluation, of 13.2, 12.8, 10.7 and 9.7 days (single first order, SFO). The experiments in which [phenyl-UL-^{14}C]-flurtamone was used gave half-lives of 10.3, 11.3, 9.4 and 8.5 days (single first order, SFO).

Aerobic degradation of metabolites, breakdown and reaction products. The results from the original soil study on the flurtamone metabolite M04 TFMBA ([redacted] C.M. 1999a, M-207971-01-1) gave laboratory DT_{50}s of 11.2 to 16.7 days (SFO, n=3, mean 13.5 days) normalised 7.3 to 10.5 days (mean 8.9 days). For M05 TFA a default value of 2 years (730 days) was assumed. In order to facilitate calculations of formation fractions new studies on M04 TFMBA were conducted at the same facility, in the same soils and at the same time as the new studies on flurtamone. Similar studies were conducted on the metabolite M05 TFA. All the new studies are fully summarized in MCA Section 7. The results are summarized below.

The degradation of [phenyl-UL-^{14}C]-3-trifluoromethylbenzoic acid (M04 TFMBA) was studied in four European soils ([redacted] N. & [redacted] T. 2012 M-443478-01-1). Due to the fast degradation and the high mineralization of the compound, the study was terminated after 28 days of incubation. M04 TFMBA was applied at a nominal rate of 25 µg/100 g soil dry weight (250 µg/kg soil dry weight) in the test systems.

Extractable ^{14}C-residues decreased from 101.6, 99.5, 100.8, and 100.5% of AR at DAT-0 to 10.5, 11.8, 10.4, and 12.3% at the study end (DAT-28). The amounts of the test item in the extracts declined from 101.5, 99.4, 100.7 and 100.3% of AR at DAT-0 to 0.9, 1.7, 0.7 and 2.4% of AR at the end of the study. Besides the test item, one major transformation product was detected in the extracts. The amounts of M05 TFA reached up to 5.5, 6.3, 6.6 and 5.7% of AR at the end of the study. Furthermore, six minor degradation products reaching up to 2.4% of AR were characterized.

The half-life of M04 TFMBA was calculated by the best fit kinetics according to FOCUS (for trigger evaluation) as 6.0, 7.4, 8.5 and 2.8 days (single first order, SFO) under aerobic conditions.

The degradation of [1-^{14}C]-trifluoroacetate (M05 TFA, the sodium salt of trifluoroacetic acid, BCS-AZ56567) was studied in four European soils ([redacted] N. 2012a M-439283-01-1). It was not degraded under laboratory conditions during an incubation time of 120 days. Significant amounts of volatiles and non-extractable residues were not formed in the course of the study. The half-life of TFA was calculated by the best fit kinetics according to FOCUS (single first order, SFO, for trigger evaluation) as >1000 days under aerobic conditions in all four tested soils.

The concentration dependent mineralization rate of [1-^{14}C] trifluoroacetate (M05 TFA, the sodium salt of trifluoroacetic acid, BCS-AZ56567), was investigated ([redacted] N. 2012b M-441101-01-1). It was examined in four different soils: a sandy loam, a clay loam, a sandy loam and a silt loam, for 120 days under aerobic conditions in the dark at 20 ± 1°C and 55 ± 5% WHC_{max} (maximum water holding capacity). No significant mineralization (≥1% of AR) could be detected in any of the samples under the used laboratory conditions during the incubation time.

Anaerobic degradation of the active substance. The anaerobic study originally submitted ([redacted] and [redacted] 1999c, M-183875-01-1) was conducted to the old EU guideline, in which treatment was made to an already anaerobic system. No significant degradation of flurtamone was observed. A new study, designed to meet current guidelines, was conducted and is fully summarized in MCA Section 7, along with a pilot study not previously available (as mentioned under 9.1). .

In the pilot study ([redacted] 1991 M-249325-02-1) flurtamone was found to be stable under anaerobic conditions. In the new study ([redacted] 2012, M-440634-01-1) flurtamone was again shown to be essentially stable.

Anaerobic degradation of metabolites, breakdown and reaction products. In an anaerobic study ([redacted] 1999 c, M-183875-01-1) conducted to the old EU guideline, in which treatment was made to an already anaerobic system, no significant degradation of flurtamone was observed. Therefore no significant metabolites were formed, the behaviour of which could be examined under anaerobic conditions. A new study, designed to meet current guidelines, was conducted and is presented below, along with a pilot study not previously available as mentioned in 91.

In the pilot study ([redacted] B.V. 1991 M-249325-02-1) it was found that the soil metabolite of flurtamone, M04 TFMBA, is stable in soil under anaerobic conditions. In the recent study ([redacted] 2012, M-440634-01-1) the main aerobic soil metabolites of flurtamone, M04 TFMBA and M05 TFA, were demonstrated to be essentially stable under anaerobic conditions.

CP 9.1.1.2 - Field studies

CP 9.1.1.2.1 - Soil dissipation studies

Although arguably not currently required, a terrestrial field soil dissipation study in Europe (Wicks 1996, M-158558-01-1) was conducted. Flurtamone and M04 TFMBA were completely degraded at all four of the test sites in Europe during the course of the field study. For flurtamone the mean DT_{50} was 58 days and the mean DT_{90} was 191 days. For total residues the mean DT_{50} was 57 days and the mean DT_{90} was 190 days. No flurtamone or M04 TFMBA could be detected after 10 months at any of the sites.

CP 9.1.1.2.2 - Soil accumulation studies

No studies are required, or offered, under this point.

Summary of rate of degradation in soil.

The geometric mean DT_{50} for flurtamone is 17.1 days (and 10.6 days if only the modern studies are considered). This value is used for PEC_{GW} and PEC_{SW} modelling.

The data from the previously submitted field study gave for flurtamone non-normalized DT_{50} values of 27.2 days to 91.6 days, with the latter (worst-case) figure being used for PEC_{Soil} calculations.

The geometric mean DT_{50} value for M04 TFMBA is 10.4 days and this value is used for PEC_{GW} and PEC_{SW} modelling. The worst-case un-normalized DT_{50} of 63 days, derived from the old parent aerobic soil study is used for PEC_{Soil} calculations. studies.

For M05 TFA no robust DT_{50} values could be derived, as was the case for the original EU approval where a value of 2 years was agreed and given in the list of endpoints. Currently the recommended default value is a DT_{50} of 1000 days (assumed to be at 20°C and pF2) and thus this has been selected as modelling endpoint.

CP 9.1.2 - Mobility in the soil

CP 9.1.2.1 - Laboratory studies

Adsorption/desorption of the active substance. In the previously submitted adsorption/desorption study ([redacted] 1990 (revised 1992), M-163688-01-1) the K_{oc} of flurtamone was 85 to 543 mL/g (n = 5, mean 329 mL/g, 1/n = 0.978). That study deviated from the current guidelines in several respects so a new study completely consistent with the guidelines was commissioned. This is fully summarized in MCA Section 7.

In a modern study conducted to current guidelines the adsorption/desorption characteristics of [trifluoromethylphenyl-UL-^{14}C]-flurtamone were studied in five soils of differing characteristics ([redacted] 2011, M-401274-02-1). The adsorption coefficients K_{Fads} of [trifluoromethylphenyl-UL-^{14}C]-flurtamone in five test soils were determined to range from 4.4692 mL/g to 10.6234 mL/g based on the Freundlich equation. The corresponding organic carbon normalised adsorption coefficients K_{FOCads} ranged from 225.1 mL/g to 287.8 mL/g (mean 257.3 mL/g). The Freundlich exponents 1/n were in the range of 0.8594 to 0.8837, indicating that the concentration of the test item affected the adsorption behaviour slightly, only. The desorption coefficients K_{FOCdes} of [trifluoromethylphenyl-UL-^{14}C]-flurtamone were found to be in the same range as the respective adsorption coefficients (236.7 mL/g - 298.5 mL/g). The mean desorption $K_{F(des)}$ and the normalized $K_{FOC(des)}$ values were 1.00 - 1.15 times higher than those obtained for adsorption phase.

Based on the soil sorption parameters measured in this study and classification of soil mobility potential according to Briggs, flurtamone can be classified as of low mobility in soil.

Adsorption/desorption of metabolites, breakdown and reaction products. In the submitted study ([redacted] 1999, M-207972-01-1) the Koc values for M04 TFMBA were 15 to 52 mL/g (n = 4, mean 32.5 mL/g, 1/n = 0.67). There were no GLP guideline studies for M05 TFA and so one was commissioned. This is presented below along with published research.

An adsorption-desorption batch-equilibrium study with fifty-four soils (topsoil and sub-soils) was performed with M05 TFA as part of a terrestrial ecosystem project, which was published in Environ. Sci. Technol. (Richey, Driscoll. and Likens 1997, M-263649-01-1). Thirty-five soil samples were obtained from 15 terrestrial sites of the National Science Foundation Long-Term Ecological Research Program. Soil samples were air-dried and passed through a 2 mm sieve prior to analysis. They were characterized. Batch equilibrium soil sorption experiments were conducted on each of the soils. A 1:5 soil/solution ratio was used for organic soil and 1:20 for mineral soils. The range of concentrations used was: 0, 2, 4, 7, 10, 20, 30 and 40 µmol sodium trifluoroacetate.

Thirty four of the soils tested showed sorption of M05 TFA. At all sites where M05 TFA was evaluated for organic and mineral soils, the organic horizon exhibited greater adsorption. Soils with high organic content were found to retain the highest concentrations of M05 TFA, adsorbing between 20 and 60% of added M05 TFA. K_{OC} values were derived from the reported Freundlich constants and the organic carbon contents (organic matter/1.724). The mean K_{OC} value for nine soils with OC <5%, considered to be most representative of agricultural soils was calculated to be 22.9 mL/g.

In a modern guideline study the adsorption/desorption characteristics of 1-^{14}C]-BCS-AZ56567 (M05 TFA sodium salt) were studied in five soils of differing characteristics (Möndel and Hein, 2011, M-406740-01-1). The adsorption phase of the study (Definitive Test) was carried out using pre-equilibrated air-dried soil with [1-^{14}C] BCS-AZ56567 at nominal concentrations of 1, 0.3, 0.1, 0.03, and 0.01 mg/L in the dark at 20 °C ± 2 °C for 24 hours. The equilibration solution used was 0.01 M aqueous $CaCl_2$ solution. The soil to solution ratio was defined for all soils as 1:1. Low to virtually no adsorption rates were determined in the preliminary testing.

As virtually no adsorption was measured it was not possible to calculate any reasonable Freundlich isotherm and therefore no data describing the Freundlich isotherm (K_F-value and 1/n) were determined.

Column leaching of the active substance. In the previously submitted column leaching studies ([redacted] 1994, M-162913-01-1) only small amounts of applied radioactivity appeared in the leachate of all but the sand soil. Most of applied radioactivity in the leachates was flurtamone, accompanied by low levels (< 1 %) of three metabolites, M02 3-trifluoro methyl-N-methyl-mandelamide (AE 0540067) M03 3-trifluoromethyl-mandelic acid (AE 0592368) and M04 TFMBA (AE C518919). No new column leaching studies have been conducted.

Column leaching of metabolites, breakdown and reaction products. The results of the aged-residue column leaching study ([redacted] 1995, M-162906-02-1) showed that the majority of applied radioactivity remained in the soil columns with only about 6% appearing in leachate. Although flurtamone remained as the major compound in the soil, there was virtually no flurtamone in the leachate. The radioactive components in the leachate were M02 3-trifluoromethyl-N-methyl-mandelamide (AE 0540067), M03 3-trifluoromethyl-mandelic acid (AE 0592368) and M04 TFMBA (AE C518919) with M04 TFMBA being the most abundant (accounting for over half of the radioactivity in the leachate). There were only traces of unidentified components in the leachate. The results of this study add weight to the notion that flurtamone will not leach significantly under real-use conditions. No new aged column leaching studies have been conducted, but a column leaching study on the metabolite M05 TFA has been conducted ([redacted] 2013, M-477737-01-1). This study showed that M05 TFA has the potential to be mobile in the soil types used in the study.

Plant uptake factor. The determination of a suitable plant uptake factor for M05 TFA, for use in modelling has recently been carried out ([redacted] B. 2013, M-468684-01-1**)**. This is summarized in MCA Section 7 and the results are presented here because the factor affects the predicted mobility of the metabolite in soil. Evidence on the occurrence of M05 TFA uptake by plants was provided by an overview of plant uptake experiments and confined rotational crop experiments. It was shown that a plant uptake factor of 0.59 is appropriate for M05 TFA when flurtamone has been applied to cereals.

CP 9.1.2.2 - Lysimeter studies

Despite the fact that in the previously submitted lysimeter study ([redacted] 1996, M-158624-01-1) the lysimeters represented particularly high risk conditions for leaching (the soil was sandier and with less silt content than defined in the guideline, and there was significant earthworm activity) parent flurtamone was hardly detectable in the leachate from the two lysimeters (average annual concentration < 0.01 µg/L). Most of the radioactivity in the leachate was identified as M05 TFA. The metabolite M04 TFMBA was also detected but at concentrations < 0.1 µg/L. Flurtamone does not present a leaching risk and M04 TFMBA, indicated by its K_{FOC} value to be more

mobile than parent compound, is unlikely to reach groundwater in significant quantities. No new lysimeter studies have been conducted.

CP 9.1.2.3 - Field leaching studies

The results from the adsorption/desorption, column leaching and lysimeter studies show that the mobility of flurtamone and its metabolites is satisfactorily understood and so studies under this point are not required.

Summary of mobility in the soil

Mobility studies show that flurtamone is not very mobile in soil. M04 TFMBA has a lower K_{FOC} but has a short half-life. M05 TFA is mobile in soil. The K_{FOC} and 1/n values used in modelling for flurtamone and its metabolites are summarized in the table below.

Table 9.1.2-1 Summary of K_{FOC} and 1/n values for flurtamone and its metabolites

Compound	K_{FOC} (mL/g)	1/n Value
Flurtamone	257.3	0.876
M04 TFMBA	32.5	0.67
M05 TFA	0	1.0

CP 9.1.3 - Estimation of concentrations in soil

Report: **KCP-9.1.3 /01; [redacted] 2014**
Title: Predicted Environmental Concentrations of Flurtamone and its Metabolites in Soil (PEC_{Soil}) Following Application to Cereal Crops
Organisation: [redacted]
Report No.: Battelle Report VC.13/012F
Bayer CropScience Document M-476712-01-1
Publication: unpublished
Dates of experimental work: Not applicable
Guidelines: **Not relevant.**
Deviations: Not relevant
GLP/GEP **No – but conducted to Good Modelling Practice**

Executive Summary

Predicted environmental concentrations in soil (PEC_{Soil}) were calculated for flurtamone and the metabolites M04 TFMBA and M05 TFA following pre-emergence application to winter or spring cereal crops at 1 x 125 g ha^{-1}.

The DT_{50} values and maximum amounts in soil used in the calculations are summarised in Table 9.1.3-1. The DT_{50} value for flurtamone is the worst case non-normalised value from the field study in Italy (see section 7.1.2.2.1). The DT_{50} value for M04 TFMBA was the outlier value from the old soil soil study of 63 days. The DT_{50} value for M05 TFA is the current default worst case assumption value. The initial PEC_{Soil} for flurtamone was calculated to be 0.1667 mg/kg following a pre-emergence application at 1x125 g/ha to cereals in Europe (Table 9.1.3-2). The maximal PEC_{soil} values for the metabolites M04 TFMBA and M05 TFA are summarised in Table 9.3.1-3.

Table 9.1.3-1: Summary of input parameters for PEC_{Soil} calculations

Compound	Molecular weight (g/mol)	DT_{50} (days)	Maximum in soil (%)
Flurtamone	333.3	91.6	-
M04 TFMBA	190.1	63.0	24.1
M05 TFA	114.0	1000	38.8

Table 9.1.3-2: Predicted environmental concentrations (mg/kg) of flurtamone in soil (PEC_{Soil}) following pre-emergence applications at 1x125 g/ha to cereals

Day	PEC_{soil} (mg/kg)	TWA (mg/kg)
0	0.1667	
1	0.1654	0.1660
2	0.1642	0.1654
4	0.1617	0.1642
7	0.1581	0.1623
14	0.1499	0.1581
21	0.1422	0.1541
28	0.1348	0.1502
50	0.1142	0.1388
100	0.0782	0.1169

Table 9.1.3-3: Maximal predicted environmental concentrations (mg kg^{-1}) of M04 TFMBA and M05 TFA in soil (PEC_{Soil})

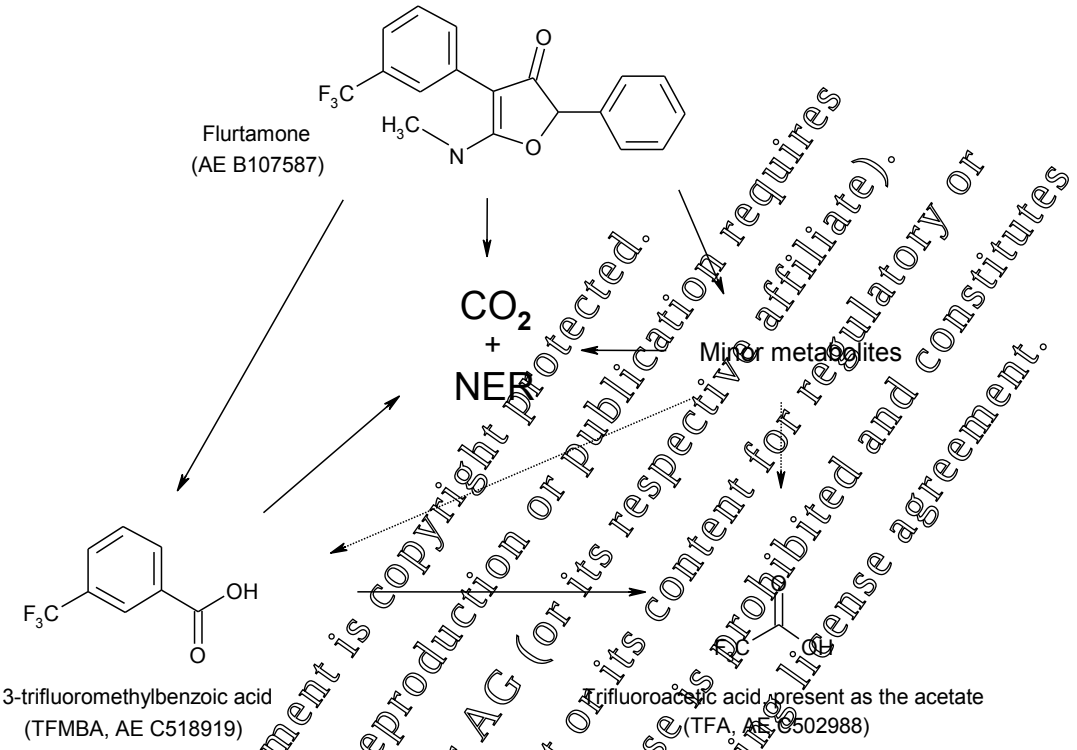
Compound	Maximal PEC_{soil} (mg/kg)
M04 TFMBA	0.0235
M05 TFA	0.0335

Material and Methods

The object of this study was to calculate the predicted environmental concentrations in soil (PEC_{soil}) of the active ingredient flurtamone and its metabolites M04 TFMBA and M05 TFA, following applications to cereals in Europe.

The soil degradation of flurtamone and its metabolites have been investigated under laboratory and field conditions. The metabolic pathway of flurtamone in soil, relevant to the calculation of PEC_{Soil} values for flurtamone and its major soil metabolites is shown below.

Figure 9.1.3-1: Degradation scheme of flurtamone in aerobic soil



The DT_{50} inputs used were the worst-case un-normalized flurtamone DT_{50} (derived from the field study) of 91.6 days, the worst-case un-normalized M04 TFMBA DT_{50} of 63 days and the default 1000 days for M05 TFA. The maximum observed percentages used were 24.7% for M04 TFMBA and 58.8% for M05 TFA. This value comes from the maximum 9.8% AR seen in laboratory studies multiplied by six to compensate for the change of specific activity following metabolism.

No crop intercept was considered (i.e. crop intercept was set to zero). PEC_{soil} values were calculated for a soil depth of 5 cm, an assumed bulk density of 1.5 g/mL. The application rate used was 125 g/ha.

The calculations were carried out on a HP personal computer with Windows XP SP3 as the operating system. Microsoft Excel was used for the PEC_{Soil} calculations.

For flurtamone, PEC_{Soil} with time and time-weighted average (TWA) values were calculated. PEC_{Soil} values for the metabolites M04 TFMBA and M05 TFA were calculated from the initial PEC_{Soil} of flurtamone with factoring for molecular weight differences and maximum residues in soil. PEC_{soil} with time and TWA values were then calculated

Findings

The short-term and long-term PEC_{soil} values for flurtamone (along with TWA values) are summarized in Table 9.1.3-1 (above). The short-term and long-term PEC_{Soil} values for M04 TFMBA (along with maximal TWA values) are shown in Table 9.1.3-4 below.

Table 9.1.3-4: Predicted environmental concentrations (mg kg^{-1}) of M04 TFMBA in soil (PEC_{Soil})

Day	PEC_{soil} (mg/kg)	TWA (mg/kg)
0	0.0235	
1	0.0232	0.0234
2	0.0230	0.0232
4	0.0225	0.0230
7	0.0217	0.0226
14	0.0201	0.0218
21	0.0186	0.0210
28	0.0173	0.0202
50	0.0135	0.0181
100	0.0078	0.0142

The initial PEC_{Soil} value for M05 TFA was calculated to be 0.0335 mg/kg.

Conclusions

PEC_{Soil} values have been calculated for flurtamone, M04 TFMBA and M05 TFA for use in risk assessments.

CP 9.2 - Fate and behaviour in water and sediment

The hydrolysis study conducted on flurtamone ([redacted] 1989, M-163684-01-1) showed that it was stable at all pHs. Hydrolysis would not be a route of degradation for flurtamone in natural water bodies. Photolytic degradation of flurtamone is rapid ([redacted] 1993, M-162275-01-1) with a photolytic half-life of 0.6 to 0.7 days of summer sunlight. One major photodegradate was formed during the study, flurtamone-carboxylic acid (AE 1083976, RPA 203597 in the report) also having a short photolytic half-life (11.8 hours), as calculated below. The quantum yield of direct photolysis of flurtamone in aqueous solution ([redacted] 1993, M-162301-01-1) was found to be 3.2×10^{-2}.

CP 9.2.1 - Aerobic mineralisation in surface water

A study was conducted to meet this new data requirement (Stupp and Beckmann 2013, M-467289-02-1) The biodegradation of [trifluoromethylphenyl-UL-^{14}C]-flurtamone was studied in surface water under aerobic conditions ("pelagic test") in the dark for up to 71 days at 20.18 ± 0.06 °C. The test water was freshly sampled from a freshwater dam close to Wiehl near Gummersbach, Germany and consisted of natural water – clear water without sediment. The test was performed in Erlenmeyer glass flasks with baffles at the bottom each containing 100 mL surface water. The flasks were equipped with traps for the collection of carbon dioxide and volatile organic compounds.

The amount of test item for the treatment of the test systems was based on the intended target concentration of flurtamone of 10 µg/L (low concentration) and 100 µg/L (high concentration). Duplicate samples were analyzed after 0, 8, 14, 23, 37, 49, 59 and 71 days after treatment (DAT). The amounts of flurtamone and its degradation products in the water were determined by liquid scintillation counting (LSC) and by HPLC/radiodetection analysis. TLC was used as confirmatory method. The amount of volatiles was determined by LSC.

Flurtamone dissipated from surface water due to degradation. The mean amounts of flurtamone in the surface water decreased from 99.3% and 98.1% AR at DAT-0 to 85.0% and 84.3% AR on DAT-71 for 10 µg/L and 100 µg/L , respectively.

Degradation of flurtamone in surface water was accompanied by the formation of M04 TFMBA (AE C518919) with 8.9% AR at DAT-59 for 10 µg/L and 3.4% AR at DAT-59 for 100 µg/L. The sum of two non-identified compounds amounted to a maximum mean value of 5.2% AR (DAT-49) at 10 µg/L and 3.6% AR (DAT-71) at 100 µg/L. No single component exceeded 3.5% AR for 10 µg/L and 2.8% AR 100 µg/L.

The maximum mean amounts of carbon dioxide were 1.1% and 0.1% AR at study end (DAT-71) for 10 µg/L (low concentration) and 100 µg/L (high concentration), respectively. The formation of volatile organic compounds was low with 0.5% and 0.1% AR at DAT-59 for 10 µg/L (low concentration) and study end (DAT-71) 100 µg/L (high concentration), respectively

The formation of non-extractable residues (NER) increased from DAT-0 towards a maximum at DAT-49 from 0.5% to 2.2% AR for 10 µg/L and from DAT-0 towards a maximum at DAT-59 from 0.5% to 2.8% AR for 100 µg/L.

When comparing sterile samples with non sterile samples on DAT-71 the sterile samples showed negligible degradation indicating degradation due to microbial activity. The half-lives for flurtamone were between 256 and 314 days in the surface water ("pelagic test") under laboratory aerobic conditions in the dark.

CP 9.2.2 - Water/sediment study

The original flurtamone water/sediment study ([redacted] 1995, M-203194-02-1) was treated at only 1/10th of the intended rate. A replacement water/sediment study was conducted with two contrasting systems treated at the correct rate. This study, ([redacted] 1997, M-158694-01-1) already evaluated at national levels is presented in MCA Section 7 and the results are summarized below. Because it was conducted with compound labelled only in one ring another study with the label in a different ring has been performed and is also presented in MCA Section 7 with the results summarized below.

The degradation of flurtamone, radiolabelled in the trifluoromethylphenyl ring and applied at a rate equivalent to 375 g/ha, was studied in two contrasting water/sediment systems over a 161-day period ([redacted] I. 1997, M-158694-01-1). The aquatic incubation units were maintained in the dark at 20°C ± 2°C. Moistened carbon dioxide-free air was passed through the water in each unit and through an ethylene glycol and two 1M potassium hydroxide traps to trap liberated carbon dioxide and other evolved volatiles. Duplicate units of each sediment type (including traps) were removed for analysis at the following intervals: zero hours (immediately after application), 6, 24 and 48 hours, 7, 14, 30, 61 100, 120, 139 and 161 days after application. Single flasks were taken at 21 days. The redox potential of the sediment and water, and the oxygen content and pH of the water were measured in each unit prior to analysis.

The results showed that flurtamone was the most abundant component of the residue in both water and sediment phases. Bound (unextractable) residues and carbon dioxide were the major degradates formed. The degradates included M02 3-trifluoromethyl-N-methyl-mandelamide (AE 0540067, RE 53285 in the report), M04 TFMBA (AE C518919, RE 54488 in the report) both minor and M08 flurtamone-desphenyl (AE 2093305, RE 591120 in the report), plus three unknowns (all < 5% applied radioactivity).

Flurtamone represented less than 5% AR in the water phases of both systems by the end of the study. M08 flurtamone-desphenyl reached a maximum of 7.8% AR in the water phase of system 2 (Manningtree Stream) and a maximum of 3.6% AR in the sediment. In the total system it reached a maximum of 10.7% AR (120 days). It was not a significant metabolite in system 1 (River Roding) in which the major metabolite was carbon dioxide, which reached 15.5% AR (139 days).

Using data derived from the HPLC examination of the samples the DT50 and DT90 values for the water phases and for the total systems were calculated by use of different mathematical models. These were linear regression on an Excel spreadsheet, the program of Timme & Frehse (v 2.0, Bayer AG) and the program KIM (v 1.0 Schering AG). The results indicated that flurtamone dissipation is not best described by simple first-order kinetics. Re-evaluation of the data showed that the DT50 for system 1 ranges from 9 to 11 days by first-order (FO), double first-order in parallel (DFOP) and double-first-order in sequence (DFOS) kinetics. First-order multiple compartment kinetics (FOMC) give a value of 6.7 days (exactly the same as the KIM result). The same exercise for the system 2 water results gave a range of 2 to 5 days (FO, DFOP, DFOS) and a result of 2.9 days using FOMC, extremely close to that given by the KIM program.

A water/sediment study using [phenyl-UL-^{14}C]-flurtamone was recently conducted ([redacted] 2012d, M-443489-01-1). The aerobic biotransformation of flurtamone was studied in two European water/sediment systems ("Anglersee" and "Wiehltalsperre") for a maximum of 100 days at

about 20.0°C in the dark. The test item was applied to the test systems with a nominal application rate of 39.0 µg/batch (approx. 75.0 µg/L) based on the 3-fold maximum single field use rate of 250 g flurtamone/ha.

The test system consisted of laboratory microcosm flasks equipped with traps for the collection of CO_2 and volatile organic compounds. The water/sediment ratio used was 3/1 (*v/v*). During incubation, the supernatant water was in smooth motion. Duplicate samples were taken and analyzed after 0, 0.25, 1, 3, 7, 14, 30, 59 and 100 days of incubation for test system Anglersee and after 0, 0.25, 1, 3, 7, 14, 30 and 100 days of incubation for test system Wiehltalsperre.

Aliquots of the water layers and the combined organic soil extracts were concentrated and analyzed by HPLC to quantify the test item as well as its transformation products. From representative water and sediment extract samples the HPLC flurtamone fractions were collected and further analyzed by a chiral HPLC method to investigate the degradation behaviour of the single enantiomers. Representative water layers and extracts were additionally analyzed using a confirmatory chromatographic method (TLC).

The total extractable radioactivity from the sediments increased in the Anglersee water/sediment systems from 4.2% AR at DAT-0 to a maximum of 53.1% AR at DAT-14 and decreased again to 11.8% AR at study termination. Total radioactive sediment extractables in the Wiehltalsperre water/sediment systems increased from 7.2% AR at DAT-0 to 53.4% AR at DAT-7 and decreased to 37.7% AR towards study termination. The maximum amounts of non-extractable residues in the Anglersee and Wiehltalsperre test systems were 32.3% AR and 33.5% AR, respectively, at study termination. For the last sampling interval, the non-extractable residues of both water/sediment systems were further characterized by fractionation into humin, humic acids and fulvic acids.

At study termination 47.9% AR and 35.8% AR were degraded to $^{14}CO_2$ in the Anglersee and Wiehltalsperre test systems, respectively, including the dissolved amount of $^{14}CO_2$ in the water layer from DAT-0.25 onwards. Significant amounts of organic volatile compounds were not detected (≤ 0.2% AR in both test systems).

The flurtamone content in the water layer of the Anglersee water/sediment systems decreased from 98.3% AR at DAT-0 to 1.3% AR at study termination. The amount of flurtamone in the water layer of the Wiehltalsperre water/sediment systems decreased from 94.5% AR at DAT-0 to 1.7% AR at study termination. The flurtamone content in the sediment of the Anglersee test systems increased from 4.2% AR at DAT-0 to 52.1% AR at DAT-14 and declined then to 10.6% AR at study termination. The flurtamone content in the sediment of the Wiehltalsperre test systems increased from 7.2% AR at DAT-0 to 52.8% AR at DAT-7 and declined then to 36.3% AR towards study termination.

Both enantiomers of flurtamone have a similar degradation behaviour in water as well as in sediment. The amount of flurtamone in the entire Anglersee water/sediment systems declined to 11.9% AR at study termination. In the Wiehltalsperre water/sediment test systems 38.0% AR was found as unchanged test item at study end. No major metabolites were observed in the water layers, the combined sediment extracts and in the entire systems. Besides flurtamone, eight minor transformation products were detected. The maximum amount of a single minor transformation product in the entire systems was 3.1% for the Anglersee water/sediment systems (DAT-100) and 2.4% AR for the Wiehltalsperre water/sediment systems (DAT-14). Due to the low amounts of the minor transformation products, identification procedures were not performed.

The dissipation time (DT_{50}) of flurtamone from the water layer (sum of degradation and translocation processes into the sediment) was calculated to be 11.2 days for the Anglersee test systems and 7.1 days for the Wiehltalsperre test systems. The degradation half-lives (DT_{50S}) of flurtamone in the entire water/sediment systems were calculated to be 51.2 days for the Anglersee test systems and 40.9 days for the Wiehltalsperre test systems, respectively.

The results from both water-sediment studies have been evaluated to obtain total system $DegT_{50}$ values ([redacted]2013d, M-475187-01-1) water phase DT_{50} values ([redacted]2013e, M-475188-01-1) and sediment phase DT_{50} values ([redacted]2013f, M-476711-01-1). The total system kinetic modelling evaluations for flurtamone showed good model fits with values ranging from 51.2 to 167 days. The geometric mean total system modelling endpoint $DegT_{50}$ value for flurtamone of 82.4 days can be used as $DegT_{50water}$ in $FOCUS_{sw}$ evaluations [in combination with a conservative $DegT_{50sediment}$ value of 1000 days]. Water phase DT_{50} values are summarized in Table 9.2.2-1 and 9.2.2-2 below and sediment phase DT_{50} values are summarized in Table 9.2.2-3.

Table 9.2.2-1: Flurtamone water phase DT_{50} values (for trigger assessment)

Sediment system	Best-fit kinetic	DT_{50} (days)	DT_{90} (days)	Chi^2 (%)	t-test (-)	Visual assessment
1	DFOP	9.2	70.7	6.1	k_1= 0.0402, k_2= 4.49E-05	+
2	DFOP	3.8	48.9	5.6	k_1= 4.54E-06, k_2= 1.91E-07	+
3	DFOP	9.4	72.9	4.6	k_1= 0.00257, k_2= 4.95E-08	+
4	DFOP	5.8	31.1	6.6	k_1= 0.019, k_2= 2.12E-07	+
Geometric Mean		**6.6**	**52.9**	Visual assessment: + = good, o = moderate, - = poor		

Table 9.2.2-2: Flurtamone water phase DT_{50} values for modelling

Sediment system	SFO DT_{50}* (days)	DT_{90} (days)	Chi^2 (%)	t-test (-)	Visual assessment
1	21.3	70.7	6.1	k_1= 0.0402, k_2= 4.49E-05	+
2	14.7	48.9	5.6	k_1= 4.54E-06, k_2= 1.91E-07	+
3	22.0	72.9	4.6	k_1= 0.00257, k_2= 4.95E-08	+
4	9.4	31.1	6.6	k_1= 0.019, k_2= 2.12E-07	+
Geometric Mean	**16.0**	**52.9**	Visual assessment: + = good, o = moderate, - = poor		

* SFO DT_{50} calculated as best-fit DT_{90}/3.32

Table 9.2.2-3: Sediment phase DT_{50} values for flurtamone

System	DT_{50} (days)	DT_{90} (days)	Chi^2 (%)	t-test (-)	Visual
River Roding	68.7	228	14.3	0.0177	o
Manningtree	114	378	7.9	0.000772	+
Anglersee	48.4	161	9.9	0.000392	+
Wiehltalsperre	175	581	5.0	0.0217	+
Geometric Man	**90.2**	**300**	Visual assessment: + = good, o = moderate, - = poor		

CP 9.2.3 - Irradiated water/sediment study

No study is offered under this point

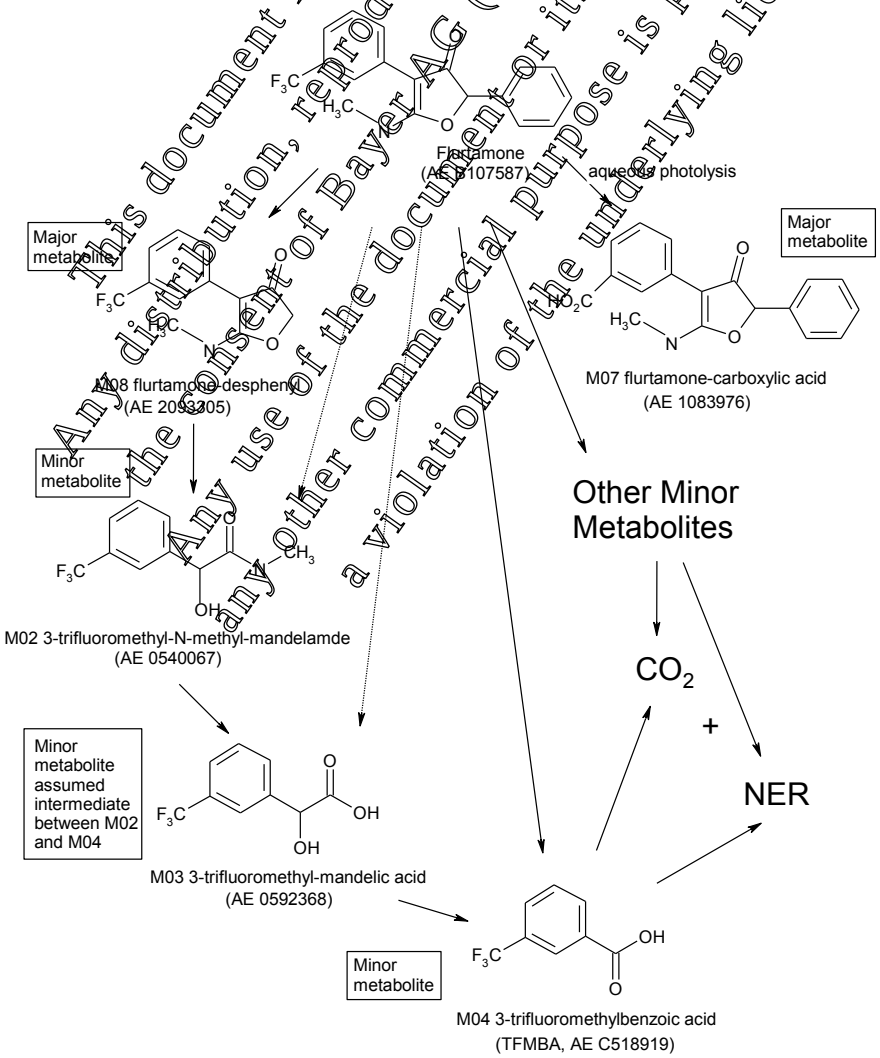
Summary of fate and behaviour in water and sediment

Flurtamone is resistant to hydrolysis. In aqueous solution it is rapidly photodegraded forming one major degradate, M07 flurtamone-carboxylic acid (AE 1083976) that also has a short photolytic half-life. The quantum yield of direct photolysis of flurtamone in aqueous solution was found to be 3.2 x 10^{-2}. Flurtamone degrades slowly in pelagic water with the formation of M04 TFMBA.

In water-sediment systems flurtamone dissipates quickly from the water phase with DT_{50}s of 3.8 to 9.4 days. The total system $DegT_{50}$ value range from 51.2 to 167 days. The geometric mean total system modelling endpoint $DegT_{50}$ value for flurtamone of 82.4 days can be used as $DegT_{50water}$ in $FOCUS_{sw}$ evaluations. The water phase modelling DT_{50} values ranged from 9.4 to 22.0 days. The mean sediment DT_{50} was 90.2 days. The major degradation product in water-sediment systems was M08 flurtamone-desphenyl (AE 2093305), although it only reached 10.7% AR in one total system (water plus sediment). It was accompanied by further degradations products at < 5% AR (M02 3-trifluoromethyl-N-methyl-mandelamide and M04 TFMBA and, presumably M03 3-trifluoromethyl-mandelic acid, as intermediate between the other two).

A proposed metabolic/degradation pathway for flurtamone in aquatic systems is shown below.

Figure 9.2-1 Proposed metabolic/degradation pathway of flurtamone in aquatic systems



CP 9.2.4 - Estimation of concentrations in groundwater

CP 9.2.4.1 - Calculation of concentrations in groundwater

Calculations of the concentrations of flurtamone and its soil metabolites M04 TFMBA and M05 TFA in groundwater have been conducted and are summarized below.

Report:	**KCP-9.2.4.1 /02; [redacted] IAJ. 2014b**
Title:	Predicted Environmental Concentrations in Groundwater (PEC_{GW}) for Flurtamone and its Metabolites Following Application to Cereal Crops
Organisation:	[redacted]
Report No.:	Battelle Report VC/13/012G Bayer CropScience Document: M-476764-01-1
Publication:	unpublished
Dates of experimental work:	Not applicable
Guidelines:	**Not relevant.**
Deviations:	Not relevant
GLP/GEP	**No – but conducted to Good Modelling Practice**

Executive Summary

Predicted environmental concentrations in groundwater (PEC_{GW}) were calculated for flurtamone and the metabolites M04 TFMBA and M05 TFA following pre-emergence application to winter or spring cereal crops at 1 x 125 g/ha.

The leaching behaviour of the active substance flurtamone and its metabolites M04 TFMBA and M05 TFA was investigated for the use on cereals (1 x 125 g/ha) according to the use pattern in Europe.

Model calculations with FOCUS PEARL 4.4.4 and FOCUS PELMO 5.5.3 were carried out according to the FOCUS groundwater requirements using input parameters summarised in Table 9.2.4.1-1.

Table 9.2.4.1-1: Key input parameters of flurtamone and its metabolites

Compound	DT_{50} [20°C and pF2] (days)	Formation fraction (-)	K_{oc} / K_{om} (ml/g)	1/n (-)
Flurtamone	1.1	-	257.3/149.2	0.876
M04 TFMBA	10.4	0.40	15.0/8.7	0.670
M05 TFA	1000	0.063[a]/0.79[b]	0	1.000

[a] direct from flurtamone [b] from TFMBA

The PEC_{gw} values (80th percentile annual average groundwater concentrations) for flurtamone and its metabolites are summarised in Table 9.2.4.1-2 to 9.2.4.1-5 following annual application to winter and spring cereals.

Table 9.2.4.1-2: Predicted 80th percentile average groundwater concentrations of flurtamone and its metabolites on winter cereals at 1 m depth with FOCUS PEARL

PEARL	PECgw (µg/l)		
	Flurtamone	TFMBA	TFA
Châteaudun	<0.001	<0.001	6.634
Hamburg	<0.001	<0.001	4.349
Jokioinen	<0.001	<0.001	6.233
Kremsmünster	<0.001	<0.001	3.356
Okehampton	<0.001	<0.001	2.731
Piacenza	<0.001	<0.001	4.186
Porto	<0.001	<0.001	2.418
Sevilla	<0.001	<0.001	3.614
Thiva	<0.001	<0.001	6.666

Table 9.2.4.1-3: Predicted 80th percentile average groundwater concentrations of flurtamone and its metabolites on winter cereals at 1 m depth with FOCUS PELMO

PELMO	PECgw (µg/l)		
	Flurtamone	TFMBA	TFA
Châteaudun	<0.001	<0.001	4.717
Hamburg	<0.001	<0.001	3.022
Jokioinen	<0.001	<0.001	4.184
Kremsmünster	<0.001	<0.001	2.824
Okehampton	<0.001	<0.001	2.425
Piacenza	<0.001	<0.001	3.306
Porto	<0.001	<0.001	1.990
Sevilla	<0.001	<0.001	3.361
Thiva	<0.001	<0.001	4.468

Table 9.2.4.1-4: Predicted 80th percentile average groundwater concentrations of flurtamone and its metabolites on spring cereals at 1 m depth with FOCUS PEARL

PEARL	PECgw (µg/l)		
	Flurtamone	TFMBA	TFA
Châteaudun	<0.001	<0.001	6.358
Hamburg	<0.001	<0.001	5.396
Jokioinen	<0.001	<0.001	6.284
Kremsmünster	<0.001	<0.001	3.474
Okehampton	<0.001	<0.001	2.750
Porto	<0.001	<0.001	2.478

Table 9.2.4.1-5: Predicted 80th percentile average groundwater concentrations of flurtamone and its metabolites on spring cereals at 1 m depth with FOCUS PELMO

PELMO	PECgw (µg/l)		
	Flurtamone	M04 TFMBA	M05 TFA
Châteaudun	<0.001	<0.001	3.326
Hamburg	<0.001	<0.001	2.534
Jokioinen	<0.001	<0.001	4.121
Kremsmünster	<0.001	<0.001	2.551
Okehampton	<0.001	<0.001	1.649
Porto	<0.001	<0.001	1.053

Materials and Methods

In order to predict the risk of groundwater contamination by plant protection products in accordance with the European Council Directive 91/414/EEC, the FOCUS (FOrum for the Co-ordination of pesticide fate models and their USe) groundwater scenario working group identified and parameterised nine European standard worst-case scenarios to be used within first-tier model calculations. These scenarios consist of soil, crop and climate data.

Four different models (PELMO, PRZM, PEARL, MACRO), which are widely used and have been extensively tested by the working group, were recommended to perform the simulations. Since the models have been shown to produce comparable results, principally, all models are considered equivalent. The models FOCUS PEARL 4.4.4 and FOCUS PELMO 5.5.3 were used for this groundwater assessment.

The purpose of this risk assessment is to investigate the long-term leaching behaviour of flurtamone and its metabolites following a repeated foliar use according to the proposed use pattern.

The soil degradation of flurtamone and its metabolites have been investigated under laboratory and field conditions. The data have been evaluated according to FOCUS Kinetics requirements [FOCUS, 2006] to derive modelling endpoint DT_{50} values [[redacted], 2013a and b].

The relevant metabolic pathway for flurtamone in soil is shown below, in Figure 9.2.4.1-1. The full input parameters for flurtamone and its metabolites used for modelling are summarized in Table 9.2.4.1-6 to 9.2.4.1-8.

Figure 9.2.4.1-1: Degradation scheme of flurtamone in aerobic soil

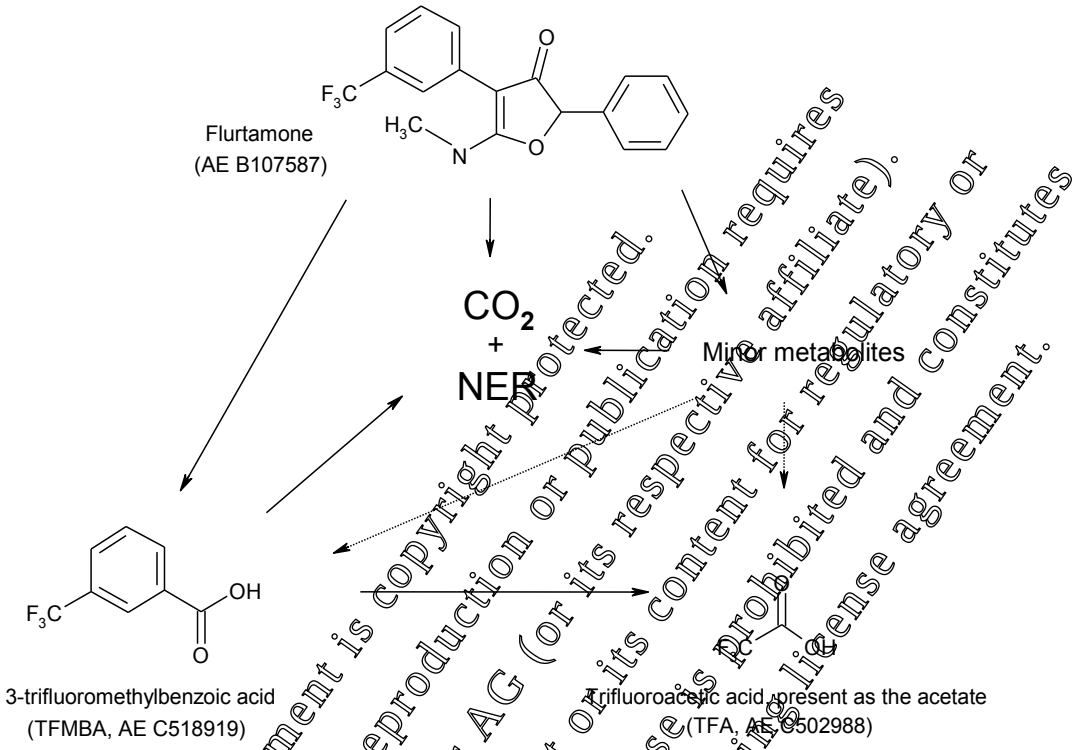


Table 9.2.4.1-6: Summary of substance input parameters, Flurtamone

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	333.3	-
Water solubility (mg L^{-1}) at 20°C; pH 7	11.5	[redacted], 1993 [M-162275-01-1]
Vapour pressure (Pa) at 20°C	7.0E-10	[redacted], 2006 [M-271433-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	17.1	[redacted], 2013a [M-475175-01-1]
Temperature correction function Reference temperature (°C) PEARL: (J mol^{-1}) PELMO: Q_{10} (-)	 20 65400 2.58	FOCUS recommendation
Moisture correction function Reference moisture (-) Moisture exponent (-)	 pF2 0.7	FOCUS recommendation
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	257.3 149.2	[redacted] 2011 [M-401274-02-1]
1/n (-)	0.876	
Management related parameters		
Crop uptake factor (-)	0	Conservative default assumption
Crop interception (%)	0	FOCUS recommendation

Table 9.2.4.1-7: Summary of substance input parameters – M04 TFMBA

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g/mol)	190.1	-
Water solubility (mg/L) at 20°C; pH 8.9	164000	[redacted], 2012 [M-442190-01-1]
Vapour pressure (Pa) at 20°C	0	Conservative assumption
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	10.4	[redacted], 2013b [M-475181-01-1]
Formation fraction (-)	0.40	[redacted], 2013b [M-475181-01-1]
Sorption to soil		
K_{foc} (mL/g) K_{fom} (mL/g)	15 8.7	[redacted], 1999 [M-209972-01-1]
1/n (-)	0.67	
Management related parameters		
Crop uptake factor (-)	0	Conservative default assumption

Table 9.2.4.1-8: Summary of substance input parameters – M05 TEA

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g/mol)	114.0	-
Water solubility (mg/L) at 20°C; pH 8.9	500000	[redacted], 2011 [M-420129-01-1]
Vapour pressure (Pa) at 20°C	1.0E-06	[redacted], 2011 [M-420190-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	1000	Default value
Formation fraction (-)	0.063/0.79	[redacted]; [redacted], 2013b [M-475181-01-1]
Sorption to soil		
K_{foc} (mL/g) K_{fom} (mL/g)	0 0	[redacted] W., 2011 [M-406740-01-1]
1/n (-)	1	
Management related parameters		
Crop uptake factor (-)	0.59	Measured for cereals; [redacted], 2013 [M-468684-01-1]

The nine FOCUS groundwater scenarios used for this groundwater exposure assessment are described in detail in the FOCUS groundwater scenario reports. The simulations were carried out over 26 years as proposed by FOCUS for pesticides which can be applied annually. The first 6 years are intended to be a so called 'warm up' period. The following 20 years were taken into account for the assessment of the potential leaching behaviour.

Flurtamone is applied to cereals between BBCH growth stages 00 and 29. For this assessment plant interception of 0 % was considered for 1 x 125 g ha^{-1} applied to soil at crop emergence. This gives conservative (worst-case) values. Application to winter cereals and to spring cereals was considered.

Findings

The PEC_{GW} values for flurtamone and its metabolites are summarized in Tables 9.2.4.1-2 to 9.2.4.1-5. PEC_{GW} values for flurtamone and M04 TFMBA were < 0.1 µg/L for all scenarios by both models. With values ranging from 1.1 to 6.6 µg/L M05 TFA clearly has the potential to leach, but it is a ubiquitously occurring non-relevant metabolite and therefore not of concern.

Conclusions

Flurtamone and its metabolites do not present a leaching issue.

CP 9.2.4.2 - Additional field tests

No additional field tests are required for flurtamone.

CP 9.2.5 - Estimation of concentrations in surface water and sediment

Report:	**KCP-9.2.5 /01; [redacted] IAJ. 2014b**
Title:	Predicted Environmental Concentrations in Surface Water (PEC_{SW}) and Sediment (PEC_{Sed}) for Flurtamone and its Metabolites Following Application to Winter Cereals
Organisation:	[redacted]
Report No.:	Battelle Report VC/13/012H Bayer CropScience Document, M-477725-01-1
Publication:	unpublished
Dates of experimental work:	Not applicable
Guidelines:	**Not relevant.**
Deviations:	Not relevant
GLP/GEP	**Not – but conducted to Good Modelling Practice**

Executive Summary

Predicted environmental concentrations in surface water (PEC_{SW}) were calculated for flurtamone and the metabolites M04 TFMBA and M05 TFA (major soil metabolites), M07 flurtamone-carboxylic acid (major photolysis degradate) and M08 flurtamone desphenyl (major water-sediment metabolite) following application of flurtamone to winter cereals at 1 x 125 g/ha.

The calculations were conducted to FOCUS recommendations to cover application to winter cereals in the autumn or in the spring. Calculations were conducted for flurtamone and its metabolites at Steps 1 and 2 and in addition for flurtamone at Step 3 and flurtamone at Step 4 for run-off scenarios only. The values generated are suitable for use in risk assessments.

Methods and Materials

An assessment of the potential environmental risk of using a plant protection product includes a prediction of the exposure of non-target aquatic organisms. Such an exposure may occur by the unintentional introduction of a substance into surface water systems via spray-drift, run-off and / or drainage flow. The objective of this evaluation was the calculation of predicted environmental concentrations in surface water and sediment (PEC_{SW} and PEC_{Sed}) for flurtamone and its metabolites following application of flurtamone to winter cereals at 125 g/ha. The calculations followed the

recommendations of the FOCUS Surface Water Scenarios Working Group [FOCUS, 2003 (Sanco/4802/2001-rev.2)], assuming spray-drift, run-off and drainage entry into three types of surface water bodies (pond, ditch, stream). The predicted concentrations can be compared to ecotoxicological effect data to derive the respective toxicity exposure ratios (TER).

Compound data. The data from soil degradation studies have been kinetically evaluated ([redacted] 2013a, M-475175-01-1 and b, M-475181-01-1) and the geometric mean DT_{50} for flurtamone was calculated as being 17.1 days, with that for M04 TFMBA being 10.4 days. For M05 TFA no robust DT_{50} values could be derived and it was given a default DT_{50} of 1000 days. These values were used in the modelling.

The data from water-sediment studies have been kinetically evaluated ([redacted] 2013c, M-475187-01-1). The geometric mean total system $DegT_{50}$ value of 82.4 days was used in the modelling for the water phase along with a conservative $DegT_{50}$ of 1000 days for the sediment phase. The only major metabolite in water-sediment systems was was M08 flurtamone-dosphenyl (AE 2093305) which reached 10.7% AR in the total system.

In the photolysis study only one major degradate was observed and that was M07 flurtamone-carboxylic acid (AE 1083976) which occurred at a maximum of 39.5% AR. This figure was used in the calculations.

From the adsorption.desorption studies the mean K_{FOC} values of 257.3 mL/g (K_{OM} 149.2 mL.g) and 32.5 mL/g (K_{OM} 18.9 mL/g) for flurtamone and M04 TFMBA respectively along with the corresponding 1/n values of 0.876 and 0.670 were used in the calculations. For M05 TFA a K_{FOC} of 0 mL/g (K_{OM} 0 mL/g) was assumed with a 1/n value of 1 and these were used in the calculations.

Method and scenario data. For Step 1 and 2 estimations a standard ditch is defined. The distance between crop and water is fixed to 1 m. For Step 1 The input of pesticides into surface water by spray-drift and run-off / erosion / drainage is evaluated as one single worst-case entry event. Also, multiple applications are typically added at one time point. After entry into surface water, drift loadings are subsequently distributed between water and sediment (within 1 d), according to the compound's K_{oc}. The run-off/erosion/drainage entry (10 % of applied amount) is distributed instantaneously between water and sediment at the time of loading, according to the K_{oc}. The degradation in the water and in the sediment compartment follows a mono-exponential first-order kinetic.

For Step 2 The pesticidal input by spray-drift is evaluated by a series of individual loadings, according to the number of applications. The substance input by run-off / erosion / drainage (2 – 5 % of the soil residue) follows 4 d after the final application. Drift inputs are distributed between water and sediment, assuming a simplified partitioning kinetic for the portion of substance in water available for sorption. The run-off/erosion/drainage entry is distributed instantaneously between water and sediment at the time of loading according to the K_{oc}. The degradation in the water and in the sediment compartment follows a mono-exponential first-order kinetic. Northern and Southern European scenarios are considered.

For Step 3 of the European surface water assessment, the FOCUS working group defined 10 realistic worst-case scenarios, which collectively represent agronomic (soil, slope, crops) and climatic conditions in the EU. The scenarios were separated into drainage (6) scenarios and run-off (4) scenarios based on the relevant entry route, in addition to the spray-drift entry which is considered

relevant for all sites. Three typical water bodies with different (and variable) residence times and different catchment areas – pond, ditch and stream – were identified and associated with the scenarios. Overall, the highest PEC_{sw} estimates from the ten scenarios are likely to represent at least a 90th percentile worst-case for surface water exposure in the EU.

A further step (Step 4) is available and this quantifies the effect of mitigation measures with regard to spray drift and run-off. Step 4 calculations were carried out for flurtamone for the run-off scenarios.

Management and crop-related parameters. The GAP stipulates a single application to winter cereals cereals of 125 g/ha at BBCH 00 to 09 (pre-emergence) or BBCH 10-29 (post-emergence). Calculations were conducted for an autumn application to winter cereals and for a spring application to winter cereals. To cover the case of the pre-emergence application a 0% crop interception was selected for the Step 2 calculations. In Step 3, the plant interception is calculated within the models depending on the application time and the corresponding crop canopy development.

Soft and hardware. The drainage input of pesticides (with up to one metabolite) into surface water is simulated using the leaching model MACRO. The model simulates pesticide losses through bulk matrix flow and through macropore flow, as a separate flow domain assuming gravity flow. FOCUS MACRO considers a 6-year warm-up period with annual applications and a subsequent 16-month assessment period.

Run-off and erosion loadings (parent with up to 2 metabolites) into surface water are calculated using the leaching model PRZM (Pesticide Root Zone Model). This is a one-dimensional, dynamic, compartmental model, which simulates hydrology and substance transport in unsaturated soil systems. The hydrological component for calculating run-off and erosion is based on the USDA Soil Conservation Service curve number methodology and a watershed-scale variation of the Universal Soil Loss Equation. The PRZM in FOCUS shell runs a 20-year simulation with annual applications. A representative 12-month period out of these 20 years for different use patterns is selected and the results imported into TOXSWA.

For the purpose of this study, the activation energy (TOXSWA, J mol^{-1}), exponent (MACRO, 1/K) and (PRZM: Q_{10}) were set to 65400 J mol^{-1}, 0.095 and Q_{10} = 2.58, respectively.

The behaviour of pesticides (only one compound) in a water body is simulated using the TOXSWA model. In FOCUS TOXSWA a standard pond, ditch and stream are assumed as stagnant or flowing water systems with time dependent water levels. TOXSWA handles transient hydrology and pesticide fluxes resulting from run-off, erosion and drainage calculated by the above described models. Entry via spray drift is additionally added here. Calculated water concentrations may vary in horizontal direction, whereas calculated sediment concentrations may be a function of both horizontal and vertical directions.

The calculations were carried out on a HP PC with Microsoft® Windows XP (SP3) as the operating system.

The input parameters are summarized in the tables that follow.

Table 9.2.5-1: Summary of substance input parameters – Flurtamone

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	333.3	-
Water solubility (mg L^{-1}) at 20°C; pH 7	11.5	[redacted], 1993 [M-162275-01-1]
Vapour pressure (Pa) at 20°C	7.0E-10	[redacted], 2006 [M-271433-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	17.1	[redacted], 2012a [M-475175-01-1]
Temperature correction function Reference temperature (°C) MACRO alpha (-) PRZM: Q_{10} (-)	 20 0.095 2.58	FOCUS recommendation
Moisture correction function Reference moisture (-) Moisture exponent (-)	 pF2 0.7	FOCUS recommendation
Degradation in water-sediment		
DT_{50} water (d)	82.40	[redacted], 2013c [M-475185-01-1]
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	82.40	[redacted], 2013c [M-475187-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	255 149.2	[redacted], 2011 [M-401274-01-1]
1/n (-)	0.876	
Management related parameters		
Crop uptake factor (-)	0	Conservative default assumption
Crop interception (%)	0	FOCUS recommendation

Table 9.2.5-2: Summary of substance input parameters – M04 TFMBA

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	190.1	-
Water solubility (mg L^{-1}) at 20°C; pH 8.9	164000	[redacted], 2012 [M-442190-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	104	[redacted], 2013b [M-475181-01-1]
Max. occur. in soil (%)	24.7	[redacted] 2012 [M-442039-01-1]
Degradation in water-sediment		
DT_{50} water (d)	1000	Consevative estimate
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	1000	Consevative estimate
Max. occur. in water/ sediment (%)	4.1	[redacted], 1997 [M-158694-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	15 8.7	[redacted], 1999 [M-207972-01-1]
Management related parameters		
Crop interception (%)	0	Conservative default assumption

Table 9.2.5-3: Summary of substance input parameters – M05 TFA

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	114.0	-
Water solubility (mg L^{-1}) at 20°C; pH 7	500000	[redacted], 2011 [M-420129-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	1000	Default value, no apparent degradation under laboratory conditions: [redacted], 2012 [M-439283-01-1] [redacted], 2013b [M-475181-01-1]
Max. occur. in soil (%)	58.8*	[redacted], 2013b [M-475181-01-1] [redacted], 1993 [M-158234-01-1]
Degradation in water-sediment		
DT_{50} water (d)	1000	Consevative estimate
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	1000	Consevative estimate
Max. occur. in water/ sediment (%)	0.01	Conservative default assumption
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	0 0	[redacted], 2011 [M-406740-01-1]
Management related parameters		
Crop interception (%)	0	Conservative default assumption

* - Maximum of 9.8% [Burr and Austin, 1993] multiplied by 6 due to specific activity change during metabolism

Table 9.2.5-4: Summary of substance input parameters – M07 flurtamone carboxylic acid (AE 1083976, RPA 203597)

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	309.3	-
Water solubility (mg L^{-1}) at 20°C; pH 7	1000	Consevative estimate
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	1000	Default value.
Max. occur. in soil (%)	0.01	Conservative default assumption
Degradation in water-sediment		
DT_{50} water (d)	1000	Consevative estimate
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	1000	Consevative estimate
Max. occur. in water/ sediment (%)	33.5	[redacted], 1993 [M-162275-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	1 0.58	Consevative estimate
Management related parameters		
Crop interception (%)	0	Conservative default assumption

Table 9.2.5-5: Summary of substance input parameters – M08 flurtamone desmethyl (AE 2093305, RPA 591120)

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	257.3	
Water solubility (mg L^{-1}) at 20°C; pH 7	1000	Conservative estimate
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	1000	Default value.
Max. occur. in soil (%)	0.01	Conservative default assumption
Degradation in water-sediment		
DT_{50} water (d)	1000	Conservative estimate
DT_{50} sediment (d)	1000	Conservative estimate
DT_{50} total system (d)	1000	Conservative estimate
Max. occur. in water/ sediment (%)	10.7	[redacted] 1997 [M-158694-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	1 0.58	Conservative estimate
Management related parameters		
Crop interception (%)	0	Conservative default assumption

Findings

The maximum Step 1 and Step 2 values for flurtamone and its metabolites are summarized in Table 9.2.5-6, below. This is followed by the actual and time-weighted averaged (TWA) PEC_{SW} values with time at Step 1 (Table 9.2.5-7) and the corresponding PEC_{Sed} values (Table 9.2.5-8).

Table 9.2.5-6: Maximum PEC_{SW} and PEC_{Sed} values at Step 1 and Step 2 values for flurtamone and its metabolites following application of flurtamone to winter cereals at 125 g/ha

Compound	Step 1		Step 2 Northern Europe		Step 2 Southern Europe	
	PEC_{SW} (µg/L)	PEC_{Sed} (µg/kg)	PEC_{SW} (µg/L)	PEC_{Sed} (µg/kg)	PEC_{SW} (µg/L)	PEC_{Sed} (µg/kg)
Flurtamone	32.17	91.34	14.00	36.05	11.46	29.27
M04 TFMBA	5.48	0.87	2.23	0.33	1.79	0.27
M05 TFA	8.39	0.00	4.18	0.00	3.35	0.00
M07 [1] flurtamone-carboxylic acid	0.36	0.00	0.36	0.00	0.36	0.00
M08 [2] flurtamone-desphenyl	0.10	0.00	0.10	0.00	0.10	0.00

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-7: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 1 for flurtamone and its metabolites with time, following application of flurtamone to winter cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	32.173	-	5.7817	-	8.3872		0.3612	-	0.0982	-
1	31.612	31.8928	5.7772	5.7794	8.3814	8.3843	0.3605	0.3609	0.0980	0.0981
2	31.347	31.6863	5.7732	5.7773	8.3756	8.3814	0.3603	0.3606	0.0979	0.0980
4	30.824	31.3858	5.7652	5.7732	8.3640	8.3756	0.3598	0.3603	0.0978	0.0979
7	30.056	30.9800	5.7532	5.7672	8.3466	8.3669	0.3590	0.3599	0.0976	0.0978
14	28.337	30.0844	5.7254	5.7532	8.3062	8.3467	0.3573	0.3590	0.0972	0.0976
21	26.717	29.2294	5.6976	5.7393	8.2660	8.3266	0.3556	0.3582	0.0966	0.0973
28	25.189	28.4085	5.6701	5.7255	8.2260	8.3064	0.3538	0.3573	0.0962	0.0971
42	22.391	26.8600	5.6153	5.6978	8.1466	8.2663	0.3504	0.3556	0.0952	0.0966
50	20.933	26.0270	5.5843	5.6822	8.1015	8.2436	0.3486	0.3546	0.0947	0.0964
100	13.746	21.5579	5.3940	5.5854	7.8156	8.1052	0.3366	0.3485	0.0915	0.0947

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-8: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 1 for flurtamone and its metabolites with time, following application of flurtamone to winter cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	79.8235	-	0.8632		0.0000	-	0.0000	-	0.0000	-
1	81.3388	80.5812	0.8666	0.8649	0.0000	0.0000	0.0036	0.0018	0.0010	0.0005
2	80.6574	80.7894	0.8660	0.8656	0.0000	0.0000	0.0036	0.0027	0.0010	0.0007
4	79.3118	80.3869	0.8648	0.8654	0.0000	0.0000	0.0036	0.0032	0.0010	0.0009
7	77.3353	79.5003	0.8630	0.8648	0.0000	0.0000	0.0036	0.0033	0.0010	0.0009
14	72.9130	77.3014	0.8588	0.8628	0.0000	0.0000	0.0036	0.0035	0.0010	0.0009
21	68.7436	75.1369	0.8546	0.8608	0.0000	0.0000	0.0036	0.0035	0.0010	0.0010
28	64.8125	73.0423	0.8505	0.8587	0.0000	0.0000	0.0035	0.0035	0.0010	0.0010
42	57.6120	69.0754	0.8423	0.8546	0.0000	0.0000	0.0035	0.0035	0.0010	0.0010
50	53.8626	66.9380	0.8376	0.8523	0.0000	0.0000	0.0035	0.0035	0.0009	0.0010
100	35.3690	55.4537	0.8091	0.8378	0.0000	0.0000	0.0034	0.0035	0.0009	0.0009

[1] RPA 203597 in report [2] RPA 591120 in report

The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone and its metabolites at Step 2 for Northern Europe and the corresponding PEC_{Sed} values are shown in Tables 9.2.5-9 and 9.2.5-10, with those for Southern Europe shown in Table 9.2.5-11 and Table 9.2.5-12.

Table 9.2.5-9: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 2 for Northern Europe for flurtamone and its metabolites following application of flurtamone to winter cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	14.0983	---	2.2305	---	4.1820	---	0.3580	---	0.0962	---
1	13.9048	14.0016	2.2288	2.2296	4.1791	4.1806	0.3576	0.3578	0.0961	0.0962
2	13.8156	13.9309	2.2272	2.2288	4.1762	4.1791	0.3573	0.3576	0.0960	0.0961
4	13.6390	13.8290	2.2242	2.2273	4.1704	4.1762	0.3569	0.3574	0.0959	0.0960
7	13.3782	13.6916	2.2195	2.2249	4.1618	4.1719	0.3561	0.3570	0.0957	0.0959
14	12.7890	13.3865	2.2088	2.2196	4.1416	4.1618	0.3544	0.3561	0.0952	0.0957
21	12.2257	13.0928	2.1981	2.2142	4.1216	4.1515	0.3527	0.3553	0.0948	0.0955
28	11.6873	12.8082	2.1875	2.2088	4.1016	4.1417	0.3510	0.3544	0.0943	0.0952
42	10.6805	12.2643	2.1663	2.1982	4.0620	4.1217	0.3476	0.3527	0.0934	0.0948
50	10.1446	11.9676	2.1544	2.1921	4.0396	4.1104	0.3457	0.3517	0.0929	0.0945
100	7.3537	10.3210	2.0810	2.1548	3.9020	4.0404	0.3339	0.3457	0.0897	0.0929

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-10: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 2 for Northern Europe for flurtamone and its metabolites following application of flurtamone to winter cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	36.0544	---	0.3343	---	0.0000	---	0.0036	---	0.0010	---
1	35.8231	35.9387	0.3341	0.3342	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
2	35.5933	35.8235	0.3339	0.3341	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
4	35.1382	35.5944	0.3334	0.3339	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
7	34.4664	35.2546	0.3327	0.3335	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
14	32.9484	34.4782	0.3311	0.3327	0.0000	0.0000	0.0035	0.0036	0.0010	0.0010
21	31.4973	33.7246	0.3295	0.3319	0.0000	0.0000	0.0035	0.0036	0.0009	0.0010
28	30.1100	32.9931	0.3279	0.3311	0.0000	0.0000	0.0035	0.0035	0.0009	0.0010
42	27.5161	31.5933	0.3247	0.3295	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
50	26.1355	30.8296	0.3229	0.3286	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
100	18.9454	26.5888	0.3119	0.3230	0.0000	0.0000	0.0033	0.0035	0.0009	0.0009

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-11: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 2 for Southern Europe for flurtamone and its metabolites following autumn application of flurtamone to winter cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Days after Max	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	11.4603	---	1.7897	---	3.3456	---	0.3576	---	0.0959	---
1	11.2889	11.3746	1.7883	1.7890	3.3433	3.3445	0.3572	0.3574	0.0958	0.0958
2	11.2165	11.3137	1.7870	1.7883	3.3410	3.3434	0.3570	0.3572	0.0957	0.0958
4	11.0731	11.2292	1.7846	1.7871	3.3364	3.3410	0.3565	0.3570	0.0956	0.0957
7	10.8614	11.1168	1.7809	1.7852	3.3294	3.3375	0.3557	0.3566	0.0954	0.0956
14	10.3830	10.8686	1.7722	1.7809	3.3133	3.3294	0.3540	0.3557	0.0949	0.0954
21	9.9257	10.6300	1.7637	1.7765	3.2975	3.3215	0.3523	0.3549	0.0945	0.0952
28	9.4886	10.3989	1.7551	1.7723	3.2813	3.3134	0.3506	0.3540	0.0940	0.0949
42	8.6712	9.9572	1.7382	1.7637	3.2496	3.2974	0.3472	0.3523	0.0931	0.0945
50	8.2361	9.7163	1.7286	1.7589	3.2317	3.2887	0.3453	0.3511	0.0926	0.0942
100	5.9703	8.3794	1.6697	1.7289	3.1210	3.2523	0.3335	0.3453	0.0894	0.0926

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-12: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 2 for Southern Europe for flurtamone and its metabolites following application of flurtamone to winter cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Days after Max	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	29.2715	---	0.2682	---	0.0000	---	0.0036	---	0.0010	---
1	29.0837	29.1776	0.2681	0.2681	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
2	28.8972	29.0840	0.2679	0.2681	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
4	28.5277	28.8981	0.2675	0.2679	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
7	27.9823	28.6221	0.2669	0.2676	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
14	26.7499	27.9918	0.2657	0.2669	0.0000	0.0000	0.0035	0.0036	0.0009	0.0010
21	25.5717	27.3800	0.2644	0.2663	0.0000	0.0000	0.0035	0.0035	0.0009	0.0010
28	24.4454	26.7861	0.2631	0.2657	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
42	22.3396	25.6497	0.2605	0.2644	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
50	21.2187	25.0296	0.2591	0.2636	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
100	15.3813	21.5867	0.2503	0.2592	0.0000	0.0000	0.0033	0.0035	0.0009	0.0009

[1] RPA 203597 in report [2] RPA 591120 in report

The maximum PEC_{SW} and PEC_{Sed} values with the dominant route of entry for each scenario at Step 3 are summarized in Table 9.2.5.13 for application in autumn. The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone at Step 3 for autumn application to winter cereals are shown in Table 9.2.5-14, and the corresponding PEC_{Sed} values, are shown in Table 9.2.5-15.

Table 9.2.5-13: Maximum PEC_{SW} and PEC_{Sed} values at Step 3 for flurtamone following autumn application to winter cereals at 125 g/ha

Scenario	Application dates	$PEC_{SW\ Max}$ (µg L^{-1})	$PEC_{Sed\ Max}$ (µg kg^{-1})	Dominant entry route
D1 Lanna Ditch	11-Sep	2.414	8.513	Drainage
D1 Lanna Stream	11-Sep	1.507	5.099	Drainage
D2 Brimstone Ditch	11-Oct	2.169	4.687	Drainage
D2 Brimstone Stream	11-Oct	1.350	2.836	Drainage
D3 Vredepeel Ditch	06-Nov	0.789	0.247	Drift
D4 Skousbo Pond	10-Sep	0.274	1.257	Drainage
D4 Skousbo Stream	10-Sep	0.685	0.529	Drift
D5 La Jailliere Pond	26-Nov	0.432	1.703	Drainage
D5 La Jailliere Stream	26-Nov	0.239	0.534	Drift
D6 Thiva Ditch	06-Dec	2.448	2.023	Drainage
R1 Weiherbach Pond	14-Nov	0.070	0.320	Run-off
R1 Weiherbach Stream	14-Nov	2.645	0.659	Run-off
R3 Bologna Stream	17-Nov	3.408	0.231	Run-off
R4 Roujan Stream	03-Nov	1.277	0.402	Run-off

Table 9.2.5-14: Actual PECsw values with time and time-weighted averaged (TWA) PECsw values at Step 3 for flurtamone following autumn application to winter cereals at 125 g/ha

Scenario	D1 Lanna Ditch		D1 Lanna Stream		D2 Brimstone Ditch		D2 Brimstone Stream		D3 Vredepeel Ditch	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	2.414	-	1.507	-	2.169	-	1.356	-	0.789	-
1	2.380	2.407	1.482	1.503	0.886	1.379	0.505	0.809	0.160	0.510
2	2.359	2.393	1.465	1.493	0.751	1.202	0.445	0.704	0.009	0.282
4	2.266	2.374	1.402	1.480	0.875	1.158	0.494	0.681	0.001	0.143
7	2.112	2.324	1.300	1.447	1.202	1.058	0.761	0.657	0.000	0.082
14	1.843	2.204	1.117	1.368	0.700	0.953	0.425	0.560	0.000	0.041
21	1.657	2.101	0.971	1.303	1.384	0.870	0.888	0.517	0.000	0.027
28	1.677	2.057	1.029	1.273	1.151	0.843	0.839	0.499	0.000	0.021
42	1.356	1.942	0.559	1.194	0.529	0.786	0.314	0.466	0.000	0.014
50	1.067	1.881	0.009	1.155	0.461	0.739	0.261	0.438	0.000	0.012
100	0.336	1.568	0.002	0.835	0.428	0.606	0.242	0.355	0.000	0.006

Scenario	D4 Skousbo Pond		D4 Skousbo Stream		D5 La Jailliere Pond		D5 La Jailliere Stream		D6 Thiva Ditch	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	0.274	-	0.000	-	0.432	-	0.739	-	2.448	-
1	0.274	0.274	0.001	0.322	0.431	0.432	0.004	0.339	1.315	1.815
2	0.273	0.274	0.000	0.300	0.428	0.431	0.001	0.331	0.990	1.531
4	0.270	0.274	0.000	0.298	0.422	0.430	0.000	0.314	0.640	1.405
7	0.264	0.274	0.000	0.267	0.410	0.427	0.000	0.282	0.277	1.138
14	0.250	0.270	0.000	0.234	0.385	0.417	0.000	0.220	0.052	0.701
21	0.236	0.266	0.000	0.202	0.363	0.406	0.000	0.167	0.064	0.516
28	0.218	0.261	0.000	0.171	0.344	0.396	0.000	0.131	0.433	0.503
42	0.191	0.249	0.000	0.125	0.292	0.375	0.000	0.091	0.044	0.366
50	0.179	0.242	0.000	0.108	0.267	0.362	0.006	0.079	0.030	0.377
100	0.129	0.206	0.175	0.058	#N/A	0.266	0.012	0.045	0.038	0.224

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	0.070	-	2.643	-	3.408	-	1.277	-
1	0.069	0.070	0.003	1.101	2.254	2.060	0.726	0.662
2	0.068	0.069	0.001	0.552	1.768	1.860	0.002	0.489
4	0.067	0.068	0.000	0.276	0.011	1.198	0.000	0.245
7	0.064	0.067	0.000	0.158	0.005	0.687	0.000	0.140
14	0.060	0.065	0.000	0.086	0.003	0.353	0.000	0.070
21	0.056	0.062	0.017	0.057	0.007	0.252	0.000	0.047
28	0.052	0.060	0.000	0.044	0.001	0.190	0.000	0.035
42	0.047	0.057	0.000	0.036	0.001	0.136	0.000	0.023
50	0.043	0.055	0.000	0.032	0.001	0.114	0.000	0.022
100	0.027	0.048	0.000	0.016	0.000	0.058	0.000	0.011

Table 9.2.5-15: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 3 for flurtamone and following autumn application to winter cereals at 125 g/ha

Scenario	D1 Lanna Ditch		D1 Lanna Stream		D2 Brimstone Ditch		D2 Brimstone Stream		D3 Vredepeel Ditch	
Time (d).	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	8.513	-	5.099	-	4.687	-	2.836	-	0.247	-
1	8.512	8.513	5.097	5.098	4.644	4.675	2.807	2.822	0.170	0.231
2	8.511	8.513	5.091	5.098	4.611	4.652	2.788	2.813	0.131	0.203
4	nc	8.512	5.059	5.096	4.613	4.628	2.797	2.797	0.095	0.163
7	nc	8.509	4.907	5.092	4.592	4.621	2.784	2.796	0.074	0.131
14	nc	8.475	4.039	5.069	4.507	4.589	2.739	2.778	0.054	0.098
21	nc	8.454	4.446	5.019	4.451	4.565	2.705	2.758	0.045	0.082
28	nc	8.443	3.757	4.959	4.422	4.529	2.666	2.743	0.039	0.072
42	nc	8.421	3.234	4.832	4.307	4.496	2.701	2.718	0.033	0.060
50	nc	8.404	3.038	4.741	4.421	4.493	2.659	2.712	0.030	0.056
100	nc	8.341	2.324	4.244	4.508	4.464	2.717	2.690	0.022	0.041

Scenario	D4 Skousbo Pond		D4 Skousbo Stream		D5 La Jaliere Pond		D5 La Jaliere Stream		D6 Thiva Ditch	
Time (d).	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	1.257	-	0.529	-	1.703	-	0.534	-	2.023	-
1	1.257	1.257	0.528	0.529	nc	1.703	0.525	0.533	2.011	2.021
2	1.257	1.257	0.525	0.528	nc	1.702	0.511	0.531	1.982	2.016
4	1.257	1.257	0.516	0.525	nc	1.700	0.479	0.524	1.855	1.994
7	1.256	1.257	0.500	0.524	nc	1.697	0.435	0.510	1.613	1.928
14	nc	1.257	0.447	0.515	nc	1.690	0.358	0.472	1.246	1.721
21	nc	1.257	1.398	0.501	nc	1.683	0.307	0.437	1.122	1.560
28	nc	1.256	0.365	0.484	nc	1.674	0.274	0.407	1.658	1.500
42	nc	1.254	0.361	0.451	nc	1.648	0.272	0.364	1.216	1.489
50	nc	1.252	0.307	0.436	nc	1.625	0.261	0.350	1.110	1.444
100	nc	1.215	0.218	0.359	nc	1.199	#N/A	0.266	0.973	1.269

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d).	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.320	-	0.658	-	6.231	-	0.402	-
1	0.320	0.320	0.362	0.529	5.619	6.002	0.257	0.352
2	0.320	0.320	0.269	0.433	5.473	5.833	0.202	0.336
4	0.320	0.320	0.201	0.338	4.924	5.538	0.156	0.276
7	0.320	0.320	0.159	0.271	4.497	5.204	0.125	0.224
14	0.319	0.320	0.138	0.204	3.896	4.712	0.094	0.169
21	0.317	0.320	0.117	0.176	3.588	4.399	0.079	0.142
28	0.316	0.320	0.095	0.158	3.249	4.160	0.070	0.126
42	0.311	0.319	0.124	0.148	2.840	3.804	0.059	0.105
50	0.308	0.319	0.104	0.143	2.660	3.641	0.055	0.098
100	0.277	0.314	0.070	0.113	2.023	2.977	0.041	0.072

The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone, at Step 4 (60% run-off mitigation, corresponding to a 10 m vegetated filter strip) for autumn application to winter cereals in run-off scenarios, are shown in Table 9.2.5-16, and the corresponding PEC_{Sed} values, are shown in Table 9.2.5-17. These values were not used in the risk assessment, since step 3 values are sufficient, but they are provided here for completeness.

Table 9.2.5-16: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 4 (60% run-off mitigation, corresponding to a 10 m vegetated filter strip) for flurtamone following autumn application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	0.037	-	1.186	-	1.556	-	0.577	-
1	0.037	0.037	0.001	0.492	1.029	0.942	0.326	0.298
2	0.036	0.037	0.001	0.247	0.793	0.854	0.061	0.220
4	0.036	0.036	0.000	0.123	0.004	0.549	0.000	0.110
7	0.034	0.036	0.000	0.071	0.001	0.315	0.000	0.063
14	0.032	0.035	0.000	0.042	0.001	0.167	0.000	0.032
21	0.030	0.033	0.007	0.028	0.003	0.115	0.000	0.021
28	0.028	0.032	0.000	0.022	0.000	0.086	0.000	0.016
42	0.025	0.030	0.000	0.016	0.000	0.064	0.000	0.011
50	0.023	0.030	0.000	0.015	0.000	0.054	0.000	0.011
100	0.014	0.028	0.000	0.008	0.000	0.027	0.000	0.006

Table 9.2.5-17: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 4 (60% run-off mitigation, corresponding to a 10 m vegetated filter strip) for flurtamone following autumn application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.189	-	0.302	-	1.413	-	0.191	-
1	0.189	0.189	0.171	0.245	1.207	1.349	0.125	0.168
2	0.189	0.189	0.127	0.202	1.178	1.294	0.099	0.160
4	0.189	0.189	0.094	0.158	0.992	1.201	0.077	0.133
7	0.189	0.189	0.075	0.127	0.878	1.095	0.062	0.108
14	0.188	0.189	0.064	0.096	0.744	0.957	0.047	0.082
21	0.187	0.189	0.054	0.082	0.710	0.882	0.040	0.070
28	0.186	0.189	0.044	0.074	0.631	0.833	0.035	0.062
42	0.183	0.188	0.058	0.069	0.555	0.759	0.030	0.052
50	0.182	0.188	0.048	0.066	0.518	0.725	0.028	0.049
100	0.165	0.185	0.032	0.052	0.394	0.587	0.021	0.036

The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone, at Step 4 (80% run-off mitigation, corresponding to a 20 m vegetated filter strip) for autumn application to winter cereals in run-off scenarios, are shown in Table 9.2.5-18, and the corresponding PEC_{Sed} values, are shown in Table 9.2.5-19. These values were not used in the risk assessment, since step 3 values are sufficient, but they are provided here for completeness.

Table 9.2.5-18: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 4 (80% run-off mitigation, corresponding to a 20 m vegetated filter strip) for flurtamone following autumn application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	0.029	-	0.618	-	0.817	-	0.524	-
1	0.028	0.029	0.001	0.256	0.540	0.495	0.000	0.156
2	0.028	0.028	0.000	0.128	0.413	0.449	0.000	0.115
4	0.027	0.028	0.000	0.064	0.002	0.289	0.000	0.057
7	0.026	0.028	0.000	0.037	0.001	0.165	0.000	0.033
14	0.024	0.026	0.000	0.025	0.000	0.093	0.000	0.016
21	0.022	0.026	0.003	0.017	0.001	0.062	0.000	0.011
28	0.021	0.025	0.000	0.013	0.000	0.047	0.000	0.008
42	0.025	0.024	0.000	0.009	0.000	0.035	0.000	0.005
50	0.023	0.024	0.000	0.009	0.000	0.029	0.000	0.007
100	0.014	0.022	0.000	0.004	0.000	0.015	0.000	0.003

Table 9.2.5-19: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 4 (80% run-off mitigation, corresponding to a 20 m vegetated filter strip) for flurtamone following autumn application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.143	-	0.164	-	0.623	-	0.106	-
1	0.143	0.143	0.097	0.136	0.521	0.594	0.071	0.094
2	0.143	0.143	0.073	0.113	0.508	0.566	0.057	0.089
4	0.143	0.143	0.055	0.090	0.414	0.521	0.044	0.075
7	0.143	0.143	0.044	0.073	0.359	0.468	0.036	0.062
14	0.143	0.143	0.037	0.055	0.299	0.401	0.028	0.047
21	0.142	0.143	0.031	0.048	0.290	0.367	0.024	0.040
28	0.141	0.143	0.026	0.043	0.255	0.345	0.022	0.036
42	0.139	0.143	0.033	0.040	0.224	0.313	0.018	0.031
50	0.138	0.142	0.028	0.038	0.209	0.298	0.017	0.029
100	0.126	0.140	0.019	0.030	0.159	0.240	0.013	0.022

The maximum PEC_{SW} and PECSed values with the dominant route of entry for each scenario at Step 3 are summarized in Table 9.2.5.20 for application in spring. The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone at Step 3 for spring application to winter cereals are shown in Table 9.2.5-21, and the corresponding PEC_{Sed} values, are shown in Table 9.2.5-22.

Table 9.2.5-20: Maximum PEC_{SW} and PEC_{Sed} values at Step 3 for flurtamone following spring application to winter cereals at 125 g/ha

Scenario	Application dates	$PEC_{SW, Max}$ (µg L^{-1})	$PEC_{Sed, Max}$ (µg kg^{-1})	Dominant entry route
D1 Lanna Ditch	25-Apr	0.860	1.556	Drift
D1 Lanna Stream	25-Apr	0.712	0.351	Drift
D2 Brimstone Ditch	07-May	0.807	1.077	Drift
D2 Brimstone Stream	07-May	0.717	0.946	Drift
D3 Vredepeel Ditch	17-Mar	0.592	0.297	Drift
D4 Skousbo Pond	18-Apr	0.028	0.104	Drift
D4 Skousbo Stream	18-Apr	0.628	0.031	Drift
D5 La Jailliere Pond	07-Mar	0.028	0.105	Drift
D5 La Jailliere Stream	07-Mar	0.623	0.018	Drift
D6 Thiva Ditch	05-Mar	0.792	0.316	Drift
R1 Weiherbach Pond	18-Mar	0.064	0.275	Run-off
R1 Weiherbach Stream	18-Mar	1.843	0.549	Run-off
R3 Bologna Stream	01-Mar	2.368	0.783	Run-off
R4 Roujan Stream	05-Mar	0.522	0.079	Drift

Table 9.2.5-21: Actual PECsw values and time-weighted averaged (TWA) PECsw values at Step 3 for flurtamone following spring application of flurtamone to winter cereals at 125 g/ha

Scenario	D1 Lanna Ditch		D1 Lanna Stream		D2 Brimstone Ditch		D2 Brimstone Stream		D3 Vredepeel Ditch	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	0.860	-	0.712	-	0.807	-	0.717	-	0.792	-
1	0.784	0.816	0.030	0.191	0.751	0.774	0.667	0.688	0.337	0.599
2	0.745	0.789	0.026	0.112	0.723	0.762	0.642	0.670	0.040	0.376
4	0.702	0.755	0.011	0.074	0.686	0.729	0.609	0.647	0.003	0.194
7	0.658	0.723	0.001	0.059	0.016	0.696	0.004	0.617	0.001	0.111
14	0.115	0.584	0.032	0.053	0.009	0.356	0.003	0.317	0.000	0.056
21	0.099	0.425	0.001	0.051	0.016	0.241	0.007	0.206	0.000	0.037
28	0.087	0.342	0.000	0.050	0.020	0.186	0.011	0.157	0.000	0.028
42	0.062	0.253	0.000	0.049	0.021	0.131	0.013	0.109	0.000	0.019
50	0.051	0.223	0.000	0.049	0.021	0.113	0.013	0.093	0.000	0.016
100	0.017	0.149	0.000	0.037	0.014	0.066	0.007	0.052	0.000	0.008

Scenario	D4 Skousbo Pond		D4 Skousbo Stream		D5 La Jailliere Pond		D5 La Jailliere Stream		D6 Thiva Ditch	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	0.028	-	0.623	-	0.928	-	0.623	-	0.792	-
1	0.027	0.027	0.000	0.043	0.027	0.028	0.000	0.024	0.388	0.622
2	0.026	0.027	0.000	0.021	0.027	0.027	0.000	0.012	0.058	0.406
4	0.026	0.026	0.000	0.011	0.026	0.027	0.000	0.006	0.004	0.212
7	0.025	0.026	0.000	0.006	0.025	0.026	0.000	0.004	0.002	0.122
14	0.023	0.025	0.000	0.005	0.023	0.025	0.000	0.002	0.001	0.062
21	0.021	0.024	0.000	0.004	0.021	0.024	0.000	0.001	0.001	0.042
28	0.020	0.023	0.000	0.004	0.019	0.023	0.000	0.001	0.001	0.032
42	0.017	0.021	0.000	0.003	0.017	0.021	0.000	0.001	0.001	0.021
50	0.016	0.021	0.000	0.003	0.016	0.020	0.000	0.001	0.000	0.018
100	0.010	0.017	0.000	0.001	0.011	0.017	0.000	0.001	0.000	0.009

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	0.064	-	1.863	-	2.368	-	0.522	-
1	0.062	0.063	0.004	0.937	0.010	1.451	0.000	0.129
2	0.061	0.063	0.001	0.470	0.003	0.733	0.000	0.065
4	0.060	0.062	0.000	0.235	0.001	0.368	0.000	0.049
7	0.057	0.060	0.000	0.135	0.000	0.210	0.000	0.034
14	0.053	0.058	0.000	0.070	0.802	0.120	0.000	0.018
21	0.049	0.055	0.000	0.050	0.000	0.097	0.000	0.012
28	0.045	0.053	0.000	0.039	0.000	0.080	0.000	0.009
42	0.039	0.049	0.000	0.026	0.000	0.053	0.000	0.006
50	0.047	0.048	0.001	0.025	0.000	0.046	0.000	0.005
100	0.029	0.043	0.000	0.014	0.000	0.024	0.000	0.004

Table 9.2.5-22: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 3 for flurtamone following spring application of flurtamone to winter cereals at 125 g/ha

Scenario	D1 Lanna Ditch		D1 Lanna Stream		D2 Brimstone Ditch		D2 Brimstone Stream		D3 Vredepeel Ditch	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	1.556	-	0.351	-	1.077	-	0.946		0.297	-
1	1.445	1.547	0.307	0.333	0.841	1.053	0.730	0.923	0.229	0.285
2	1.338	1.534	0.289	0.317	0.738	1.025	0.633	0.897	0.174	0.258
4	1.219	1.503	0.266	0.299	0.626	0.966	0.531	0.844	0.127	0.213
7	1.128	1.452	0.237	0.282	0.537	0.881	0.451	0.766	0.099	0.173
14	1.026	1.339	0.245	0.270	0.440	0.735	0.360	0.632	0.072	0.130
21	0.966	1.255	0.212	0.264	0.400	0.645	0.323	0.549	0.060	0.109
28	0.918	1.193	0.192	0.259	0.377	0.587	0.301	0.496	0.053	0.096
42	0.838	1.107	0.168	0.251	0.350	0.516	0.276	0.430	0.044	0.080
50	0.799	1.069	0.158	0.248	0.340	0.497	0.263	0.406	0.041	0.074
100	0.618	0.904	0.122	0.219	0.302	0.484	0.213	0.324	0.029	0.054

Scenario	D4 Skousbo Pond		D4 Skousbo Stream		D5 La Jailliere Pond		D5 La Jailliere Stream		D6 Thiva Ditch	
Time (d).	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.104	-	0.031	-	0.105	-	0.018	-	0.316	-
1	0.104	0.104	0.018	0.024	0.105	0.105	0.011	0.014	0.251	0.305
2	0.104	0.104	0.013	0.020	0.105	0.105	0.008	0.012	0.192	0.279
4	0.104	0.104	0.010	0.016	0.105	0.105	0.007	0.010	0.141	0.232
7	0.104	0.104	0.008	0.016	0.105	0.105	0.005	0.008	0.111	0.190
14	0.104	0.104	0.006	0.015	0.104	0.105	0.004	0.006	0.082	0.144
21	0.104	0.104	0.005	0.015	0.104	0.105	0.004	0.006	0.069	0.122
28	0.103	0.104	0.005	0.015	0.103	0.105	0.004	0.005	0.061	0.108
42	0.103	0.104	0.004	0.014	0.102	0.105	0.004	0.005	0.052	0.091
50	0.102	0.104	0.004	0.014	0.100	0.104	0.003	0.005	0.048	0.084
100	#N/A	0.103	0.003	0.012	0.093	0.103	0.002	0.004	0.034	0.062

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.275	-	0.549	-	0.783	-	0.079	-
1	0.275	0.275	0.312	0.452	0.472	0.678	0.050	0.069
2	0.275	0.275	0.235	0.375	0.359	0.570	0.039	0.067
4	0.274	0.275	0.177	0.294	0.272	0.451	0.069	0.060
7	0.274	0.275	0.141	0.238	0.217	0.365	0.045	0.057
14	0.272	0.274	0.113	0.185	0.450	0.278	0.034	0.049
21	0.269	0.274	0.095	0.158	0.206	0.278	0.028	0.043
28	0.266	0.274	0.084	0.141	0.171	0.256	0.024	0.039
42	0.258	0.272	0.079	0.122	0.138	0.222	0.020	0.033
50	0.253	0.272	0.122	0.118	0.148	0.213	0.019	0.031
100	0.224	0.264	0.065	0.101	0.099	0.166	0.014	0.024

The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone, at Step 4 (60% run-off mitigation, corresponding to a 10 m vegetated filter strip) for spring application to winter cereals in run-off scenarios, are shown in Table 9.2.5-23, and the corresponding PEC_{Sed} values, are shown in Table 9.2.5-24. These values were not used in the risk assessment, since step 3 values are sufficient, but they are provided here for completeness.

Table 9.2.5-23: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 4 (60% run-off mitigation, corresponding to a 10 m vegetated filter strip) for flurtamone following spring application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	0.039	-	0.834		1.077		0.022	-
1	0.038	0.038	0.002	0.423	0.005	0.660	0.000	0.099
2	0.037	0.038	0.001	0.212	0.002	0.334	0.000	0.050
4	0.036	0.038	0.000	0.106	0.001	0.167	0.000	0.025
7	0.035	0.037	0.000	0.061	0.000	0.096	0.000	0.015
14	0.032	0.035	0.000	0.032	0.351	0.063	0.000	0.008
21	0.030	0.034	0.000	0.026	0.000	0.049	0.000	0.005
28	0.028	0.033	0.000	0.020	0.000	0.040	0.000	0.004
42	0.024	0.030	0.000	0.013	0.000	0.027	0.000	0.003
50	0.027	0.029	0.000	0.011	0.000	0.023	0.000	0.002
100	0.016	0.026	0.000	0.007	0.000	0.012	0.000	0.002

Table 9.2.5-24: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 4 (60% run-off mitigation, corresponding to a 10 m vegetated filter strip) for flurtamone following spring application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.168		0.255	-	0.374	-	0.063	-
1	0.168	0.168	0.149	0.212	0.233	0.327	0.036	0.051
2	0.168	0.168	0.112	0.177	0.178	0.277	0.026	0.042
4	0.168	0.168	0.084	0.139	0.135	0.221	0.019	0.032
7	0.168	0.168	0.067	0.113	0.107	0.179	0.014	0.029
14	0.166	0.168	0.053	0.087	0.214	0.137	0.010	0.025
21	0.165	0.168	0.044	0.074	0.100	0.136	0.008	0.023
28	0.163	0.167	0.039	0.066	0.083	0.125	0.012	0.021
42	0.158	0.167	0.037	0.057	0.067	0.108	0.008	0.018
50	0.155	0.166	0.057	0.055	0.071	0.104	0.007	0.017
100	0.137	0.162	0.030	0.047	0.048	0.081	0.013	0.013

The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone, at Step 4 (80% run-off mitigation, corresponding to a 20 m vegetated filter strip) for spring application to winter cereals in run-off scenarios, are shown in Table 9.2.5-25 and the corresponding PEC_{Sed} values, are shown in Table 9.2.5-26. These values were not used in the risk assessment, since step 3 values are sufficient, but they are provided here for completeness.

Table 9.2.5-25: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 4 (80% run-off mitigation, corresponding to a 20 m vegetated filter strip) for flurtamone following spring application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	0.030	-	0.524		0.733		0.322	-
1	0.030	0.030	0.000	0.221	0.000	0.346	0.000	0.099
2	0.030	0.030	0.000	0.111	0.000	0.175	0.000	0.050
4	0.029	0.030	0.000	0.056	0.000	0.088	0.000	0.025
7	0.028	0.029	0.000	0.032	0.543	0.055	0.000	0.014
14	0.026	0.028	0.425	0.018	0.000	0.040	0.000	0.007
21	0.024	0.027	0.000	0.016	0.242	0.030	0.000	0.005
28	0.022	0.026	0.000	0.012	0.000	0.023	0.000	0.004
42	0.019	0.025	0.000	0.008	0.000	0.017	0.000	0.003
50	0.020	0.025	0.029	0.007	0.022	0.014	0.000	0.002
100	0.011	0.021	0.000	0.004	0.000	0.007	0.000	0.002

Table 9.2.5-26: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 4 (80% run-off mitigation, corresponding to a 20 m vegetated filter strip) for flurtamone following spring application to winter cereals at 125 g/ha

Scenario	R1 Weiherbach Pond		R1 Weiherbach Stream		R3 Bologna Stream		R4 Roujan Stream	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.131		0.140	-	0.213	-	0.063	-
1	0.131	0.131	0.086	0.118	0.139	0.188	0.036	0.051
2	0.131	0.131	0.066	0.100	0.108	0.161	0.026	0.042
4	0.131	0.131	0.050	0.080	0.083	0.131	0.019	0.032
7	0.131	0.131	0.040	0.065	0.067	0.108	0.014	0.025
14	0.130	0.131	0.032	0.051	0.122	0.083	0.010	0.019
21	0.129	0.131	0.027	0.044	0.060	0.082	0.008	0.016
28	0.127	0.131	0.024	0.039	0.050	0.075	0.010	0.014
42	0.123	0.131	0.022	0.034	0.041	0.067	0.007	0.012
50	0.121	0.130	0.033	0.033	0.043	0.063	0.006	0.011
100	0.107	0.127	0.018	0.028	0.029	0.050	0.009	0.011

Conclusions

PEC_{SW} and PEC_{Sed} values for flurtamone and its metabolites at Steps 1 and 2 and in addition for flurtamone at Step 3 and flurtamone at Step 4 for run-off scenarios only, were calculated for application of flurtamone to winter cereals in the autumn or in spring. These values are suitable for use in risk assessments.

Report:	**KCP-9.2.5 /02; [redacted] IAJ. 2014b**
Title:	Predicted Environmental Concentrations in Surface Water (PEC_{SW}) and Sediment (PEC_{Sed}) for Flurtamone and its Metabolites Following Application to Spring Cereals
Organisation:	[redacted]
Report No.:	Battelle Report VC/13/0121 Bayer CropScience Document M-477734-01-1
Publication:	unpublished
Dates of experimental work:	Not applicable
Guidelines:	**Not relevant.**
Deviations:	Not relevant
GLP/GEP	**No – but conducted to Good Modelling Practice**

Executive Summary

Predicted environmental concentrations in surface water (PEC_{SW}) were calculated for flurtamone and the metabolites M04 TFMBA and M05 TFA (major soil metabolites), M07 flurtamone-carboxylic acid (major photolysis degradate) and M08 flurtamone desphenyl (major water-sediment metabolite) following application of flurtamone to spring cereals at 1 x 125 g/ha.

The calculations were conducted to FOCUS recommendations. Calculations were conducted for flurtamone and its metabolites at Steps 1 and 2 and in addition for flurtamone at Step 3. The values generated are suitable for use in risk assessments.

Methods and Materials

An assessment of the potential environmental risk of using a plant protection product includes a prediction of the exposure of non-target aquatic organisms. Such an exposure may occur by the unintentional introduction of a substance into surface water systems via spray-drift, run-off and / or drainage flow. The objective of this evaluation was the calculation of predicted environmental concentrations in surface water and sediment (PEC_{SW} and PEC_{Sed}) for flurtamone and its metabolites following application of flurtamone to spring cereals at 125 g/ha. The calculations followed the recommendations of the FOCUS Surface Water Scenarios Working Group [FOCUS**,** 2003 (Sanco/4802/2001-rev.2)], assuming spray-drift, run-off and drainage entry into three types of surface water bodies (pond, ditch, stream). The predicted concentrations can be compared to ecotoxicological effect data to derive the respective toxicity exposure ratios (TER).

Compound data. The data from soil degradation studies have been kinetically evaluated ([redacted] 2013a, M-475175-01-1 and b, M-475181-01-1) and the geometric mean DT_{50} for flurtamone was calculated as being 17.1 days, with that for M04 TFMBA being 10.4 days. For M05 TFA no robust

DT_{50} values could be derived and it was given a default DT_{50} of 1000 days. These values were used in the modelling.

The data from water-sediment studies have been kinetically evaluated ([redacted] 2013c, M-475187-01-1). The geometric mean total system $DegT_{50}$ value of 82.4 days was used in the modelling for the water phase along with a conservative $DegT_{50}$ of 1000 days for the sediment phase. The only major metabolite in water-sediment systems was was M08 flurtamone-desphenyl (AE 2093305) which reached 10.7% AR in the total system.

In the photolysis study only one major degradate was observed and that was M07 flurtamone carboxylic acid (AE 1083976) which occurred at a maximum of 33.5% AR. This figure was used in the calculations.

From the adsorption.desorption studies the mean K_{FOC} values of 257.1 mL/g (K_{OM} 149.2 mL/g) and 32.5 mL/g (K_{OM} 18.9 mL/g) for flurtamone and M04 TFMBA respectively along with the corresponding 1/n values of 0.876 and 0.670 were used in the calculations. For M05 TEA a K_{FOC} of 0 mL/g (K_{OM} 0 mL/g) was assumed with a 1/n value of 1 and these were used in the calculations.

Method and scenario data. For Step 1 and 2 estimations a standard ditch is defined. The distance between crop and water is fixed to 1 m. For Step 1 The input of pesticides into surface water by spray-drift and run-off / erosion / drainage is evaluated as one single worst-case entry event. Also, multiple applications are typically added at one time point. After entry into surface water, drift loadings are subsequently distributed between water and sediment (within 1 d), according to the compound's K_{oc}. The run-off/erosion/drainage entry (10 % of applied amount) is distributed instantaneously between water and sediment at the time of loading, according to the K_{oc}. The degradation in the water and in the sediment compartment follows a mono-exponential first-order kinetic.

For Step 2 The pesticidal input by spray-drift is evaluated by a series of individual loadings, according to the number of applications. The substance input by run-off / erosion / drainage (2 – 5 % of the soil residue) follows 4 d after the final application. Drift inputs are distributed between water and sediment, assuming a simplified partitioning kinetic for the portion of substance in water available for sorption. The run-off/erosion/drainage entry is distributed instantaneously between water and sediment at the time of loading according to the K_{oc}. The degradation in the water and in the sediment compartment follows a mono-exponential first-order kinetic. Northern and Southern European scenarios are considered.

For Step 3 of the European surface water assessment, the FOCUS working group defined 10 realistic worst-case scenarios, which collectively represent agronomic (soil, slope, crops) and climatic conditions in the EU. The scenarios were separated into drainage (6) scenarios and run-off (4) scenarios based on the relevant entry route, in addition to the spray-drift entry which is considered relevant for all sites. Three typical water bodies with different (and variable) residence times and different catchment areas – pond, ditch and stream – were identified and associated with the scenarios. Overall, the highest PEC_{sw} estimates from the ten scenarios are likely to represent at least a 90th percentile worst-case for surface water exposure in the EU.

A further step (Step 4) is available and this quantifies the effect of mitigation measures with regard to spray drift and run-off. Step 4 calculations were not necessary as the values obtained from Step 3 passed the ecotoxicological risk assessments.

Management and crop-related parameters. The GAP stipulates a single application to spring cereals of 125 g/ha at BBCH 00 to 09 (pre-emergence) or BBCH 10-29 (post-emergence). To cover the case of the pre-emergence application a 0% crop interception was selected for the Step 2 calculations. In Step 3, the plant interception is calculated within the models depending on the application time and the corresponding crop canopy development.

Soft and hardware. The drainage input of pesticides (with up to one metabolite) into surface water is simulated using the leaching model MACRO. The model simulates pesticide losses through bulk matrix flow and through macropore flow, as a separate flow domain assuming gravity flow. FOCUS MACRO considers a 6-year warm-up period with annual applications and a subsequent 16-month assessment period.

Run-off and erosion loadings (parent with up to 2 metabolites) into surface water are calculated using the leaching model PRZM (Pesticide Root Zone Model). This is a one-dimensional, dynamic, compartmental model, which simulates hydrology and substance transport in unsaturated soil systems. The hydrological component for calculating run-off and erosion is based on the USDA Soil Conservation Service curve number methodology and a watershed-scale variation of the Universal Soil Loss Equation. The PRZM in FOCUS shell runs a 20-year simulation with annual applications. A representative 12-month period out of these 20 years for different use patterns is selected and the results imported into TOXSWA.

For the purpose of this study, the activation energy (TOXSWA, J mol^{-1}), exponent (MACRO, 1/K) and (PRZM: Q_{10}) were set to 65400 J mol^{-1}, 0.095 and Q_{10} = 2.58, respectively. .

The behaviour of pesticides (only one compound) in a water body is simulated using the TOXSWA model. In FOCUS TOXSWA a standard pond, ditch and stream are assumed as stagnant or flowing water systems with time dependent water levels. TOXSWA handles transient hydrology and pesticide fluxes resulting from run-off, erosion and drainage calculated by the above described models. Entry via spray drift is additionally added here. Calculated water concentrations may vary in horizontal direction, whereas calculated sediment concentrations may be a function of both horizontal and vertical directions.

The calculations were carried out on a HP PC with Microsoft® Windows XP (SP3) as the operating system.

The input parameters are summarized in the tables that follow.

Table 9.2.5-27: Summary of substance input parameters – Flurtamone

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	333.3	-
Water solubility (mg L^{-1}) at 20°C; pH 7	11.5	[redacted], 1993 [M-162275-01-1]
Vapour pressure (Pa) at 20°C	7.0E-10	[redacted], 2006 [M-271433-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	17.1	[redacted], 2013a [M-475175-01-1]
Temperature correction function Reference temperature (°C) MACRO alpha (-) PRZM: Q_{10} (-)	 20 0.095 2.58	 FOCUS recommendation
Moisture correction function Reference moisture (-) Moisture exponent (-)	 pF2 0.7	 FOCUS recommendation
Degradation in water-sediment		
DT_{50} water (d)	82.40	[redacted], 2013c [M-475187-01-1]
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	82.40	[redacted], 2013c [M-475187-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	253.3 149.2	[redacted], 2011 [M-401274-01-1]
1/n (-)	0.876	
Management related parameters		
Crop uptake factor (-)	0	Conservative default assumption
Crop interception (%)	0	FOCUS recommendation

Table 9.2.5-28: Summary of substance input parameters – M04 TFMBA

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	190.1	-
Water solubility (mg L^{-1}) at 20°C; pH 8.9	164000	[redacted], 2012 [M-442190-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	10.4	[redacted], 2013b [M-475181-01-1]
Max. occur. in soil (%)	24.7	[redacted] 2012 [M-442039-01-1]
Degradation in water-sediment		
DT_{50} water (d)	1000	Consevative estimate
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	1000	Consevative estimate
Max. occur. in water/ sediment (%)	4.1	[redacted], 1997 [M-158694-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	15 8.7	[redacted], 1999 [M-207972-01-1]
Management related parameters		
Crop interception (%)	0	Conservative default assumption

Table 9.2.5-29: Summary of substance input parameters – M05 TFA

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	114.0	-
Water solubility (mg L^{-1}) at 20°C; pH 7	500000	[redacted], 2011 [M-420129-01-1]
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	1000	Default value, no apparent degradation under laboratory conditions: [redacted], 2012 [M-439283-01-1] [redacted], 2013b [M-475191-01-1]
Max. occur. in soil (%)	58.8*	[redacted], 2013b [M-475191-01-1] [redacted], 1993 [M-158234-01-1]
Degradation in water-sediment		
DT_{50} water (d)	1000	Consevative estimate
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	1000	Consevative estimate
Max. occur. in water/ sediment (%)	0.01	Conservative default assumption
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	0 0	[redacted], 2011 [M-406740-01-1]
Management related parameters		
Crop interception (%)	0	Conservative default assumption

* - Maximum of 9.8% [Burr and Austin, 1993] multiplied by 6 due to specific activity change during metabolism

Table 9.2.5-30: Summary of substance input parameters – M07 flurtamone carboxylic acid (AE 1083976, RPA 203597)

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g/mol^{-1})	309.3	-
Water solubility (mg L^{-1}) at 20°C; pH 7	1000	Consevative estimate
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	1000	Default value.
Max. occur. in soil (%)	0.01	Conservative default assumption
Degradation in water-sediment		
DT_{50} water (d)	1000	Consevative estimate
DT_{50} sediment (d)	1000	Consevative estimate
DT_{50} total system (d)	1000	Consevative estimate
Max. occur. in water/ sediment (%)	33.5	[redacted], 1993 [M-162275-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	1 0.58	Consevative estimate
Management related parameters		
Crop interception (%)	0	Conservative default assumption

Table 9.2.5-31: Summary of substance input parameters – M08 flurtamone desmethyl (AE 2093305, RPA 591120)

Parameter	Value	Remarks
Physico-chemical properties		
Molecular weight (g mol^{-1})	257.3	
Water solubility (mg L^{-1}) at 20°C; pH 7	1000	Conservative estimate
Degradation in soil		
DT_{50} soil (d) at 20°C and pF2	1000	Default value.
Max. occur. in soil (%)	0.01	Conservative default assumption
Degradation in water-sediment		
DT_{50} water (d)	1000	Conservative estimate
DT_{50} sediment (d)	1000	Conservative estimate
DT_{50} total system (d)	1000	Conservative estimate
Max. occur. in water/ sediment (%)	10.7	[redacted] 1997 [M-158694-01-1]
Sorption to soil		
K_{foc} (L kg^{-1}) K_{fom} (L kg^{-1})	1 0.58	Conservative estimate
Management related parameters		
Crop interception (%)	0	Conservative default assumption

Findings

The maximum Step 1 and Step 2 values for flurtamone and its metabolites are summarized in Table 9.2.5-32, below. This is followed by the actual and time-weighted averaged (TWA) PEC_{SW} values with time at Step 1 (Table 9.2.5-33) and the corresponding PEC_{Sed} values (Table 9.2.5-34).

Table 9.2.5-32: PEC_{SW} and PEC_{Sed} values at Step 1 and Step 2 for flurtamone and its metabolites following application of flurtamone to spring cereals at 125 g/ha

Compound	Step 1		Step 2 Northern Europe		Step 2 Southern Europe	
	PEC_{SW} (µg/L)	PEC_{Sed} (µg/kg)	PEC_{SW} (µg/L)	PEC_{Sed} (µg/kg)	PEC_{SW} (µg/L)	PEC_{Sed} (µg/kg)
Flurtamone	32.12	81.34	6.18	15.71	11.46	29.27
M04 TFMBA	5.78	0.83	0.91	0.14	1.79	0.27
M05 TFA	8.39	0.00	1.67	0.00	3.35	0.00
M07 [1] flurtamone-carboxylic acid	0.36	0.00	0.36	0.00	0.36	0.00
M08 [2] flurtamone-desphenyl	0.10	0.00	0.10	0.00	0.10	0.00

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-33: Actual PEC_{SW} values and time-weighted averaged (TWA) PEC_{SW} values at Step 1 for flurtamone and its metabolites , following application of flurtamone to spring cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	32.173	-	5.7817	-	8.3872		0.3612	-	0.0982	-
1	31.612	31.8928	5.7772	5.7794	8.3814	8.3843	0.3605	0.3609	0.0980	0.0981
2	31.347	31.6863	5.7732	5.7773	8.3756	8.3814	0.3603	0.3606	0.0979	0.0980
4	30.824	31.3858	5.7652	5.7732	8.3640	8.3756	0.3598	0.3603	0.0978	0.0979
7	30.056	30.9800	5.7532	5.7672	8.3466	8.3669	0.3590	0.3599	0.0976	0.0978
14	28.337	30.0844	5.7254	5.7532	8.3062	8.3467	0.3575	0.3590	0.0971	0.0976
21	26.717	29.2294	5.6976	5.7393	8.2660	8.3265	0.3556	0.3582	0.0966	0.0973
28	25.189	28.4085	5.6701	5.7255	8.2260	8.3064	0.3538	0.3573	0.0962	0.0971
42	22.391	26.8600	5.6153	5.6978	8.1466	8.2663	0.3504	0.3556	0.0952	0.0966
50	20.933	26.0270	5.5843	5.6822	8.1015	8.2436	0.3486	0.3546	0.0947	0.0964
100	13.746	21.5579	5.3940	5.5854	7.8156	8.1052	0.3366	0.3485	0.0915	0.0947

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-34: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 1 for flurtamone and its metabolites, following application of flurtamone to spring cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	79.8235	-	0.8632		0.0000	-	0.0000	-	0.0000	-
1	81.3388	80.5812	0.8666	0.8649	0.0000	0.0000	0.0036	0.0018	0.0010	0.0005
2	80.6574	80.7894	0.8660	0.8656	0.0000	0.0000	0.0036	0.0027	0.0010	0.0007
4	79.3118	80.3866	0.8648	0.8655	0.0000	0.0000	0.0036	0.0032	0.0010	0.0009
7	77.3353	79.5003	0.8630	0.8648	0.0000	0.0000	0.0036	0.0033	0.0010	0.0009
14	72.9130	77.3014	0.8588	0.8628	0.0000	0.0000	0.0036	0.0035	0.0010	0.0009
21	68.7436	75.1369	0.8546	0.8608	0.0000	0.0000	0.0036	0.0035	0.0010	0.0010
28	64.8125	73.0423	0.8505	0.8587	0.0000	0.0000	0.0035	0.0035	0.0010	0.0010
42	57.6120	69.0754	0.8423	0.8546	0.0000	0.0000	0.0035	0.0035	0.0010	0.0010
50	53.8626	66.9380	0.8376	0.8523	0.0000	0.0000	0.0035	0.0035	0.0009	0.0010
100	35.3690	55.4537	0.8091	0.8378	0.0000	0.0000	0.0034	0.0035	0.0009	0.0009

[1] RPA 203597 in report [2] RPA 591120 in report

The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone and its metabolites at Step 2 for Northern Europe and the corresponding PEC_{Sed} values are shown in Tables 9.2.5-35 and 9.2.5-36, with those for Southern Europe shown in Table 9.2.5-37 and Table 9.2.5-38.

Table 9.2.5-35: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 2 for Northern Europe for flurtamone and its metabolites following application of flurtamone to spring cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	6.1843	---	0.9081	---	1.6728	---	0.3574	--0	0.0953	-
1	6.0571	6.1207	0.9073	0.9077	1.6717	1.6723	0.3568	0.3571	0.0951	0.0952
2	6.0183	6.0792	0.9066	0.9073	1.6705	1.6717	0.3566	0.3569	0.0951	0.0952
4	5.9413	6.0295	0.9054	0.9067	1.6682	1.6705	0.3568	0.3567	0.0949	0.0951
7	5.8277	5.9673	0.9035	0.9057	1.6647	1.6688	0.3559	0.3566	0.0947	0.0950
14	5.5711	5.8329	0.8991	0.9035	1.6567	1.6647	0.3542	0.3558	0.0943	0.0948
21	5.3257	5.7044	0.8948	0.9013	1.6487	1.6607	0.3525	0.3550	0.0938	0.0945
28	5.0911	5.5802	0.8903	0.8992	1.6407	1.6567	0.3508	0.3542	0.0934	0.0943
42	4.6525	5.3430	0.8819	0.8948	1.6248	1.6487	0.3474	0.3525	0.0925	0.0938
50	4.4191	5.2137	0.8770	0.8924	1.6158	1.6442	0.3455	0.3515	0.0920	0.0936
100	3.2034	4.4962	0.8471	0.8772	1.5608	1.6162	0.3337	0.3455	0.0888	0.0920

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-36: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 2 for Northern Europe for flurtamone and its metabolites following application of flurtamone to spring cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PECSed (µg/kg)	TWA PECSed (µg/kg)	Actual PECSed (µg/kg)	TWA PECSed (µg/kg)	Actual PECSed (µg/kg)	TWA PECSed (µg/kg)	Actual PECSed (µg/kg)	TWA PECSed (µg/kg)	Actual PECSed (µg/kg)	TWA PECSed (µg/kg)
0	15.7057	--	0.1361	---	0.0000	---	0.0036	--	0.0010	-
1	15.6050	15.6554	0.1360	0.1360	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
2	15.5049	15.6052	0.1359	0.1360	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
4	15.3067	15.5054	0.1357	0.1359	0.0000	0.0000	0.0036	0.0036	0.0009	0.0010
7	15.0140	15.3573	0.1354	0.1358	0.0000	0.0000	0.0035	0.0036	0.0009	0.0009
14	14.3528	15.0191	0.1348	0.1354	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
21	13.7206	14.6909	0.1341	0.1351	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
28	13.1163	14.3722	0.1335	0.1348	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
42	11.9864	13.7625	0.1322	0.1341	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
50	11.3850	13.4298	0.1315	0.1338	0.0000	0.0000	0.0034	0.0035	0.0009	0.0009
100	8.2529	11.5824	0.1270	0.1315	0.0000	0.0000	0.0033	0.0034	0.0009	0.0009

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-37: Actual PEC_{SW} values with time and time-weighted averaged (TWA) PEC_{SW} values at Step 2 for Southern Europe for flurtamone and its metabolites following application of flurtamone to spring cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)	Actual PEC_{SW} (µg/L)	TWA PEC_{SW} (µg/L)
0	11.4603	---	1.7897	---	3.3456	---	0.3576	---	0.0959	--
1	11.2889	11.3746	1.7883	1.7890	3.3433	3.3445	0.3572	0.3574	0.0958	0.0958
2	11.2165	11.3137	1.7870	1.7883	3.3410	3.3433	0.3570	0.3572	0.0957	0.0958
4	11.0731	11.2292	1.7846	1.7871	3.3364	3.3410	0.3565	0.3570	0.0956	0.0957
7	10.8614	11.1168	1.7809	1.7852	3.3294	3.3375	0.3557	0.3566	0.0954	0.0956
14	10.3830	10.8686	1.7722	1.7800	3.3133	3.3294	0.3540	0.3557	0.0949	0.0954
21	9.9257	10.6300	1.7637	1.7706	3.2973	3.3214	0.3523	0.3549	0.0945	0.0952
28	9.4886	10.3989	1.7551	1.7723	3.2813	3.3134	0.3506	0.3540	0.0940	0.0949
42	8.6712	9.9572	1.7382	1.7637	3.2496	3.2974	0.3472	0.3523	0.0931	0.0945
50	8.2361	9.7163	1.7286	1.7589	3.2317	3.2883	0.3453	0.3513	0.0926	0.0942
100	5.9703	8.3794	1.6697	1.7289	3.1216	3.2323	0.3335	0.3453	0.0894	0.0926

[1] RPA 203597 in report [2] RPA 591120 in report

Table 9.2.5-38: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 2 for Southern Europe for flurtamone and its metabolites following application of flurtamone to spring cereals at 125 g/ha

Compound	Flurtamone		M04 TFMBA		M05 TFA		M07 [1] flurtamone-carboxylic acid		M08 [2] flurtamone-desphenyl	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	29.2715	---	0.2682	-	0.0000	---	0.0036	-	0.0010	-
1	29.0837	29.1776	0.2681	0.2681	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
2	28.8972	29.0840	0.2679	0.2681	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
4	28.5277	28.8981	0.2675	0.2679	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
7	27.9823	28.6221	0.2669	0.2676	0.0000	0.0000	0.0036	0.0036	0.0010	0.0010
14	26.7499	27.9918	0.2657	0.2669	0.0000	0.0000	0.0035	0.0036	0.0009	0.0010
21	25.5717	27.3800	0.2644	0.2663	0.0000	0.0000	0.0035	0.0035	0.0009	0.0010
28	24.4454	26.7861	0.2631	0.2657	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
42	22.3396	25.6497	0.2605	0.2644	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
50	21.2187	25.0296	0.2591	0.2636	0.0000	0.0000	0.0035	0.0035	0.0009	0.0009
100	15.3813	21.5867	0.2503	0.2592	0.0000	0.0000	0.0033	0.0035	0.0009	0.0009

[1] RPA 203597 in report [2] RPA 591120 in report

The maximum PEC_{SW} and PEC_{Sed} values with the dominant route of entry for each scenario at Step 3 are summarized in Table 9.2.5.39. The actual and time-weighted averaged (TWA) PEC_{SW} values with time for flurtamone at Step 3 for autumn application to winter cereals are shown in Table 9.2.5-40, and the corresponding PEC_{Sed} values, are shown in Table 9.2.5-41.

Table 9.2.5-39: Maximum PEC_{SW} and PEC_{Sed} values at Step 3 for flurtamone following application to spring cereals at 125 g/ha

Scenario	Application dates	$PEC_{SW, Max}$ ($\mu g\ L^{-1}$)	$PEC_{Sed, Max}$ ($\mu g\ kg^{-1}$)	Dominant entry route
D1 Lanna Ditch	25-Apr	0.857	1.036	Drift
D1 Lanna Stream	25-Apr-	0.693	0.307	Drift
D3 Vredepeel Ditch	17-Mar	0.791	0.295	Drift
D4 Skousbo Pond	18-Apr	0.028	0.099	Drift
D4 Skousbo Stream	18-Apr	0.616	0.026	Drift
D5 La Jailliere Pond	07-Mar	0.028	0.100	Drift
D5 La Jailliere Pond	07-Mar	0.612	0.016	Drift
R4 Roujan Stream	05-Mar	0.521	0.072	Drift

Table 9.2.5-40: Actual PECsw values with time and time-weighted averaged (TWA) PECsw values at Step 3 for flurtamone applied to spring cereals at 125 g/ha

Scenario	D1 Lanna Ditch		D1 Lanna Stream		D3 Vredepeel Ditch		D4 Skousbo Pond	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	0.857	-	0.693	-	0.791		0.028	-
1	0.747	0.795	0.034	0.112	0.327	0.595	0.027	0.027
2	0.666	0.751	0.034	0.074	0.038	0.371	0.026	0.027
4	0.430	0.658	0.036	0.055	0.003	0.191	0.025	0.026
7	0.083	0.451	0.035	0.054	0.001	0.110	0.024	0.026
14	0.057	0.258	0.034	0.052	0.000	0.055	0.023	0.025
21	0.053	0.194	0.031	0.050	0.000	0.037	0.021	0.024
28	0.050	0.162	0.030	0.049	0.000	0.028	0.019	0.023
42	0.043	0.133	0.017	0.047	0.000	0.018	0.016	0.021
50	0.035	0.126	0.000	0.046	0.000	0.016	0.015	0.020
100	0.011	0.093	0.000	0.041	0.000	0.008	0.009	0.016
Scenario	**D4 Skousbo Stream**		**D5 La Jailliere Pond**		**D5 La Jailliere Pond**		**R4 Roujan Stream**	
Time (d)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)	Actual PECsw (µg/L)	TWA PECsw (µg/L)
0	0.616	-	0.028	-	0.613		0.521	-
1	0.000	0.035	0.027	0.027	0.000	0.021	0.000	0.119
2	0.000	0.018	0.026	0.027	0.000	0.011	0.000	0.060
4	0.000	0.009	0.025	0.026	0.000	0.005	0.000	0.044
7	0.000	0.005	0.024	0.026	0.000	0.003	0.000	0.030
14	0.000	0.004	0.022	0.025	0.000	0.002	0.000	0.016
21	0.000	0.003	0.020	0.024	0.000	0.001	0.000	0.011
28	0.000	0.003	0.019	0.023	0.000	0.001	0.000	0.008
42	0.000	0.002	0.016	0.021	0.000	0.001	0.000	0.005
50	0.000	0.002	0.015	0.020	0.000	0.001	0.000	0.004
100	0.000	0.001	0.010	0.016	0.000	0.000	0.000	0.003

Table 9.2.5-41: Actual PEC_{Sed} values with time and time-weighted averaged (TWA) PEC_{Sed} values at Step 3 for flurtamone applied to spring cereals at 125 g/ha

Scenario	D1 Lanna Ditch		D1 Lanna Stream		D3 Vredepeel Ditch		D4 Skousbo Pond	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	1.036	-	0.307	-	0.295		0.099	-
1	0.967	1.031	0.283	0.295	0.225	0.282	0.099	0.099
2	0.891	1.020	0.274	0.287	0.171	0.256	0.099	0.099
4	0.794	0.985	0.269	0.279	0.125	0.210	0.099	0.099
7	0.723	0.925	0.269	0.278	0.097	0.171	0.099	0.099
14	0.648	0.823	0.270	0.278	0.071	0.128	0.099	0.099
21	0.615	0.765	0.271	0.278	0.059	0.108	0.098	0.099
28	0.595	0.728	0.272	0.278	0.052	0.095	0.098	0.099
42	0.564	0.681	0.264	0.278	0.043	0.079	0.096	0.099
50	0.543	0.662	0.224	0.273	0.040	0.073	0.095	0.099
100	0.423	0.575	0.157	0.252	0.029	0.053	0.089	0.097
Scenario	**D4 Skousbo Stream**		**D5 La Jailliere Pond**		**D5 La Jailliere Pond**		**R4 Roujan Stream**	
Time (d)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)	Actual PEC_{Sed} (µg/kg)	TWA PEC_{Sed} (µg/kg)
0	0.026	-	0.100	-	0.018		0.072	-
1	0.015	0.020	0.100	0.100	0.010	0.013	0.045	0.062
2	0.011	0.017	0.100	0.100	0.008	0.011	0.035	0.058
4	0.008	0.013	0.100	0.100	0.006	0.009	0.060	0.052
7	0.007	0.011	0.100	0.100	0.005	0.007	0.038	0.050
14	0.005	0.012	0.100	0.100	0.004	0.006	0.029	0.042
21	0.005	0.012	0.099	0.100	0.004	0.005	0.023	0.037
28	0.004	0.012	0.099	0.100	0.003	0.005	0.021	0.033
42	0.004	0.011	0.097	0.100	0.003	0.004	0.017	0.028
50	0.003	0.011	0.096	0.100	0.003	0.004	0.016	0.027
100	0.002	0.010	0.089	0.099	0.002	0.003	0.011	0.020

Conclusions

PEC_{SW} and PEC_{Sed} values for flurtamone and its metabolites at Steps 1 and 2 and in addition for flurtamone at Step 3 and flurtamone at Step 4 for run-off scenarios only, were calculated for application of flurtamone to spring cereals in the autumn or in spring. These values are suitable for use in risk assessments.

CP 9.3 - Fate and behaviour in air

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

Data on volatility submitted for Annex I inclusion and documented in the Review Report on flurtamone have been revised and new values determined under guideline OECD 104 have already been submitted at national level.

Flurtamone has vapour pressure values between 7.0 x 10^{-10} at 20°C and 2.0 x 10^{-9} Pa at 25°C and a Henry's law constant of 2.03 x 10^{-8} Pa m^3 mol^{-1} at 20°C ([redacted] 2006a M-271433-01-1 and b M-271434-01-1, see below). It therefore has a low potential to volatilise.

The results from studies on volatility from soil and plant surfaces ([redacted] 1995 M-219948-01-1 and [redacted] 1995 M-210853-01-1) showed that there was very little volatilization of the compound over a 24 hour period, in line with what be expected when the vapour pressure and Henry's law constant values are considered. In addition theoretical calculation of the potential for photo-oxidation ([redacted] 1994 M-162358-01-1) resulted in a half-life of 2 hours based on an OH radical concentration of 1.5 10^6 cm^{-3} on a 12 h day basis. Volatilization is not considered to be a route of dissipation of flurtamone in the environment.

The vapour pressure of flurtamone was determined by use of the gas saturation method, according to OECD 104 ([redacted] 2006a M-271433-01-1). Three different test temperatures were used (50, 60 and 70°C). The results were used in the calculation of the vapour pressures of flurtamone at 20 and 25°C. Values of 7 x 10^{-10} Pa (20°C) and 2.0 x 10^{-9} Pa (25°C) were obtained.

The Henry's law constant for flurtamone was determined at 20°C ((Bogdoll and Lemke, 2006b M-271434-01-1). It was determined according to the following formula:

$$K = \frac{P \times M}{Cs}$$

The Henry's law constant K was found to be 2.03 x 10^{-8} Pa m^3 mol^{-1}.

Summary of route of degradation in air and transport in air.

The vapour pressure of flurtamone means that it will not make its way into the atmosphere and so no degradation products will be formed in that compartment. The vapour pressures of its metabolites mean that they will not make their way into the atmosphere when formed in other environmental compartments such as soil and water. Thus it is not necessary to calculate PEC values in air.

CP 9.4 - Estimation of concentrations for other routes of exposure

There are no other routes of exposure for flurtamone and its metabolites.