European Commission

Renewal Assessment Report prepared according to the Commission Regulation (EU) N° 1107/2009

Triticonazole

Volume 3 – B.8 (AS)

Rapporteur Member State: Austria
Co-Rapporteur Member State: United Kingdom

Version History

When	What
September/2003	Initial DAR
September/2004	Addendum 1
January/2005	Addendum 2
July/2018	DRAR

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B.8. ENVIRONMENTAL FATE AND BEHAVIOUR AND ENVIRONMENTAL EXPOSURE ASSESSMENT

Triticonazole was originally included in Annex I of the EU Council Directive 91/414/EEC with Commission Directive 2006/39/EC (entry into force on 12th of April 2006). The active substance was subsequently approved under Regulation (EC) 1107/2009 via Implementing Regulation (EU) 540/2011. The associated review report is published under SANCO/10442/2005, final, rev 12, March 2010.

On the basis of the proposed and supported uses (as listed in Appendix II of the review report), the following particular issues have been identified as requiring particular and short term attention from all Member States, in the framework of any authorisations to be granted, varied or withdrawn, as appropriate:

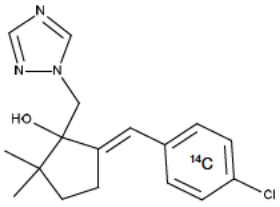
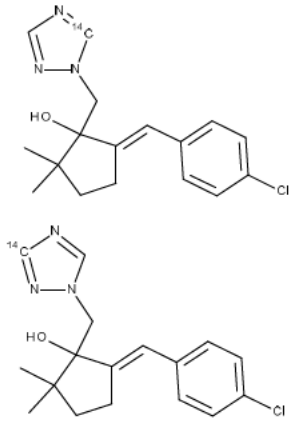
- must pay particular attention to the operator safety. Conditions of authorisation should include protective measures, where appropriate.
- must pay particular attention to the potential for groundwater contamination, in particular from the highly persistent active substance and its metabolite RPA 406341, in vulnerable zones;
- must pay particular attention to the protection of granivorous birds (long term risk).

Conditions of authorisation should include risk mitigation measures, where appropriate.

Data on the fate and behaviour of triticonazole in soil, water and air had been submitted for Annex I inclusion of triticonazole by the notifier BASF in 2003. This data were the basis for the DAR and its Addenda and are considered the Baseline Dossier for renewal. In accordance with Commission Regulation (EU) 844/2012 of 18th of September 2012, BASF submitted a Supplementary Dossier to support the renewal of the approval of triticonazole.

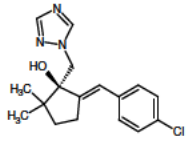
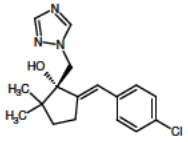
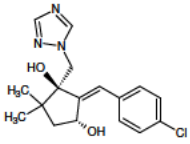
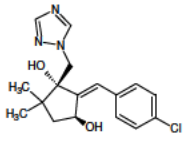
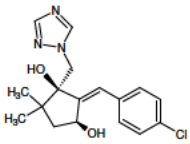
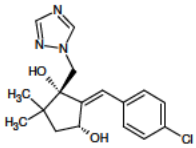
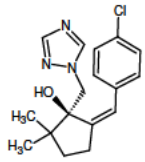
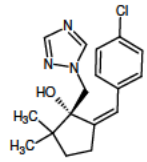
Baseline Dossier and Supplementary Dossier have been combined by the RMS AT into one consistent document and were evaluated altogether.

The studies investigating the environmental fate of triticonazole were performed with the following positions of ^{14}C-radiolabel:

	
[Phenyl-U-^{14}C]-triticonazole - 'Ph label'	[Triazole-3(5)-^{14}C]-triticonazole - 'T label'

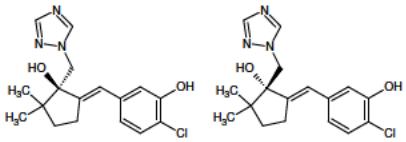
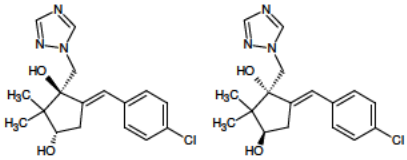
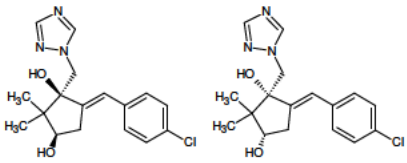
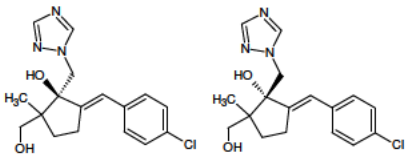
Details of the literature search undertaken can be found in chapter B.8.6, references relied on. With the exception of on paper on surface and groundwater monitoring in the US (Reilly et al., 2012) no relevant scientifically peer-reviewed open literature reference has been identified by the applicant for triticonazole or its metabolites with respect to fate and behaviour in the environment.

Table B.8-1 Parent triticonazole and metabolites of triticonazole identified in environmental fate studies

Code number (Synonyms)	Chemical name and molecular formula	Mol weight (g/mol)	Occurrence (% AR)	Structure
Triticonazole E-isomer (BAS 595 F, RPA 400727, M595F000)	(1*RS*, 5*E*)-5-(4-chlorobenzylidene)-2,2-dimethyl-1-(1*H*-1,2,4-triazol-1-ylmethyl) cyclopentanol $C_{17}H_{20}ClN_3O$	317.8	Not applicable (parent)	 *R*-isomer  *S*-isomer
RPA 406341 Trans-diol (Alpha-hydroxy-triticonazole, M595F002, AE 0540093, Reg. No. 5059144)	(1*RS*,2*E*,3*SR*)-2-(4-chlorobenzylidene)-5,5-dimethyl-1-(1*H*-1,2,4-triazol-1-ylmethyl)-1,3-cyclopentanediol $C_{17}H_{20}ClN_3O_2$	333.8	**Aerobic soil: 20.2** Anaerobic soil: 1.8 Soil photolysis: 3.5 Aquatic hydrolysis: ni Aquatic photolysis: ni Aerobic surface water: 1.8 Water/sediment: ni	 *RS*-isomer  *SR*-isomer
RPA 404766 Cis-diol (Beta-hydroxy-triticonazole, M595F001, AE 0591653, Reg. No. 5079285)	(1*RS*,2*E*,3*RS*)-2-(4-chlorobenzylidene)-5,5-dimethyl-1-(1*H*-1,2,4-triazol-1-ylmethyl)-1,3-cyclopentanediol $C_{17}H_{20}ClN_3O_2$	333.8	**Aerobic soil: 13.9**[a] Anaerobic soil: 2.0 Soil photolysis: 3.3 Aquatic hydrolysis: ni Aquatic photolysis: ns Aerobic surface water: 1.3 Water/sediment: ni	 *RR*-isomer  *SS*-isomer
RPA 406203 Z-isomer (M595F014, Reg. No. 5079359)	(1*RS*, 5*Z*)-5-(4-chlorobenzylidene)-2,2-dimethyl-1-(1*H*-1,2,4-triazol-1-ylmethyl) cyclopentanol $C_{17}H_{20}ClN_3O$	317.8	Aerobic soil: 4.4 Anaerobic soil: - **Soil photolysis: 11.0** Aquatic hydrolysis: 2.6 **Aquatic photolysis: 42.3**[b] Aerobic surface water: 4.2[c] Water/sediment: ni	 *R*-isomer  *S*-isomer

ni denotes not investigated (below 5 % AR)
ns denotes not stated (below 5 % AR)
(a) 10 °C study (max. 9.9 % AR in 20 - 25 °C studies)
(b) Without sensitizer
(c) Arithmetic mean of phenyl and triazole label

Table B.8-2 **Other metabolites of triticonazole originally considered as possible metabolites of triticonazole (considered not to occur at significant amounts in environmental compartments following re-evaluation)**

Code number (Synonyms)	Chemical name and molecular formula	Mol weight (g/mol)	Occurrence (% AR)	Structure
RPA 407922 (M595F013, Reg. No. 5079288)	2-chloro-5-{(E)-[(2RS)-2-hydroxy-3,3-dimethyl-2-(1H-1,2,4-triazol-1-ylmethyl)cyclopentylidene]methyl}phenol $C_{17}H_{20}ClN_3O_2$	333.8	Unlikely to occur at significant (> 5 % AR) amounts in environmental compartments	 *R*-isomer *S*-isomer
RPA 406780[(a)]	(1SR,3RS,5E)-5-(4-chlorobenzylidene)-2,2-dimethyl-1-(1H-1,2,4-triazol-1-ylmethyl)cyclopentane-1,3-diol $C_{17}H_{20}ClN_3O_2$	333.8	Unlikely to occur at significant (> 5 % AR) amounts in environmental compartments	 *RS*-isomer *SR*-isomer  *RR*-isomer *SS*-isomer
RPA 404886 (M595F005, Reg. No. 5079247)	(1*RS*,5*E*)-5-(4-chlorobenzylidene)-2-(hydroxymethyl)-2-methyl-1-(1*H*-1,2,4-triazol-1-ylmethyl) cyclopentanol $C_{17}H_{20}ClN_3O_2$	333.8	Unlikely to occur at significant (> 5 % AR) amounts in environmental compartments	 *R*-isomer *S*-isomer

(a) Isomeric composition not specified further (Trans- vs. Cis-diol)

B.8.1. FATE AND BEHAVIOUR IN SOIL

B.8.1.1. Route of degradation in soil

B.8.1.1.1. Aerobic degradation

Studies submitted for first Annex I inclusion:

- **Ayliffe & Austin (1993)**, investigating phenyl labelled triticonazole in three soils at 22 °C
- **Ayliffe & McMillan-Staff (1994)**, investigating phenyl labelled triticonazole in one soil at 22 °C
- **Ayliffe & Godward (1993)**, investigating phenyl labelled triticonazole in three soils at 10 °C and in one soil at 10 and 22 °C
- **Doble et al. (1996)**, investigating triazole labelled triticonazole in one soil at 25 °C
- **Simmonds et al. (1996)**, investigating phenyl labelled triticonazole in one soil at contrasting incubation conditions
- **Simmonds & Lowden (2002)**, generating metabolites of triticonazole for identification

New studies submitted:

- **Ta & Strobush (2012)**, investigating phenyl and triazole labelled triticonazole in three US soils at 20 °C
- **Ta & Strobush (2015)**, investigating phenyl and triazole labelled triticonazole in one soil at 20 °C
- **Szegedi (2018)**, investigating the structure of the two metabolite fractions 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' observed > 5 % AR at two consecutive sampling points in Ayliffe & Austin (1993)

Reference:	**Fungicides: RPA 400727-^{14}C: Aerobic soil metabolism in three soils (Final report)**
Author(s), year:	Ayliffe, J. M., Austin, D. J., 1993
Report/Doc. Number:	C017917, 428635, P91/326, 200159
Guideline(s):	US-EPA N, 162-1 (1982) (not stated in report)
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

An aerobic soil metabolism study was performed over 363 days with [phenyl-U-^{14}C]-triticonazole (called RPA 400727 in the study report) in a UK clay loam, UK sandy loam and a Speyer 2.2 loamy sand (German standard) soils. The nominal dose rate was equivalent to 385 g ai/ha or 1.70 mg/kg triticonazole (assuming 200 g ai/100 kg seeds applied at 180 kg seed/ha). Each soil sample was brought to nominally 75 % of 0.33 bar water capacity. The study was performed in the dark at 22 ± 2 °C.

The soils were Soxhlet extracted with 140 ml acetonitrile/water (4:1, v/v). Analytical analyses were carried out with TLC and HPLC (isocratic method for metabolite quantification). Reference substances used: RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 404886, RPA 406780, RPA 407341.

Table B.8.1.1.1-1 Soil Characteristics

Soil[(a)]	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H[(b)]	CEC (meq/ 100 g)	WHC at 33 kPa (%)	Biomass (start) µg C/g soil	Biomass (168 DAT) µg C/g soil	Biomass (365 DAT) µg C/g soil
UK sandy loam	73	15	12	1.24	6.42	8.2	11.6	130	88	104
UK clay loam	45	33	22	9.76	6.18	34.6	31.4	1032	897	783
Speyer 2.2 loamy sand	83	9	8	5.7	6.3	10.8	10.65	376	257	182

(a) Texture classification not specified

(b) Matrix not specified

Findings:

Table B.8.1.1.1-2 Recovery (% AR, mean of duplicate samples, HPLC)

DAT	Extractable	NER	CO_2	Other volatiles	Total
			UK sandy loam		
0	89.9	0.3	na	na	90.2
1	89.9	0.6	0.0	0.0	90.5
7	90.0	1.2	0.1	0.1	91.4
14	92.0	1.9	0.2	0.1	94.1
28	89.7	2.8	0.4	0.1	93.0
56	86.3	4.8	1.0	0.1	92.2
84	82.5	5.9	2.0	0.1	90.6
112	77.9	7.5	3.0	0.2	88.5
140	80.0	7.9	4.1	0.2	92.2
168	79.6	7.9	5.2	0.2	92.8
224	73.8	10.0	6.3	0.2	90.3
266	65.0	12.7	7.5	0.2	85.4
363	66.2	14.7	8.4	0.2	89.5
			UK clay loam		
0	93.4	0.2	na	na	93.6
1	101.9	0.6	0.0	0.0	102.5
7	101.4	0.9	0.2	0.0	102.4
14	98.5	2.0	0.5	0.0	101.0
28	96.6	2.8	1.3	0.0	100.7
56	87.4	4.7	2.6	0.5	95.2
84	86.2	5.9	5.2	0.6	97.9
112	78.5	9.4	8.1	0.6	96.8
140	75.1	10.2	10.7	0.6	96.7
168	69.1	10.8	13.3	0.6	93.8
224	62.5	13.1	15.8	1.0	92.3
266	53.1	14.8	19.1	1.0	88.0
363	47.4	17.9	23.9	1.0	90.2
			Speyer 2.2 loamy sand		
0	94.9	0.3	na	na	95.3
1	94.7	2.2	0.0	0.0	96.9
7	95.7	0.6	0.1	0.0	96.3
14	96.0	1.4	0.1	0.0	97.5
28	89.7	1.9	0.2	0.0	91.8
56	91.7	2.3	0.3	0.0	94.4
84	90.7	2.3	0.4	0.0	93.3
112	88.5	3.1	0.5	0.0	92.2
140	93.9	2.8	0.6	0.0	97.4
168	88.9	3.5	0.9	0.0	93.3
224	86.0	3.7	1.4	0.1	91.1
266	86.7	5.2	1.6	0.1	93.5
363	89.6	8.0	2.1	0.1	99.7

For each soil at all time points and for each pair of soil duplicate samples, a good radiochemical balance was achieved with the mean recoveries (of the duplicate means) of applied radioactivity greater than 90 %.

The unextractable soil bound residue reached 7.5, 9.4 and 3.1 % of applied radioactivity 112 days after application for the UK sandy loam, UK clay loam and Speyer 2.2 loamy sand soils, respectively. Trapped ^{14}C-carbon dioxide amounted to 3.0, 8.1 and 0.5 % of applied radioactivity 112 days after application, respectively. Other trapped volatiles amounted to a maximum of 1 % of applied radioactivity after 363 days. The radioactivity of bound residues is distributed amongst the soil fractions, the major portion is seen in the humin fraction.

In the UK sandy loam soil, the proportion of parent triticonazole present decreased to 44.5 % of applied radioactivity 363 days after application. In the UK clay loam soil, the proportion of parent present decreased to 18 % of applied radioactivity 363 days after application.

In the Speyer 2.2 loamy sand soil, the proportion of parent triticonazole present only decreased to 70 % of applied radioactivity 363 days after application. In addition, only 2.1 % of applied radioactivity had been trapped as ^{14}C-carbon dioxide by the end of the incubation time (363 days after application). Therefore, it was concluded that the soil batch used for the investigation was microbially compromised, and the results obtained unreliable. As such, an additional investigation with another batch of the Speyer 2.2 loamy sand soil was conducted and is reported in the next study (Ayliffe & McMillan-Staff, 1994).

Table B.8.1.1.1-3 Characterisation of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR)

DAT	Triti-conazole	RPA 404766[(a)] (Cis-diol)	RPA 404886	RPA 406341 (Trans-diol)	MWT 333[(b)]	MWT 349	MWT 333[(c)]	MWT 315	-	-	-	-
Code	-	Met 1	Met 2	Met 3	Met 4	Met 5	Met 6	Met 7	Met 8	Met 9	Met 10	Met 11
rRT	*1.00*	*0.33*	*0.38*	*0.45*	*0.51*	*0.55*	*0.63*	*0.70*	*0.80*	*1.05*	*1.13*	*1.29*
UK sandy loam												
0	90.0	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1	89.9	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
7	87.5	1.2	nd	1.4	nd	nd	nd	nd	nd	nd	nd	nd
14	88.2	2.1	nd	1.8	nd	nd	nd	nd	nd	nd	nd	nd
28	80.3	3.6	0.3	4.4	nd	nd	0.3	nd	1.0	nd	nd	nd
56	67.4	5.4	1.1	8.6	nd	0.9	nd	3.0	nd	nd	nd	nd
84	71.3	2.3	nd	6.6	nd	nd	nd	2.4	nd	nd	nd	nd
112	57.5	3.9	2.5	7.2	nd	1.6	nd	4.3	1.0	nd	nd	nd
140	63.5	3.4	1.0	5.3	nd	1.7	nd	4.6	nd	nd	nd	nd
168	60.6	5.1	2.7	7.2	nd	0.9	nd	2.8	0.6	nd	nd	nd
224	46.9	3.5	3.5	5.8	nd	2.4	2.5	6.1	nd	nd	3.3	nd
266	40.6	6.1	nd	6.1	0.5	3.2	1.4	6.5	nd	nd	nd	0.8
363	44.7	6.6	nd	3.0	nd	2.7	4.2	5.3	nd	nd	nd	nd
UK clay loam												
0	93.4	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
1	101.9	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
7	95.4	3.2	nd	2.5	nd	nd	nd	nd	0.3	nd	nd	nd
14	87.9	5.6	nd	4.6	nd	nd	nd	0.4	nd	nd	nd	nd
28	84.4	6.3	0.3	5.5	nd	nd	nd	nd	0.3	nd	nd	nd
56	67.6	6.7	1.2	8.1	nd	1.6	2.0	0.4	nd	nd	nd	nd
84	69.6	5.7	nd	6.9	nd	1.6	2.5	nd	nd	nd	nd	nd
112	52.7	6.4	1.0	9.0	nd	3.9	4.5	0.7	0.3	nd	nd	nd
140	51.8	5.4	1.1	8.1	0.2	4.2	5.8	nd	nd	nd	nd	nd
168	39.7	4.7	0.9	8.5	nd	5.5	7.9	0.3	nd	nd	1.1	2.6
224	31.5	4.9	1.0	7.4	nd	5.9	9.0	nd	nd	1.0	1.3	0.6
266	24.0	4.6	0.3	6.3	nd	5.2	12.8	nd	nd	nd	nd	nd
363	17.7	3.0	nd	7.5	nd	6.8	11.7	0.9	nd	nd	nd	nd

nd denotes not detected
(a) In this study erroneously considered to be RPA 406780, identified as RPA 404766 (Cis-diol) in later studies when analytical systems became more sophisticated (RPA 406780 and RPA 404766 (Cis-diol) co-elute under the isocratic HPLC method as 'Met 1')
(b) Claimed in Ayliffe & Godward (1994) having a MWT of 333
(c) Claimed in Ayliffe & Godward (1994) being identified as RPA 407922 (refer to comments)

Metabolites

In the UK sandy loam soil up to 10 metabolites were quantified. Met 1 (RPA 404766, Cis-diol) (in this study erroneously considered to be RPA 406780, identified as RPA 404766 in later studies) up to 6.6 % AR (DAT 363), Met 3 (RPA 406341, Trans-diol) up to 8.6 % AR (DAT 56) and Met 7 (MWT 315) was measured in amounts up to 6.5 % AR (DAT 266). The other metabolites were found with amounts < 5 % AR.

Up to 11 metabolites were quantified in the UK clay loam soil. Met 6 (MWT 333) was found in amounts up to 12.8 % AR (DAT 266), Met 1 (RPA 404766, Cis-Diol) up to 6.7 % AR, Met 3 (RPA 406341, Trans-diol) up to 9.0 % AR and Met 5 (MWT 349) up to 6.8 % AR. The other metabolites were not seen consistently and reached a maximum individual value of 2.6 % AR.

RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) are stereoisomers.

Conclusion:

In the metabolism study with 3 soils with phenyl ring labelled triticonazole at least 11 metabolites were quantified. Three of them amounted for more than 10 % AR in at least one of the test soils or reached almost 10 % AR at study termination. These major metabolites are:

- Met 1 = RPA 404766 (Cis-diol) (in this study erroneously considered to be RPA 406780, identified as RPA 404766 in later studies)
- Met 3 = RPA 406341 (Trans-diol)
- Met 6 (MWT 333)

Two metabolites, Met 5 (MWT 349) and Met 7 (MWT 315), reached amounts > 5 % AR in two consecutive measurements during the study.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some deviations:
  - The test duration of 363 days is beyond the recommended study duration of about 120 days recommended in the OECD guideline 307. However, OECD guideline 307 indeed recommends continuing the incubation for longer periods (e.g. 6 or 12 months) where necessary to characterise the decline of the test substance and the formation and decline of major transformation products. In view of the limited degradation of triticonazole in aerobic laboratory soil incubation experiments accompanied by late formation of degradation products the RMS AT considers the entire one-year incubation period representative for triggering identification of metabolites in line with Regulation (EU) No. 283/2013. Notice that on basis of soil microbial biomass measurements at the start and end of incubation the two UK soils are indeed not considered being microbially exhausted during the incubation. Microbial biomass C was well above 1 % of total organic C at the start and end of incubation in the UK sandy loam and UK clay loam. In the Speyer 2.2 loamy sand microbial biomass C was 0.8 % of total organic C when initiating the incubation declining to 0.6 % by study end. Subsequently, an additional incubation was conducted with a different and more viable batch of this soil (refer to Ayliffe & McMillan-Staff, 1994, next study). The RMS AT agrees to replace data obtained in this study with data obtained from the more viable batch used in Ayliffe & McMillan-Staff (1994).
  - With a nominal dose rate of 385 g ai/ha the study is clearly overdosed considering the intended field application rate of 12.5 g ai/ha only
  - Mass balance was below 90 % in some rare cases
  - There is no information available about the duration of soil storage (storage temperature was stated being 20 °C)
  - No information is available on the history of the field site, the way of sampling and the transportation of the soil
  - No information is available on the pre-equilibration phase
  - The organic carbon content of the UK clay loam is not within the range recommended by OECD 307 (i.e. 0.5 to 2.5 %)
  - The LOD and LOQ of the analytical method were not specified in the study report

  On overall the study is still considered reliable, results obtained are not in contradiction with results obtained in more recent studies.

- The RMS AT notes that at time of study conduction knowledge on possible triticonazole metabolites and most suitable HPLC separation techniques to separate them was fairly limited. The study authors used an isocratic HPLC method (acetonitrile/water/acetic acid, 40:60:2, v/v/v) for metabolite profiling, which in later studies (Doble et al., 1996, Simmonds et al., 1996, Simmonds & Lowden, 2002) was shown not to be capable to adequately separate all metabolites of triticonazole.

This particularly refers to RPA 406780 considered to represent 'Met 1' in this study. In Doble et al. (1996) and Simmonds et al. (1996), both applying a more advanced gradient HPLC method, it became evident that RPA 406780 is unlike to occur in soils at significant amounts at all. Instead, RPA 404766 (Cis diol), more or less co-eluting with RPA 406780 under conditions of the isocratic method, is representing 'Met 1' observed in this study.

Based on Doble et al. (1996) and Simmonds et al. (1996) it is also unlikely that 'Met 2' in this study can be unambiguously identified being RPA 404886. In view of the RMS AT 'Met 2' (below 5 % AR in any case) remains unidentified. As indicated in Doble et al. (1996) and Simmonds et al. (1996) RPA 404886 is unlikely to occur at significant amounts in soils.

In the next study, Ayliffe & McMillan-Staff (1994), 'Met 6 (MWT 333)' observed in this study at 12.8 % AR in the UK clay loam was claimed being identified as RPA 407922. The RMS strongly challenges this finding as explained more in detail in Ayliffe & McMillan-Staff (1994). Notice that the applicant proposal for 'Met 6 (MWT 333)' being RPA 407922 was indeed accepted for first Annex I inclusion, triggering several further studies conducted with RPA 407922 (amongst them metabolite dosed degradation, sorption and ecotox studies). For renewal the applicant was requested by the RMS AT to further underpin their identification proposal with additional data (preferably with HPLC chromatograms on authentic reference substances applying the same HPLC methods as used in these early reports demonstrating that RPA 407922 may have eluted in the range of 'Met 6 (MWT 333)' at the time of study conduction). As discussed more in detail in the next study the applicant finally agreed with the conclusion of the RMS AT that 'Met 6 (MWT 333)' in the chromatograms of this study does not belong to the metabolite RPA 407922 but to an unidentified structure. In a new position paper (Szegedi, 2018) the applicant indicates possible structures for 'Met 6 (MWT 333)' as well as for 'Met 7 (MWT 315)'.

- As investigated further in Simmonds & Lowden (2002), metabolite fraction 'Met 5 (MWT 349)' is likely to comprise two unidentified metabolites, which can be separated under conditions of gradient HPLC, one with a MWT of 333 g/mol, one with a MWT of 349 g/mol. In Simmonds & Lowden (2002) these two compounds were observed at almost equimolar amounts (one soil). On basis of these findings, 'Met 5 (MWT 349)' is unlikely to exceed 5 % AR in the UK clay loam soil on basis of its individual constitutes.

- The RMS notes that HPLC peaks eluting after triticonazole (rRT > 1) were tentatively assigned having a MWT of 333 as well (possibly corresponding to 'Met 11').

- It may be noted that final residue data on triticonazole and its metabolites in the UK sandy loam and in the UK clay loam presented in Table B.8.1.1.1-3 are based on values given in the addendum report of this study (i.e. Ayliffe & McMillan-Staff, 1994, next study).

Reference:	**Addendum Report: Fungicides: RPA 400727-^{14}C: Aerobic soil metabolism in three soils**
Author(s), year:	Ayliffe, J. M., McMillan-Staff, S. L., 1994
Report/Doc. Number:	R012981, P91/326, 200471
Guideline(s):	USEPA (= EPA) N, 162-1 (1982) (not stated in report)
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

An additional aerobic soil metabolism study was performed over 357 days with [phenyl-U-^{14}C]-triticonazole (called RPA 400727 in the report) in a Speyer 2.2 loamy sand (German standard) soil. The nominal dose rate

was equivalent to 360 g ai/ha or 1.46 ppm triticonazole (assuming 200 g ai/100 kg seeds applied at 180 kg seed/ha). Each soil sample was brought to nominally 75 % of 0.33 bar water capacity. The study was performed in the dark at 22 ± 2 °C. Soil samples were extracted by Soxhlet with acetonitrile/water (4:1, v/v) for three hours. Each extract was subjected to quantitative radioassay by direct liquid scintillation counting. Determinations of parent compound and its metabolites in the soil extracts were carried out by thin-layer chromatography (TLC) and high performance liquid chromatography (HPLC) (isocratic method for metabolite quantification).

Further work based on gradient HPLC and MS was also carried out to identify the major metabolites found in the UK clay loam extracts from the main study above (Ayliffe & Austin, 1993). Reference substances used: RPA 407922.

Table B.8.1.1.1-4 Soil Characteristics

Soil[(a)]	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H[(a)]	CEC (meq/100 g)	WHC at 33 kPa (%)	Biomass (start) µg C/g soil	Biomass (end) µg C/g soil
Speyer 2.2 loamy sand	89	6	5	4.05	6.8	10.0	16.6	394	186

(a) Texture classification not specified
(b) Matrix not specified

Findings:

Table B.8.1.1.1-5 Recovery (% AR, HPLC, mean of duplicate samples)

DAT	Extractable	NER	CO_2	Other volatiles	Total
0	96.2	0.8	na	na	97.0
14	89.9	1.1	0.1	0.1	91.2
28	80.2	2.6	0.3	0.1	83.2
56	85.6	3.3	0.8	0.1	89.7
84	89.1	3.4	1.0	0.1	93.5
140	89.3	4.5	1.5	0.3	95.6
210	76.2	6.4	1.6	0.3	84.5
280	77.8	5.1	1.8	0.3	85.0
357	77.1	6.4	2.1	0.3	86.0

na denotes not analysed

Table B.8.1.1.1-6 Characterisation of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR)

DAT	Triti-conazole	RPA 404766[(a)] (Cis-diol)	RPA 404886	RPA 406341 (Trans-diol)	MWT 333	MWT 349	MWT 333[(b)]	MWT 315	-	-	-	-
Code		Met 1	Met 2	Met 3	Met 4	Met 5	Met 6	Met 7	Met 8	Met 9	Met 10	Met 11
rRT	*1.00*	*0.33*	*0.38*	*0.45*	*0.51*	*0.55*	*0.63*	*0.70*	*0.80*	*1.05*	*1.13*	*1.29*
0	96.2	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
14	84.0	2.8	nd	2.8	0.5	nd	nd	nd	nd	nd	nd	nd
28	69.9	4.8	nd	5.1	nd	nd	nd	nd	0.8	nd	nd	nd
56	66.8	7.0	0.6	8.0	nd	nd	nd	0.9	2.5	nd	nd	nd
84	67.9	9.9	nd	11.4	nd	nd	nd	nd	nd	nd	nd	nd
140	55.4	8.8	1.5	13.3	nd	1.1	nd	2.2	3.6	0.1	3.4	nd
210	sample not analysed by HPLC											
280	40.4	7.5	1.5	13.4	nd	1.6	0.3	3.6	3.6	1.4	2.6	nd
357	37.5	8.7	0.6	15.3	nd	0.9	1.6	1.0	4.2	0.9	2.9	nd

nd denotes not detected
(a) In this study erroneously considered to be RPA 406780, identified as RPA 404766 (Cis-diol) in later studies when analytical systems became more sophisticated
(b) Claimed identified as RPA 407922 in this study (refer to comment section)

A radiochemical balance was achieved with a mean recovery (of the duplicate means) of applied radioactivity of 89.5 % (83.2 – 97.0 % AR). The unextractable soil bound residue reached 4.5 % of applied radioactivity and trapped ^{14}C carbon dioxide amounted to 1.5 % of applied radioactivity, 140 days after application. Other trapped volatiles amounted to less than 1 % AR after 357 days.

Up to 6 metabolites were quantified. Beside this small amount of polar compounds were found. Met 1 (= RPA 404766, Cis-Diol) (in this study erroneously considered to be RPA 406780) was found in amounts up to 9.9 % AR (DAT 84) and Met 3 (= RPA 406341, Trans diol) in amounts up to 15.3 % AR (DAT 357). Other metabolites were all present at < 5 % AR.

On basis of retention time (gradient HPLC) Met 6 (MWT 333, see previous study, Ayliffe & Austin, 1993) was identified as RPA 407922. This was confirmed by LC-MS.

At the completion of both phases of the study 84 % of the extractable material in the UK clay loam soil experiment was positively identified with a further 14 % being fully characterised. For the UK sandy loam experiment the figures were 88 % and 4 % respectively, whilst for the second Speyer 2.2 loamy sand experiment they were 82 % and 1 %.

Conclusions (including Ayliffe & Austin, 1993):

Under aerobic conditions triticonazole was metabolised in soil to a variety of compounds that were chemically and chromatographically very similar. RPA 404766 (Cis-diol), RPA 406341 (Trans-diol) and RPA 407922 (= Met 6), were found to be major soil metabolites. Triticonazole was metabolised in all soils via hydroxylation (yielding up to 11 metabolites) followed by degradation via the formation of unextractable soil bound residues and ultimately CO_2.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some deviations:
  - The test duration of 363 days is beyond the recommended study duration of about 120 days recommended in the OECD guideline 307. The same as mentioned in Ayliffe & Austin (1993) applies for this study as well. Microbial biomass C was well above 1 % of total organic C at the start of incubation (1.7 %) declining to 0.8 % of total organic C by study end.
  - With a nominal dose rate of 385 g ai/ha the study is clearly overdosed considering the intended field application rate of 12.5 g ai/ha only
  - Mass balance was below 90 % in some cases leading to some uncertainties regarding maximum occurrence of metabolites.
  - There is no information available about the duration of soil storage (storage temperature was 20 °C)
  - No information is available on the history of the field site, the way of sampling and the transportation of the soil
  - No information is available on the pre-equilibration phase
  - The LOD and LOQ of the analytical method were not specified in the study report

  On overall the study is still considered reliable, results obtained are not in contradiction with results obtained in more recent studies.

- The RMS AT agrees with the applicant, that this additional incubation with another, more viable batch of the Speyer 2.2 loamy sand should replace results obtained by Ayliffe & Austin (1993) applying a less viable batch of this soil (with a microbial biomass C below 1 % of total organic C already at start of incubation).

- As the study authors used the same isocratic HPLC method for metabolite profiling as used in Ayliffe & Austin (1993), the same shortcomings as mentioned in Ayliffe & Austin (1993) apply to this study as well.

- Metabolite fraction 'Met 6 (MWT 333)' was not observed at significant amounts in the Speyer 2.2 loamy sand. However, the study authors investigated samples from the UK clay loam originating from Ayliffe & Austin (1993) further, applying a more sophisticated gradient HPLC method. On basis of retention times 'Met 6 (MWT 333)' was tentatively identified as RPA 407922. Later this was claimed

being confirmed by atmospherically pressure chemical ionisation (APCI) mass spectroscopy on basis of a slightly modified isocratic HPLC method. Finally, the peak assignment of 'Met 6 (MWT 333)' being RPA 407922 was accepted for first Annex I listing and triggered several further studies (fate and ecotox studies) as 'Met 6 (MWT 333)' was considered a major metabolite of triticonazole ins soil exceeded 10 % in the UK clay loam.

On closer inspection, the RMS AT came to the conclusion that the limited information provided in this study report (HPLC chromatograms as well as mass spectra) does not allow to unambiguously verifying this structure proposal. As demonstrated e.g. in Simmonds and Lowden (2002) RPA 407922 usually does not eluate that late under conditions of the isocratic method used in Ayliffe & Austin (1993). Instead, RPA 407922 was shown to practically co-eluates with RPA 406341 (Trans-diol) if applying the isocratic method. The more advanced gradient HPLC, additionally applied in this study to elucidate 'Met 6 (MWT 333)' is very close to the HPLC method applied in Doble et al. (1996) and Simmonds et al. (1996). In the latter two studies, RPA 407922 immediately eluted after RPA 406341 (Trans-diol) and could in principal be separated from RPA 406341 (Trans-diol). However, without carefully considering both substances as reference material in accompanying HPLC runs, there is a risk of misinterpreting these two closely eluting peaks also under conditions of gradient HPLC. Finally, mass spectroscopic identification (APCI) in this study was once again based on a slightly modified isocratic method, which is unlikely to adequately separate RPA 407922 from RPA 406341 (Trans-diol) as well. Notice that mass spectroscopic identification of mono-hydroxylated triticonazole derivatives (all with MWT 333) is strongly hindered as all these compounds show practically identical APCI mass spectra.

In conclusion, the RMS AT could not verify that 'Met 6 (MWT 333)' observed in Ayliffe & Austin (1993) up to 12.8 % AR applying the isocratic HPLC method can be unambiguously assigned being RPA 407922. Therefore the applicant was requested by the RMS AT to further underpin their peak assignment. In view of the RMS AT this may be best done by providing illustrative original or new HPLC chromatograms of authentic reference compounds of triticonazole including RPA 406341 (Trans-diol) and RPA 407922 on basis of the isocratic and gradient HPLC methods used in Ayliffe & Austin (1993) and in this study. The applicant performed HPLC analysis of reference substances RPA 407922 and RPA 406341 (Trans-diol) with the same type of columns and same isocratic and gradient conditions as in Ayliffe & Austin (1993) and Ayliffe & McMillan-Staff (1994). The retention times obtained by the study authors could indeed not be reproduced. A complete separation of the two peaks could not be shown unambiguously. Finally, the applicant agreed with the conclusion of the RMS AT that 'Met 6 (MWT 333)' in the chromatogram does not belong to metabolite RPA 407922 but to an unidentified structure. The RMS AT notes that the supporting additional HPLC runs conducted by the applicant have not been submitted to the RMS AT. In a new position paper (Szegedi, 2018) the applicant indicates possible structures for 'Met 6 (MWT 333)' as well as for 'Met 7 (MWT 315)'.

Reference:	**Fungicides: RPA 400727-^{14}C: Rate of degradation in four soils**
Author(s), year:	Ayliffe, J. M., Godward, P. J., 1993
Report/Doc. Number:	R012979, 200234, P91/411, GOoD2486
Guideline(s):	Dutch Guidelines for the Submission of Applications for Registration of Pesticides, Part G.1
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The degradation of [phenyl-U-^{14}C]-triticonazole (called RPA 400727 in the report) under aerobic conditions was investigated in three agricultural soils (UK sandy loam, UK clay loam, UK loamy sand) and one German standard loamy sand soil (Speyer 2.2) at 10 °C and in the UK loamy sand at 22 °C. Soils were treated with an initial concentration of 1.64 ppm triticonazole (based on soil d.w.) – except the UK loamy sand which reached

2.46 ppm. The dose was equivalent to nominally 360 g ai/ha (related to 15 cm soil depth), equivalent to a seed treatment rate of 200 g ai/100 kg seed, with seeds sown at 180 kg/ha. Soil moisture was kept at 75 % of the 0.33 bar water capacity. Samples were incubated in the dark for 363 days. The soil samples were Soxhlet extracted with 140 ml acetonitrile/water (4:1, v/v).

Analytics: Isocratic HPLC for metabolite quantification, confirmation (triticonazole only) by LC-MS. Reference substances used: None.

Table B.8.1.1.1-7 Soil Characteristics

Soil[(a)]	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H[(b)]	CEC (meq/ 100 g)	WHC at 33 kPa (%)	Biomass (start) µg C/g soil	Biomass (end) µg C/g soil
UK sandy loam	73	13.5	13.5	1.43	6.3	6.0	12.0	118	115
UK clay loam	47	32	21	5.65	6.08	28.5	30.0	760	903
Speyer 2.2 loamy sand	83	9	8	5.7	6.3	10.8	10.65	284	361
UK loamy sand	79	11.5	9.5	32.24	6.24	51.1	38.5	912	769 (10 °C) 631 (22 °C)

(a) Texture classification not specified
(a) Matrix not specified

Findings:

Table B.8.1.1.1-8 Distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) - UK sandy loam, 10 °C

DAT	Extract-able	NER	CO_2	Total	Triti-cona-zole	RPA 404766[(a)] (Cis-diol)	RPA 404886	RPA 406341 (Trans-diol)	MWT 349	MWT 333[(b)]	MWT 315
Code					-	Met 3	Met 4	Met 5	Met 6	Met 7	Met 8
rRT	-		-	-	*1.00*	*0.35*	*0.41*	*0.48*	*0.57*	*0.64*	*0.70*
0	97.5	0.4	0.0	97.9	97.5	nd	nd	nd	nd	nd	nd
1	101.0	0.5	0.0	101.6	101.0	nd	nd	nd	nd	nd	nd
7	97.4	0.8	0.1	98.3	96.9	0.5	nd	nd	nd	nd	nd
14	94.0	1.2	0.2	95.4	88.9	2.5	nd	2.6	nd	nd	nd
28	93.2	1.7	0.3	95.2	82.8	4.4	nd	6.0	nd	nd	nd
56	94.5	2.6	0.6	97.6	81.3	2.6	1.2	4.2	1.4	nd	0.6
84	90.0	2.7	0.8	93.5	77.6	2.4	1.4	4.2	nd	nd	1.5
112	89.7	3.5	1.1	94.3	70.2	2.8	1.3	6.3	nd	2.5	2.2
140	88.8	3.9	1.5	94.2	74.5	5.7	nd	7.4	1.2	nd	nd
168	90.3	5.7	1.9	97.9	67.2	3.8	2.1	6.2	1.9	2.7	1.5
245	85.1	7.7	2.3	95.1	55.0	7.4	nd	8.6	2.0	6.9	nd
306	85.6	7.4	2.7	95.6	58.6	6.9	nd	10.5	2.9	4.7	2.0
363	85.6	7.0	3.1	95.7	44.8	7.1	nd	10.5	10.5	nd	4.2

nd denotes not detected
(a) In this study erroneously considered to be RPA 406780, identified as RPA 404766 (Cis-diol) in later studies when analytical systems became more sophisticated
(b) Claimed in Ayliffe & Godward (1994) being identified as RPA 407922 (refer to comments)

Table B.8.1.1.1-9 Distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) - UK clay loam, 10 °C

DAT	Extract-able	NER	CO_2	Total	Triti-cona-zole	RPA 404766[(a)] (Cis-diol)	RPA 404886	RPA 406341 (Trans-diol)	MWT 349	MWT 333[(b)]	MWT 315
Code					-	Met 3	Met 4	Met 5	Met 6	Met 7	Met 8
rRT	-	-	-	-	*1.00*	*0.35*	*0.41*	*0.48*	*0.57*	*0.64*	*0.70*
0	97.1	0.6	0.0	97.7	97.1	nd	nd	nd	nd	nd	nd
1	91.5	1.4	0.0	93.0	91.5	nd	nd	nd	nd	nd	nd
7	91.8	1.1	0.1	93.0	86.1	2.4	nd	3.3	nd	nd	nd
14	95.4	1.1	0.2	96.7	81.7	6.9	nd	6.8	nd	nd	nd
28	93.6	1.8	0.4	95.8	66.7	13.9	nd	13.0	nd	nd	nd
56	92.6	1.8	0.7	95.1	63.0	13.5	nd	12.2	nd	nd	nd

84	84.6	5.4	1.1	91.1	59.8	6.6	0.8	8.7	0.6	2.0	1.7
112	84.0	4.1	1.4	89.5	50.4	8.5	1.7	10.3	1.8	2.3	2.6
140	85.0	5.5	1.8	92.3	60.4	11.4	nd	13.3	nd	nd	nd
168	84.5	8.3	2.3	95.0	46.8	8.6	nd	13.2	1.9	5.0	3.4
245	81.6	8.9	2.7	93.2	42.6	9.9	nd	13.4	3.7	3.0	2.1
306	75.1	7.7	3.3	86.1	36.7	12.6	nd	16.1	2.2	5.3	2.2
363	78.7	8.8	4.1	91.6	25.1	8.1	nd	12.9	11.1	1.7	6.1

nd denotes not detected
(a) In this study erroneously considered to be RPA 406780, identified as RPA 404766 (Cis-diol) in later studies when analytical systems became more sophisticated
(b) Claimed in Ayliffe & Godward (1994) being identified as RPA 407922 (refer to comments)

Table B.8.1.1.1-10 Distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) - Speyer 2.2 loamy sand, 10 °C

DAT	Extract-able	NER	CO_2	Total	Triti-cona-zole	RPA 404766[a] (Cis-diol)	RPA 404886	RPA 406341 (Trans-diol)	MWT 349	MWT 333[b]	MWT 315
Code					-	Met 3	Met 4	Met 5	Met 6	Met 7	Met 8
rRT	-	-	-	-	*1.00*	*0.35*	*0.41*	*0.48*	*0.57*	*0.64*	*0.70*
0	97.7	0.2	0.0	97.9	97.7	nd	nd	nd	nd	nd	nd
1	98.8	0.4	0.0	99.2	98.8	nd	nd	nd	nd	nd	nd
7	94.4	0.8	0.1	95.3	94.4	nd	nd	nd	nd	nd	nd
14	92.5	0.9	0.1	93.5	82.3	5.3	nd	4.9	nd	nd	nd
28	90.5	1.3	0.2	92.0	76.0	7.1	nd	7.4	nd	nd	nd
56	95.1	1.7	0.3	97.2	81.3	6.2	0.6	6.3	0.7	nd	nd
84	92.0	2.1	0.4	94.5	73.3	5.9	0.8	6.6	0.2	nd	0.8
112	91.7	2.4	0.6	94.7	72.7	6.4	0.5	6.8	nd	nd	nd
140	94.0	2.2	0.7	96.9	75.4	8.4	nd	10.2	nd	nd	nd
168	88.7	3.8	0.8	93.3	72.8	7.1	nd	7.9	0.4	nd	0.4
245	89.1	5.0	1.1	95.2	67.6	9.0	nd	8.7	0.7	nd	nd
306	88.7	4.1	1.2	94.0	71.9	9.0	nd	7.7	nd	nd	nd
363	94.4	4.3	1.4	100.1	66.7	8.2	nd	8.7	2.1	1.0	1.3

nd denotes not detected
(a) In this study erroneously considered to be RPA 406780, identified as RPA 404766 (Cis-diol) in later studies when analytical systems became more sophisticated
(b) Claimed in Ayliffe & Godward (1994) being identified as RPA 407922 (refer to comments)

Table B.8.1.1.1-11 Distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) - UK loamy sand, 10 °C

DAT	Extract-able	NER	CO_2	Total	Triti-cona-zole	RPA 404766[a] (Cis-diol)	RPA 404886	RPA 406341 (Trans-diol)	MWT 349	MWT 333[b]	MWT 315
Code					-	Met 3	Met 4	Met 5	Met 6	Met 7	Met 8
rRT	-	-	-	-	*1.00*	*0.35*	*0.41*	*0.48*	*0.57*	*0.64*	*0.70*
0	96.5	0.5	0.0	97.0	96.5	nd	nd	nd	nd	nd	nd
1	100.7	0.6	0.0	101.3	100.7	nd	nd	nd	nd	nd	nd
7	96.5	1.2	0.1	97.8	94.2	1.1	nd	1.3	nd	nd	nd
14	94.4	0.9	0.2	95.4	94.4	nd	nd	nd	nd	nd	nd
28	94.9	1.3	0.2	96.4	81.8	6.6	nd	6.4	nd	nd	nd
56	91.8	1.5	0.4	93.6	74.4	8.2	nd	9.2	nd	nd	nd
84	92.5	2.4	0.5	95.4	82.7	2.5	0.3	4.1	nd	nd	nd
112	87.4	2.8	0.7	90.8	74.0	2.8	0.8	4.5	nd	0.6	0.2
140	89.0	3.3	0.9	93.1	83.0	0.9	nd	5.1	nd	nd	nd
168	89.8	4.5	1.0	95.4	75.1	2.6	0.3	3.7	3.1	2.1	0.6
245	86.7	5.2	1.3	93.2	70.7	3.6	nd	7.1	nd	2.3	nd
306	88.0	5.0	1.5	94.4	73.3	3.9	nd	8.4	nd	1.5	0.9
363	93.6	6.0	1.7	101.2	62.2	5.7	0.7	9.1	6.5	nd	1.9

nd denotes not detected
(a) In this study erroneously considered to be RPA 406780, identified as RPA 404766 (Cis-diol) in later studies when analytical systems became more sophisticated
(b) Claimed in Ayliffe & Godward (1994) being identified as RPA 407922 (refer to comments)

Table B.8.1.1.1-12 Distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) - UK loamy sand, 22 °C

DAT	Extract-able	NER	CO_2	Total	Triti-cona-zole	RPA 404766[(a)] (Cis-diol)	RPA 404886	RPA 406341 (Trans-diol)	MWT 349	MWT 333[(b)]	MWT 315
Code					-	Met 3	Met 4	Met 5	Met 6	Met 7	Met 8
rRT	-	-	-	-	*1.00*	*0.35*	*0.41*	*0.48*	*0.57*	*0.64*	*0.70*
0	96.3	0.5	0.0	96.8	96.3	nd	nd	nd	nd	nd	nd
1	94.9	0.8	0.0	95.7	94.9	nd	nd	nd	nd	nd	nd
7	93.3	1.1	0.2	94.6	91.5	1.2	nd	0.7	nd	nd	nd
14	93.8	1.6	0.3	95.6	79.6	7.4	nd	6.8	nd	nd	nd
28	89.4	2.1	0.5	92.0	71.5	8.4	nd	9.5	nd	nd	nd
56	89.5	3.7	1.1	84.2	65.7	7.8	nd	14.8	1.2	nd	nd
84	87.8	4.6	2.3	94.7	66.1	3.1	1.5	8.6	1.5	0.3	2.1
112	83.3	5.6	3.4	92.4	60.1	2.9	1.6	8.4	1.3	1.3	3.0
140	80.6	7.3	4.5	92.3	67.4	5.0	nd	8.2	nd	nd	nd
168	80.1	9.4	5.6	95.1	56.0	2.7	0.7	8.4	3.2	1.2	3.2
245	71.8	12.7	7.9	92.3	45.4	3.5	nd	4.9	4.3	4.0	5.3
306	69.4	11.6	9.4	90.4	51.2	2.4	nd	7.8	2.4	4.8	0.8
363	71.2	11.3	11.0	93.5	42.9	3.2	0.7	7.2	3.5	6.2	3.9

nd denotes not detected
(a) In this study erroneously considered to be RPA 406780, identified as RPA 404766 (Cis-diol) in later studies when analytical systems became more sophisticated (refer to comment section)
(b) Claimed in Ayliffe & Godward (1994) being identified as RPA 407922 (refer to comments)

For each soil at all time points and for each pair of soil duplicate samples, a good radiochemical balance was achieved with the mean recoveries (of the duplicate means) of applied radioactivity ranging between 93.1 % and 96.3 % AR.

The unextractable soil bound residue reached 3.5, 4.1, 2.4 and 2.8 % of applied radioactivity 112 days after application for the UK sandy loam, UK clay loam, Speyer 2.2 loamy sand and the UK loamy sand at 10 °C, respectively. The unextractable soil bound residue reached 5.6 % of applied radioactivity 112 days after application for the UK loamy sand at 22 °C. Trapped ^{14}C-carbon dioxide amounted to 1.1, 1.4, 0.6 and 0.7 % of applied radioactivity at 10 °C 112 days after application, respectively, and 3.4 % 112 days after application for the UK loamy sand at 22 °C.

Up to thirteen metabolites were detected and quantified. Of these, RPA 406341 (Trans-diol), RPA 404766 (Cis-diol) (in this study erroneously considered being RPA 406780, identified as RPA 404766 in later studies) and Met 6 (MWT 349) exceeded 10 % AR at 10 °C in at least one soil. Only RPA 406341 (Trans-diol) exceeded 10 % AR in the UK loamy sand at 22 °C.

Unknown Met 7 (MWT 333) and Met 8 (MWT 315) were found in amounts > 5 % AR. Met 7 (MWT 333) reached a maximum amount of 6.9 % AR (DAT 245) in the UK sandy loam at 10 °C. Other unknown metabolites did not exceed 5 % AR.

Conclusion:

Degradation of phenyl ring labelled triticonazole was tested in 4 soils at 10 °C. Five metabolites > 5 % AR were detected:

- RPA 404766 (Cis-diol) (in this study erroneously considered to be RPA 406780, identified as RPA 404766 in later studies)
- RPA 406341 (Trans-diol)
- Met 6 (MWT 349) reaching a maximum of 11.1 % AR at the end of the study
- Met 7 (MWT 333) reaching a maximum in the UK loamy sand (22 °C) of 6.2 % AR at the end of the study
- Metabolite 8 (MWT) detected > 5 % AR in two soils (UK clay loam, UK loamy sand) only once

The content of this report is complementary to the study described in Ayliffe & Austin (1993). All four soils showed a decrease in the rate of degradation of parent at the lower temperature (compared with the 22 °C experiment results reported in this document, in Ayliffe & Austin (1993) and Ayliffe & McMillan-Staff (1994).

For all soils less carbon dioxide was produced at the lower temperature together with an increase in the relative amounts of soil extractable radioactivity.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some deviations:
  - The test duration of 363 days is beyond the recommended study duration of about 120 days recommended in the OECD guideline 307. The same as mentioned in Ayliffe & Austin (1993) applies for this study as well. Microbial biomass C was well above (or close to) 1 % of total organic C at the start of and end of incubation in the UK sandy loam, UK clay loam and Speyer 2.2 loamy sand. In the UK loamy sand, biomass C was actually only around 0.5 % of total organic C (10 and 20 °C study). However, as demonstrated later, degradation rates of parent and metabolites in the UK loamy sand where well within the range of degradation rates observed in the other soils. Thus degradation rates observed in this soil were included in the final dataset.
  - With a nominal dose rate of 385 g ai/ha the study is clearly overdosed considering an intended field application rate of 12.5 g ai/ha only
  - Mass balance was below 90 % in some cases leading to some uncertainties regarding maximum occurrence of metabolites.
  - There is no information available about the duration of soil storage (storage temperature was 20 °C)
  - No information is available on the history of the field site, the way of sampling and the transportation of the soil
  - No detailed information is available on the 14 days pre-equilibration phase
  - The organic carbon content of the UK loamy sand is definitely outside the range recommended by OECD 307 (i.e. 0.5 to 2.5 %) indicating that this field site may have been a forest in former times. However, as results obtained in this high-organic soil are not deviating from other soils the RMS AT considers these data equally representative.
  - The LOD and LOQ of the analytical method were not specified in the study report

  On overall the study is still considered reliable, results obtained are not in contradiction with results obtained in more recent studies.

- On basis of the year (1993) of investigation and on soil properties stated it is evident that the UK sandy loam, UK clay loam and Speyer 2.2 loamy sand used in Ayliffe & Austin (1993), Ayliffe & Godward (2014) and in this study are the same (same batches with the exception of the more viable batch of the Speyer 2.2 loamy sand used in Ayliffe & McMillan-Staff, 1994). This implies that finally a consistent set on 10 and 22 °C studies is available on four soils (including the UK loamy sand).

- The RMS AT notes that the study authors did not further investigate (identify) metabolites observed in this report e.g. by mass spectroscopy, but simply made reference to Ayliffe & Austin (1993) on basis of peak pattern and HPLC retention times using the same isocratic method for metabolite profiling. Notice that 'Met 6 (MWT 349)', 'Met 7 (MWT 333)' and 'Met 8 (MWT 315)' in this report refer to 'Met 5 (MWT 349)', 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' in Ayliffe & Austin (1993), respectively. As the study authors used the same isocratic HPLC method for metabolite profiling as used in Ayliffe & Austin (1993), the same shortcomings as mentioned in Ayliffe & Austin (1993) apply to this study as well.

- In line with Ayliffe & Austin (1993) metabolite fraction 'Met 6' in this study report ('Met 5' in Ayliffe & Austin, 1993) with a MWT of 349 g/mol is likely to comprise two unidentified metabolites, which can be separated under conditions of gradient HPLC, one with a MWT of 333 g/mol and one with a MWT of 349 g/mol (Simmonds & Lowden, 2002). In Simmonds & Lowden (2002) these two compounds were observed at almost equimolar amounts (one soil). On basis of these findings, 'Met 6' in this study ('Met 5' in Ayliffe & Austin, 1993) is unlikely to exceed 5 % AR on basis of its individual constitutes.

- The study was kinetically re-assessed by Jarvis & Montesano (2014a).

Reference:	**^{14}C-Triazole labelled triticonazole: Rate of degradation in clay soil under aerobic conditions**
Author(s), year:	Doble, M. L., Ferreira, E. M., Hardy, I. A. J., 1996
Report/Doc. Number:	R012994, 201171, P94/158, GOoD8999
Guideline(s):	US-EPA N, 162-1 (1982), Draft European Uniform Guidelines (Lynch 1993)
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The rate of degradation of [triazole-3(5)-^{14}C]-triticonazole (called RPA 400727 in the report), applied at an application rate equivalent to 385 g ai/ha, has been studied in a clay soil (Mississippi, USA) over a 12 month period. Samples were incubated in the dark at 25 ± 2 °C. The moisture content of the soil samples were maintained at 75 ± 5 % of the maximum moisture holding capacity at 0.33 bar suction. Soil samples were Soxhlet extracted with mixtures of acetonitrile/water (4:1, v/v). Each extract was subjected to quantitative radioassay by direct liquid scintillation counting. Determinations of parent compound and its metabolites in the soil extracts were carried out by thin-layer chromatography (TLC) and high performance liquid chromatography (HPLC) applying a gradient method. Reference substances used: RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406203 (Z-isomer), RPA 404886, RPA 406780, RPA 407922.

Table B.8.1.1.1-13 Soil Characteristics

Soil (USDA)	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H ($CaCl_2$)	CEC (mEq/ 100 g)	WHC at 33 kPa (%)	WHC at 10 kPa (%)	MWHC (%)	Study MC (%)	Biomass (start) µg C/ g soil	Biomass (end) µg C/ g soil
US clay soil	4.1	31.6	64.3	2.04	5.7	32.2	31.71	62.37	70.76	23.78	119	304

Findings:

Table B.8.1.1.1-14 Recovery of radioactivity (% AR, mean of duplicate samples, numbers shaded in grey exceed 5 % AR)

DAT	Extractable	NER	CO_2	Other volatiles	Total	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)	RPA 406203 (Z-isomer)
0	101.4	0.7	-	-	102.1	100.8	-	-	0.7
1	93.0	3.2	0.0	0.0	96.2	92.2	-	-	0.7
7	98.0	2.2	0.0	0.0	100.3	97.1	-	-	0.9
15	91.0	3.9	0.1	0.0	100.3	94.9	0.8	0.6	-
30	97.1	3.0	0.1	0.0	100.3	95.7	1.5	-	-
50	92.4	5.9	0.1	0.0	98.3	85.6	1.8	5.0	-
77	93.4	6.0	0.2	0.0	99.6	84.6	4.6	4.3	-
100	93.8	8.3	0.2	0.0	102.2	77.7	7.6	7.6	-
129	93.3	6.8	0.3	0.0	100.4	75.2	5.9	7.9	1.7
189	91.4	9.1	0.6	0.0	101.1	73.6	5.8	8.2	0.9
240	87.2	6.2	0.8	0.0	99.8	67.3	6.9	10.7	1.4
365	96.3	6.8	0.8	0.0	107.5	74.9	9.5	10.6	-

The mean recoveries ranged from 96.2 to 107.5 % of the applied radioactivity. The unextractable soil bound residue reached 6.8 % of applied radioactivity mainly associated with humin fraction. The trapped ^{14}C carbon dioxide amounted to 0.3 % of applied radioactivity, 120 days after application. Other trapped volatiles amounted to less than 0.1 % of applied radioactivity after 365 days.

The proportion of parent present decreased to 75.2 % of applied radioactivity 120 days after application, but very little breakdown occurred after 120 days (presumably due to the effects of incubation on the soil viability).

The major metabolites were identified as RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol), both isomers formed by 3-hydroxylation of the cyclopentane ring, reaching 10.7 % and 9.5 % AR, respectively, after 12 months. RPA 406203 is the Z isomer of the parent compound. Four unknown metabolites were quantified, none of each exceeding 3.7 % AR.

Conclusions:

The route of degradation of triticonazole when labelled in the triazole ring was identical to that found in other studies where the label was in the phenyl ring. As major metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) were found.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some deviations:
  - The test duration of 365 days is beyond the recommended study duration of about 120 days recommended in the OECD guideline 307. The same as mentioned in Ayliffe & Austin (1993) applies for this study as well. Microbial biomass C was well above 1 % of total organic C at the start and at the end of incubation (indeed increasing in this soil).
  - With a nominal dose rate of 385 g ai/ha the study is clearly overdosed considering the intended field application rate of 12.5 g ai/ha only
  - There is no information available about the duration of soil storage
  - No information is available on the history of the field site, the way of sampling and the transportation of the soil
  - No detailed information is available on the pre-equilibration phase
  - The LOD and LOQ of the analytical method were not specified in the study report

  On overall the study is still considered reliable. Results obtained are not in contradiction with results obtained in more recent studies.

- Altogether, this study as well as Simmonds et al (1996) and the most recent study conducted by Ta & Strobush (2012) and Ta & Strobush (2015) give the most advanced insights into the metabolite profile to be expected from degradation of triticonazole in aerobic soils (for details refer to next study, Simmonds et al., 1996).

- The study was kinetically re-assessed by Jarvis & Montesano (2014a).

Reference:	**Triticonazole: Rate of degradation in one soil type under aerobic conditions with regard to varying temperature, soil moisture, treatment rate and soil viability**
Author(s), year:	Simmonds, M. B., Hardy, I. J., Ferreira, E. M., 1996
Report/Doc. Number:	R012995, 201173, P94/141, GOoD7834
Guideline(s):	Danish Agency of Environmental Protection Guidelines, Paragraph 21 (1988) and Draft European Guidelines (Lynch, 1993)
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

A study was designed to investigate the rate of aerobic degradation of [phenyl-U-^{14}C]-triticonazole in a sandy loam soil under different conditions:

Table B.8.1.1.1-15 Different study conditions

Investigation	Temperature	Application rate	Moisture content
Standard	25 ± 2 °C	385 g ai/ha	50 % field capacity
Low temperature:	10 ± 2 °C	385 g ai/ha	50 % field capacity
Reduced soil moisture content:	25 ± 2 °C	385 g ai/ha	20 % field capacity
Reduced application rate:	25 ± 2 °C	38.5 g ai/ha	50 % field capacity
Sterile	25 ± 2 °C	385 g ai/ha	50 % field capacity

Table B.8.1.1.1-16 Soil Characteristics

Soil (USDA)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/ 100 g)	Field capacity (%)	Biomass (start) µg C/g soil	Biomass (end) µg C/g soil
Manningtree, sandy loam	76.2	16.1	7.7	0.8	6.1	3.4	30.9	192	222

Portions of soil were incubated in the dark in glass incubation flasks at the appropriate temperature under aerobic conditions over a period of 365 days. Moistened carbon dioxide-free air was blown through each flask before being passed through an ethylene glycol and two potassium hydroxide traps.

Duplicate samples of soil were removed for analysis, at each selected time interval, for each regime. The traps associated with each flask taken for sampling were sampled at the same time.

The soil samples were Soxhlet extracted with mixtures of acetonitrile/water (4:1, v/v) and the concentrated extracts were analysed for parent compound and degradation products by gradient HPLC and TLC. Representative samples were also analysed by LC-MS-MS. Reference substances used: RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406203 (Z-isomer), RPA 404886, RPA 406780, RPA 407922.

Findings:

Table B.8.1.1.1-17 Characterisation/distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) – standard conditions

DAT	Extract-able	NER	CO_2	Total[a]	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)	Collective minor metabolites[b]
0	95.5	1.3	0.0	96.8	94.2	0.0	0.0	1.4
1	94.9	0.7	0.1	95.7	92.5	0.5	0.7	1.3
7	93.0	1.3	0.2	94.5	85.0	0.5	2.2	3.9
15	95.4	2.1	0.3	97.8	85.8	3.0	6.5	0.0
30	89.9	2.6	0.8	93.3	77.1	4.1	7.1	1.5
50	88.8	6.2	1.9	96.8	68.3	6.3	10.0	4.1
77	88.8	6.3	3.0	98.1	65.1	7.2	11.7	4.8
100	84.0	6.1	2.7	92.7	55.5	8.7	13.3	6.4
129	86.0	7.2	4.7	97.9	57.3	6.7	13.5	8.6
189	84.5	12.8	6.9	104.2	42.3	8.5	16.7	14.1
240	80.9	10.5	7.9	99.3	38.3	7.9	16.7	16.9
365	68.3	15.8	17.6	101.8	30.5	4.4	14.7	16.5

(a) Including non ^{14}C-CO_2
(b) Including RPA 406203 (Z-isomer; no individual > 4.1 % AR) and collective unknown components (no individual > 5.9 % AR)

Table B.8.1.1.1-18 Characterisation/distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) – reduced temperature (10 °C)

DAT	Etract-able	NER	CO_2	Total[a]	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)	Collective minor metabolites[b]
0	90.3	2.5	0.0	92.8	88.7	0.0	0.0	1.6

1	102.1	0.9	0.0	103.0	99.4	0.0	0.0	1.9
7	89.0	1.9	0.0	90.9	83.3	2.1	2.5	1.1
15	98.4	2.9	0.1	101.5	87.6	2.6	3.9	3.2
29	92.0	2.2	0.3	94.5	84.0	0.7	4.1	2.4
50	95.7	2.6	0.6	98.9	82.8	2.8	5.9	4.3
71	97.2	2.2	0.8	100.1	86.7	3.5	7.0	0.0
99	96.1	2.7	1.0	99.7	77.8	3.8	6.9	7.6
130	104.6	3.6	1.4	109.5	82.6	5.5	10.0	6.5
188	95.7	4.7	1.5	102.0	70.8	5.5	11.7	7.6
238	91.8	7.4	1.2	100.5	66.3	6.2	13.2	6.0
365	94.2	5.4	1.4	101.0	64.7	6.5	14.6	7.2

(a) Including non ^{14}C-CO_2
(b) Including RPA 406203 (Z-isomer; no individual > 4.4 % AR) and collective unknown components (no individual > 4.1 % AR)

Table B.8.1.1.1-19 Characterisation/distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) – reduced moisture

DAT	Etract-able	NER	CO_2	Total[(a)]	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)	Collective minor metabolites[(b)]
0	98.3	0.1	0.0	98.4	96.4	0.0	0.0	1.9
1	97.7	0.3	0.0	98.0	93.0	0.0	0.6	4.1
7	98.2	1.2	0.2	99.6	91.4	1.8	2.8	2.2
15	95.9	1.6	0.3	97.8	80.1	3.3	5.3	7.2
30	94.7	3.2	0.9	98.8	76.1	4.9	8.3	6.3
50	91.9	6.3	0.9	99.0	70.3	5.7	9.3	6.1
77	88.4	6.4	1.7	96.5	68.8	6.7	10.4	2.6
100	84.9	9.6	2.4	96.9	58.1	5.5	11.1	10.3
129	84.6	8.8	2.4	95.7	55.9	7.2	11.9	9.6
189	82.4	13.9	3.8	100.1	53.1	6.6	10.9	10.1
240	79.2	11.3	5.4	95.9	45.7	6.0	12.2	14.6
365	79.4	16.0	10.6	106.0	44.0	6.7	15.8	13.0

(a) Including non ^{14}C-CO_2
(b) Including RPA 406203 (Z-isomer; no individual > 2.2 % AR) and collective unknown components (no individual > 5.2 % AR)

Table B.8.1.1.1-20 Characterisation/distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) – reduced application rate

DAT	Etract-able	NER	CO_2	Total[(a)]	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)	Collective minor metabolites[(b)]
0	92.1	3.0	0.0	95.0	90.7	0.0	0.0	1.4
1	93.7	3.8	0.1	97.5	93.2	0.0	0.0	0.5
7	86.5	8.5	0.5	95.5	84.0	0.2	2.5	0.2
15	103.2	2.3	0.7	106.2	98.0	1.5	3.7	0.0
30	90.8	4.3	1.1	96.3	81.7	3.1	6.0	0.0
50	90.3	4.0	1.4	95.7	73.8	5.9	8.8	1.8
77	88.0	6.8	2.8	97.5	64.8	7.3	12.2	3.7
100	86.8	6.3	3.9	97.0	61.3	7.5	14.8	3.3
129	90.2	7.9	3.8	102.0	63.9	8.2	14.6	1.6
189	84.8	12.0	7.8	104.7	49.0	8.2	17.7	9.9
240	81.7	11.1	7.2	100.0	37.4	7.3	20.2	16.1
365	77.5	12.9	12.7	103.2	39.4	6.5	17.6	14.1

(a) Including non ^{14}C-CO_2
(b) Including RPA 406203 (Z-isomer; no individual > 1.1 % AR) and collective unknown components (no individual > 5.2 % AR)

Table B.8.1.1.1-21 Characterisation/distribution of radioactivity (% AR, HPLC, mean of duplicate samples, numbers shaded in grey exceed 5 % AR) – sterile conditions

DAT	Etract-able	NER	CO_2	Total[(a)]	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)	Collective minor metabolites[(b)]
0	102.8	0.1	-	102.9	101.4	0.0	0.0	1.4
1	96.2	0.9	0.0	97.2	88.2	2.1	3.4	1.1
7	100.9	4.0	0.0	104.9	99.4	0.0	0.0	1.6

15	97.3	1.4	0.0	98.7	95.7	0.0	0.0	1.6
30	104.9	1.0	0.0	105.9	103.2	0.0	0.0	1.7
50	96.9	4.5	0.3	101.8	82.8	3.2	3.4	4.0
77	94.9	5.6	0.4	100.9	78.0	0.0	8.9	4.6
100	102.3	2.6	0.0	104.9	100.7	0.0	0.0	0.7
129	94.3	4.4	0.0	98.6	92.7	0.0	0.0	0.7
189	99.8	2.9	0.1	102.9	99.8	0.0	0.0	0.0
240	100.4	3.7	0.1	104.2	99.3	0.0	0.0	1.1
365	107.5	3.8	0.4	111.7	102.3	2.4	2.8	0.0

(a) Including non ^{14}C-CO_2
(b) Including RPA 406203 (Z-isomer; no individual > 4.1 % AR) and collective unknown components (no individual > 1.9 % AR)

An acceptable radiochemical balance was obtained for all regimes studied. Mean values ranged between 91 % and 112 % of applied radioactivity.

Formation of unextractable residues was slower at reduced temperature and under sterile conditions with maximum values reaching 7.4 % and 4.4 % respectively. Unextractable residues from day 240 and 238 replicates were fractionated and their distributions between humic acid, fulvic acid and humin fractions were shown. Radioactivity was found in all three soil fractions, the highest amount found in the humin fraction followed by fulvic acid and humic acid in the case of all treatment regimes.

CO_2 production was significantly slower at reduced temperature and under sterile conditions reaching maximum values of only 1.4 % and < 0.4 % AR respectively.

Two main metabolites were identified in all experimental regimes except under sterile conditions: RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) exceeding 5 % AR. Further RPA 406203 (Z-isomer; up to 4.4 % AR) and collective unknown compounds were detected with individual amounts up to 5.9 % AR (standard conditions).

Conclusions:

The rate of degradation was significantly influenced primarily by the temperature and the microbial activity and, to a lesser extent, by the moisture content of the soil. Under sterile conditions no degradation can be observed. Metabolite RPA 406341 (Trans-diol) amounted for > 10 % AR under all conditions tested except in sterile soil. The maximum amount reached of RPA 404766 (Cis-diol) was 8.7 % AR (standard conditions). RPA 406203 (Z-isomer) was also observed in some sample extracts up to 4.4 % AR (reduced temperature). In addition, several other minor components, some of which were tentatively identified as tri-hydroxy degradates, were observed. The maximum of an individual unknown component was about 5.9 % AR (DAT 365, standard conditions).

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some deviations:
  - The test duration of 365 days is beyond the recommended study duration of about 120 days recommended in the OECD guideline 307. The same as mentioned in Ayliffe & Austin (1993) applies for this study as well. Microbial biomass C was well above 1 % of total organic C at the start and at the end of incubation.
  - With a nominal dose rate of 385 g ai/ha the study is clearly overdosed considering the intended field application rate of 12.5 g ai/ha only. However, results from the experiment conducted at 38.5 g/ha only do not indicate that the high application rate may have adversely affected degradation and metabolism of triticonazole in soil.
  - There is no information available about the soil storage conditions.
  - The LOD and LOQ of the analytical method were not specified in the study report.

  On overall the RMS AT considers this study still reliable. Results obtained are not in contradiction with results obtained in more recent studies.

- The RMS AT notes, that the information provided in the study report does not allow verifying whether individual unidentified components (max. at 5.9 % AR at DAT 365 under standard conditions)

summarized as 'collective minor metabolites' exceed 5 % AR at two consecutive sampling points. The applicant was requested by the RMS AT to submit further information. On inspection of GLP raw data provided by the applicant the RMS AT could verify that none of the unidentified metabolites ('collective minor metabolites') exceeded 5 % AR at two consecutive sampling points on individual basis in any of the experiments.

- The two studies, Doble et al. (1996) and this study, conducted in the same laboratory at the same time, give fundamental insights into the metabolite profile to be expected from degradation of triticonazole in aerobic soils. Two soils, the US clay soil and the UK Manningtree sandy soil, have been investigated and the obtained metabolite profiles, which are consistent in both soils, have been thoroughly investigated by adequate gradient HPLC and mass spectroscopy including reference substances. Figures on example HPLC chromatograms of authentic reference standard mixtures and of both soils are given below (on basis of 'HPLC gradient 1' used for metabolite profiling and 'HPLC gradient 2' used for mass spectroscopic work).

  Particularly, the two studies give strong indication that:

  - RPA 406780, considered to represent 'Met 1' in Ayliffe & Austin (1993) and Ayliffe & McMillan-Staff (1994), is unlikely to occur in aerobic soils at significant amounts. Instead, RPA 404766 (Cis-diol), closely eluting with RPA 406780 under conditions of isocratic HPLC, represents 'Met 1' (refer to chromatograms given below showing standard mix chromatograms and samples of both soils).

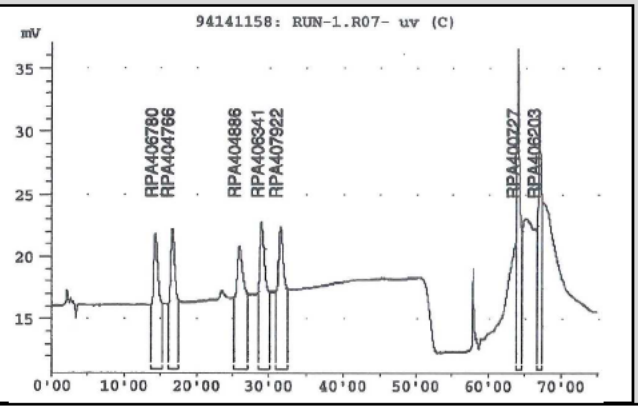
  - RPA 404886 is unlikely to occur in aerobic soils at significant amounts. 'Met 2' in Ayliffe & Austin (1993) and Ayliffe & McMillan-Staff (1994) is most probably an unknown metabolite with a MWT of 331 (refer to chromatograms given below).

  - RPA 407922 is unlikely to occur in aerobic soils at significant amounts. This finding is in strong contrast to the occurrence of metabolite 'Met 6 (MWT 333)' in Ayliffe & Austin (1993) originally claimed by Ayliffe & McMillan-Staff (1994) to represent RPA 407922. This finding is not supported anymore by the applicant (refer to chromatograms given below).

  Concluding, on basis of Doble et al. (1993) and this study, the only three metabolites which can be unambiguously identified in aerobic soils in view of the RMS AT are RPA 404766 (Cis-diol), RPA 406341 (Trans-diol) and RPA 406203 (Z-isomer). All other metabolites remain unidentified having indicative MWTs of 315, 331, 333, 347 and 349, amongst them other unknown mono- (MWT 333) and di-hydroxylated (MWT 349) derivatives of triticonazole.

Table B.8.1.1.1-22 **Example HPLC chromatograms of a mix of authentic reference substances, of the 240 DAT sample of the UK Manningtree sandy loam (standard conditions) and of the 245 DAT sample of the US clay applying 'HPLC gradient 1' (used for metabolite profiling) - RMS AT assessment on basis of raw data in the study reports**

Reference substances mix, UV
(this study, page 62)



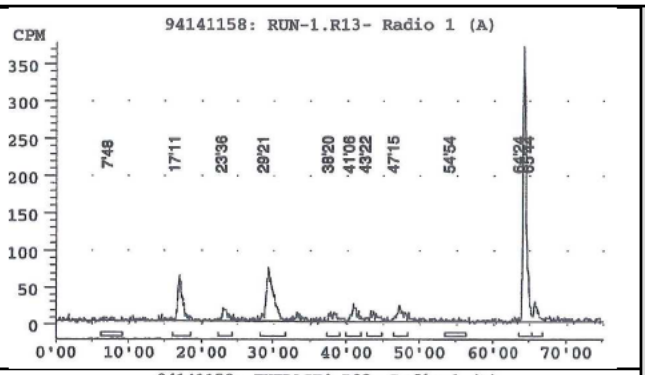
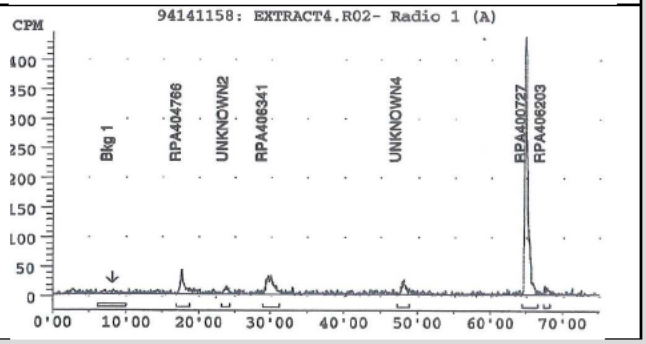
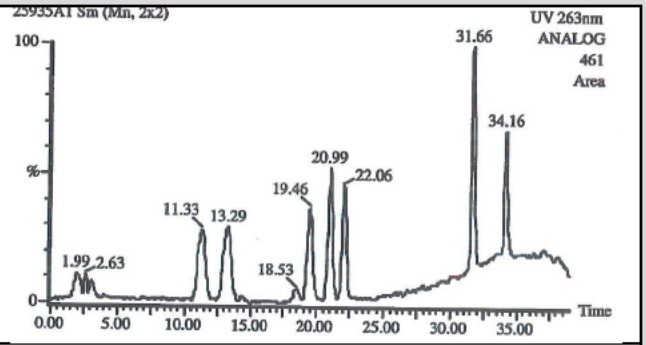
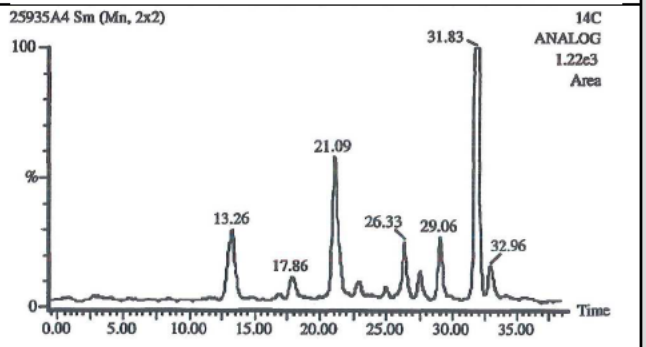
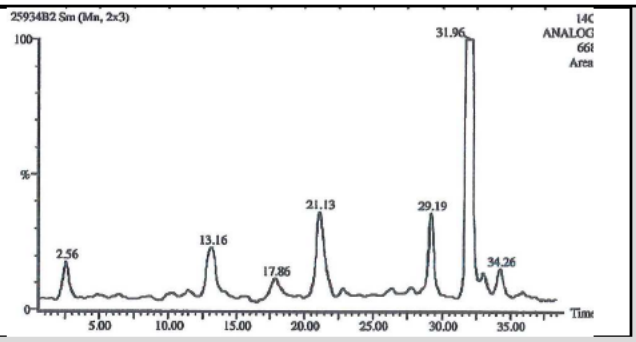
UK Manningtree sandy loam, standard conditions, 240 DAT, ^{14}C (this study, page 46) 17.11 **RPA 404766 (Cis-diol)** 29.21 **RPA 406341 (Trans-diol)** 64.24 **Triticonazole**	
US clay, 245 DAT, ^{14}C (Doble et al., 1996, page 44)	

Table B.8.1.1.1-23 **Example HPLC chromatograms of a mix of authentic reference substances, of the 240 DAT sample of the UK Manningtree sandy loam (standard conditions) and of the 245 DAT sample of the US clay applying 'HPLC gradient 2' (used for mass spectroscopic work) - RMS AT assessment on basis of raw data in the study reports**

Reference substances mix, UV (this study, p. 119): 11.33 RPA 406780 13.29 RPA 404766 (Cis-diol) 19.46 RPA 404886 20.99 RPA 406341 (Trans-diol) 22.06 RPA 407922 31.66 Triticonazole 34.16 RPA 406203 (Z-isomer)	
UK Manningtree sandy loam, standard conditions, 240 DAT, ^{14}C (this study, p. 127): 13.26 **RPA 404766 (Cis-diol)** 17.86 MWT 331 21.09 **RPA 406341 (Trans-diol)** 22.96 MWT 347 24.96 MWT 349 26.33 MWT 315 27.49 MWT 333 + MWT 349 29.06 MWT 331 31.83 **Triticonazole** 32.96 MWT 347	

US clay, 245 DAT, ^{14}C
(Doble et al., 1996, p. 80)

13.16 **RPA 404766 (Cis-diol)**
17.86 MWT 331
21.13 **RPA 406341 (Trans-diol)**
29.19 MWT 331
31.96 **Triticonazole**
34.26 **RPA 406203 (Z-isomer)**



- The study was kinetically re-assessed by Jarvis & Montesano (2014a).

Reference:	**[^{14}C]-Triticonazole: Generation and identification of soil metabolites**
Author(s), year:	Simmonds, M., Lowden, P., 2002
Report/Doc. Number:	C021044, CX/01/011, GOoD 28047
Guideline(s):	EU 95/36/EC, Section 7.1.1.2.2 (1995)
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

This study was designed to generate metabolites of triticonazole and, in particular, that which had been seen at significant levels in earlier studies but had not been identified (i.e. MWT 349). The study was, therefore, quantitative only with respect to the amounts of particular degradates formed and obtaining a mass balance was not an objective.

[Phenyl-U-^{14}C]-triticonazole was applied to samples of a soil that was similar to that used in earlier route and rate of degradation studies in which an apparently major metabolite had been detected but not identified (Ayliffe & Austin, 1993, and Ayliffe & Godward, 1993). The soil characteristics are shown in the Table below.

Table B.8.1.2.1.1-24: Soil Characteristics

Soil	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/100g)	Biomass (start) µg C/g soil	Biomass (end) µg C/g soil
Clay loam	27.3	38.7	34.0	4.3	7.4	53.6	978	722

Soil samples of 100 g or 300 g (oven dried weight) were placed in flasks and were then treated with triticonazole at a rate equivalent to 1650 g/ha. This relatively high rate was used in order to increase the chances of reasonable amounts of metabolites being produced which would assist the analytical process. The samples were then incubated in the dark at 10 or 20 °C with a stream of carbon dioxide-free air being passed over the surface of the soil sample. The soil flasks were connected to water-traps as a visual check for correct airflow through the flasks. Flasks were removed for analysis at selected intervals throughout the study (up to approximately one year). Samples from both 10 and 20 °C incubations were taken at 4 months and 7.5 months after application. Further 20 °C incubation samples were taken at 10, 10.25, 10.5 and 10.75 months after application. Further 10 °C incubation samples were taken at 12.25 and 12.5 months after application.

The extraction procedure (Soxhlet extraction using acetonitrile/water, 80:20) was the same as that used in earlier triticonazole soil metabolism studies in which the unidentified degradates were initially observed. Samples that contained an acceptable quantity of the metabolites of interest were processed further. The components of interest were isolated by repeated HPLC analysis (using a gradient method which utilised a Kromasil KR100 5C18 column (250 × 4.6 mm i.d.) and a mobile phase of acetonitrile/water/acetic acid in varying proportions)

and fraction collection. The fraction-collected samples were concentrated by rotary evaporation to low volume followed by adjustment to a known volume with acetonitrile/water (1:1). The concentrated sample extracts from the 100 g soil samples incubated at 20 °C were combined prior to profiling, while the 300 g sample concentrates were profiled separately. The same process was carried out for the 10 °C sample concentrates.

In addition, a selected sample was profiled using the original conditions first used in the aerobic rate of degradation studies (Ayliffe & Austin, 1993, Ayliffe & McMillan-Staff, 1994, Ayliffe & Godward, 1993). These conditions comprised an isocratic mobile phase (water/acetonitrile/glacial acetic acid, 60:40:2, v/v/v) instead of a gradient.

The concentrated samples were also examined by liquid chromatography-mass spectrometry (LC-MS), employing the same HPLC conditions as were used for the fraction collecting and a Micromas Quattro LC mass spectrometer in positive ion electrospray (ESP+) mode.

Findings:

The overall recovery of radioactivity was not an objective of this study and, due to the absence of trap data and combustion data, could not be determined. The Soxhlet method extracted between 73 % and 92 % of applied radioactivity. Procedural recoveries on concentration were very good, with all samples within the acceptable range of 90 - 110 % of recovered radioactivity.

Gradient HPLC profiles demonstrated two unknown metabolites of interest. Both were tentatively identified as having a molecular weight of 349 g/mol, and eluted in the same region of the chromatograms. These two metabolites were isolated together by fraction collection and analysed by LC-MS and later identified as having molecular weights of 333 g/mol (mono-hydroxylated metabolite) and 349 g/mol (di-hydroxylated metabolite).

No significant differences in the metabolic profile were observed between samples when profiled under the gradient conditions previously described. All showed chromatography and metabolite profiles consistent with those observed in previous soil studies (Ayliffe & Austin, 1993, Ayliffe & McMillan-Staff, 1994, Ayliffe & Godward, 1993).

Isocratic HPLC analysis of the 20 °C bulk sample concentrate, selected for profiling using the conditions adopted in the original rate of degradation studies (Ayliffe & Austin, 1993, Ayliffe & McMillan-Staff, 1994, Ayliffe & Godward, 1993), gave rise to a single peak under isocratic conditions where two peaks had been observed under gradient conditions. It was therefore concluded that the single peak assigned as MWT 349 in the isocratic profile, would actually consist of more than one constituent if analysed under the gradient conditions.

Conclusions:

The structural identity of these two hydroxylated metabolites was not be achieved by the LC-MS techniques used in this study. The MS data did, however, suggest that it was unlikely that either the phenyl or the triazole rings were further OH substituted.

The analysis of samples during this study with a gradient HPLC method resulted in further resolution of what was thought to be a single component in the original studies. The two resolved components were found in this study to be present in roughly equal amounts. The component in the original study designated as an unknown with MW 349 exceeded 10 % of applied radioactivity in selected samples. It is concluded from this study that this 10 % was in fact two components each present at approximately 5 % of applied radioactivity.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 and is still considered reliable for the intended purpose (metabolite identification).
- The main focus of this study was to further investigate a metabolite fraction observed above 10 % AR in Ayliffe & Austin (1993) and Ayliffe & Godward (1993), called 'Met 5 (MWT 349)' in Ayliffe & Austin (1993) and 'Met 6' in Ayliffe and Godward (1993). The authors did this by comparing the isocratic HPLC method used in these two studies with a more advanced gradient HPLC method. The

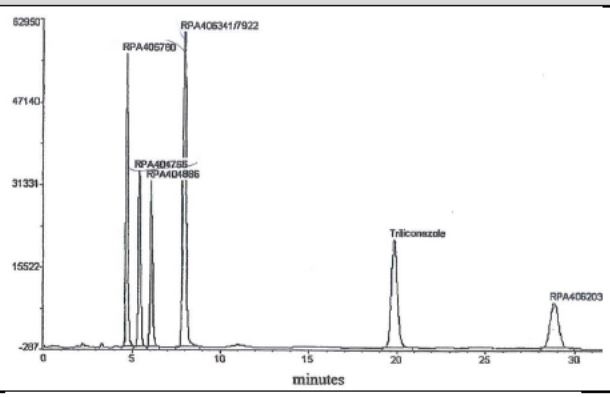
RMS AT agrees with the study author, that what was originally thought to be one compound (one peak) is likely to comprise two compounds (two separate peaks) with a MWT of 333 and 349, representing unknown mono- and di-hydroxylated derivatives of triticonazole.

- Although not in the author's focus this study demonstrates that the relative retention time (rRT) of RPA 407922 observed under conditions of the isocratic HPLC method does not match the rRT of 'Met 6 (MWT 333)' observed in Ayliffe & Austin (1993), claimed to be RPA 407922 by Ayliffe & McMillan-Staff (1994) (see figures on the 'isocratic HPLC method' below). It also demonstrates that the isocratic method is not capable to adequately separate RPA 406431 (Trans-diol) from RPA 407922 with both substances eluting much earlier (see below). With respect to the metabolite profiling in Ayliffe & Austin (1993) both substances are most probably co-eluting as 'Met 3'. Notice that RPA 407922 is unlikely to occur at significant amounts in soil on basis of Doble et al. (1996) and Simmonds et al. (1996).

- The RMS AT notes that the peak assignment of RPA 404886 and RPA 407922 in the soil sample of this study applying the gradient HPLC method (see figure on the 'gradient HPLC method' below) is probably wrong (on basis of retention times compared to the standard mix). This is also more in line with findings in Doble et al. (1996) and Simmonds et al. (1996) indicating that these two substances are unlikely to occur in aerobic soils at significant amounts. Notice that the study authors only investigated peak MWT 333 and MWT 349 (gradient HPLC) by mass spectroscopy.

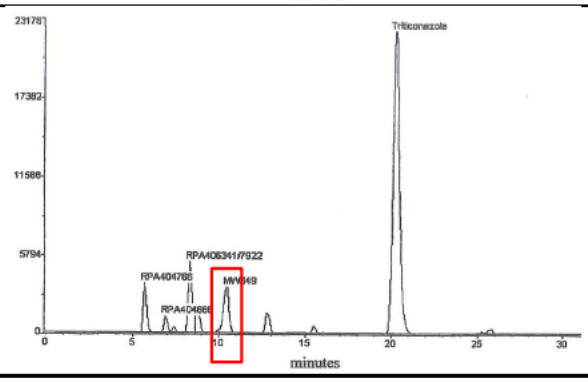
Table B.8.1.1.1-25 Example HPLC chromatograms of a mix of authentic reference substances, of the 100 g sample (20 °C) and of the 84 DAT sample of the UK sandy loam (Ayliffe & Austin, 1993) applying the isocratic HPLC method (used for metabolite profiling) - RMS AT assessment on basis of raw data in the study reports

Reference standard mix, UV
(this study, page 49)



100 g 20 °C soil sample, ^{14}C
(this study, page 50)

red box: area of interest in this study



UK sandy loam, 84 DAT, ^{14}C
(Ayliffe & Austin, 1993, page 40)

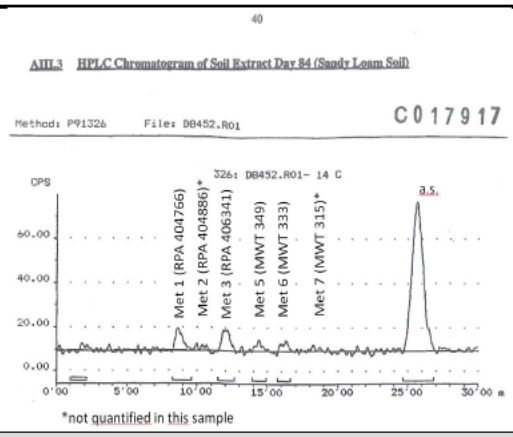
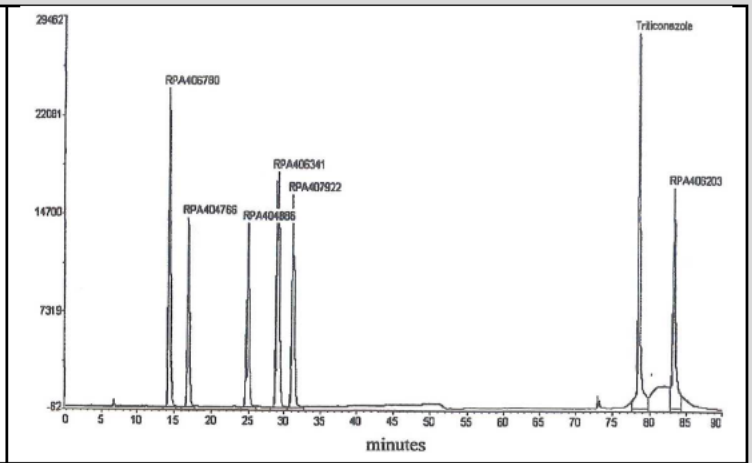


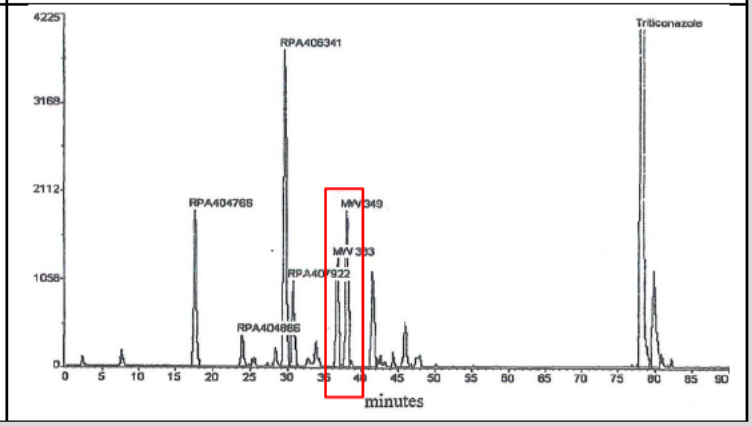
Table B.8.1.1.1-26 **Example HPLC chromatograms of a mix of authentic reference substances and of the 100 g sample (20 °C) applying the gradient HPLC method (used for mass spectroscopic work) - RMS AT assessment on basis of raw data in the study reports**

Reference standard mix, UV
(this study, page 42)



100 g 20 °C soil sample, ^{14}C
(this study, page 43)

red box: area of interest in this study



Reference:	**Aerobic soil metabolism of ^{14}C-BAS 595 F**
Author(s), year:	Ta, C., Strobush, A., 2012
Report/Doc. number:	2012/7004893
Guideline(s):	EPA 835.4100, OECD 307 (2002), SETAC (1995)
GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Test material

[Phenyl-U-^{14}C]-triticonazole (BAS 595 F)

Reg. No.	4378513
Lot/Batch number	866-1201
Molecular Weight	317.82 g/mol (non-labelled)
Site of radiocarbon labelling:	phenyl-U-^{14}C
Radiochemical purity:	98.9 %
Specific activity of ai:	6.76 MBq/mg

[Triazole-3(5)-^{14}C]-triticonazole (BAS 595 F)

Reg. No.	4378513
Lot/Batch number	867-1201
Molecular Weight	317.82 g/mol (non-labelled)
Site of radiocarbon labelling:	triazole-3(5)-^{14}C
Radiochemical purity:	99.6 %
Specific activity of ai:	5.07 MBq/mg

Soil

Three soils of different textures: One sand soil collected from California, one loamy sand soil from Wisconsin, and one loam soil from New Jersey were used. After removing the vegetation, larger soil fauna and stones, the soil was sieved through a 2-mm sieve before used. Prior to dosing, the moistures of the soils were adjusted to approximately 50 % of its maximum water holding capacity (MWHC) by adding the appropriate amount of HPLC water. The dry weight was determined by weighing the soils (3 reps) after they had been in an oven at approximately 100 °C overnight.

Soil characterization is presented in the table below.

Table B.8.1.1.1-27 Properties of the test soils

Name	California USA	New Jersey USA	Wisconsin USA
USDA Textural class	Sand	Loam	Loamy Sand
Sand [%]	94	30	86
Silt [%]	4	44	7
Clay [%]	2	26	7
Cation Exchange Capacity [meq/100 g]	4.7	8.3	7.5
Max. Water Hold. Capacity [g/100 g dry soil]	19.3	42.6	22.3
Total Organic Matter [%]	0.13	1.8	2.0
Total Organic Carbon [%]	0.08	1.0	1.16
pH (water)	8.1	6.8	6.0
Microbial Biomass Carbon at 0 DAT [µg/g dry soil]	90.9	58.6	71.6
Microbial Biomass Carbon at 120 DAT [µg/g dry soil]	14.2	10.5	21.2
Microbial Biomass Carbon at 366 DAT [µg/g dry soil]	27.9	48.9	118.2
Bulk Density [g/cc]	1.42	0.99	1.38

(a) Total organic carbon percent = percent organic matter / 1.724
DAT = days after treatment

Test system

The sieved soils were weighed into individual 250 mL polypropylene wide mouth centrifuge bottles as test vessels. Approximately 50 g of soil (dry weight basis) was added to each bottle. The moisture content of each sample was adjusted to 50 % of its maximum water holding capacity (MWHC) by adding HPLC water if necessary. The soil samples were then allowed to acclimate in a chamber at 20 ± 2 °C for 3 to 11 days in the dark under aerobic conditions. The test vessels were connected to an air flow-through system in series in which each vessel received a constant air-flow at a rate of approximately 20 mL/min downward over the soil surface and were incubated in the dark at 20 ± 2°C in constant temperature chambers. Before entering the bottles, air was bubbled through a 1N sodium hydroxide scrubber to remove carbon dioxide and to moisturize it. This procedure helped to minimize the drying of the soil samples and the saturation of the carbon dioxide traps during

incubation. Air leaving the test vessels was passed through 30 mL of 1N sodium hydroxide absorbers to collect any carbon dioxide evolved.

A total of 23 soil samples were prepared for each soil and each label. In addition, 10 non-treated samples and 2 high dose samples for each soil were prepared. Non treated soil was used to determine the microbial activity at study initiation, at the middle, and at the end of the incubation period. High dose samples were used to generate metabolites for identification and were treated with the same application solution at 6X rate.

The application solution of ^{14}C-labeled triticonazole was prepared in acetonitrile at a concentration of approximately 0.4 mg/mL. Aliquots of 100-µL of the application solution containing approximately 40 µg of test substance were applied into each test vessel (50 g of soil) resulting in a concentration of ^{14}C-triticonazole of 0.8 ppm in soil. This nominal final concentration of triticonazole was equivalent to a maximum single application rate of 0.58 lb/a (equivalent to 580 g/ha assuming the applied material distributed evenly into 5 cm depth of soil and bulk density of soil as 1.5 g/cm^3). The radiopurity (> 95 %) of the application solutions were verified by HPLC.

Test System Maintenance and Sampling
During the incubation period, the samples were checked approximately once every two weeks for the first month and once every month for the rest of the incubation period to determine the soil moisture content. The soil moisture was maintained at approximately 50 % of the maximum water holding capacity by periodically adding HPLC water to the soil samples, as necessary. The test vessels were connected to an air flow-through system in series and incubated in the dark at 20 ± 2 °C in constant temperature chambers.

Two samples for each soil were removed at intervals of 0-time (immediately after application), 14, 30, 63, 91, 120, 184, 274, and 366 days after treatment (DAT).

The liquid traps were assayed at all sampling times (except time-0) by directly adding aliquots of the trapping solution into liquid scintillation cocktail and counting by liquid scintillation counting (LSC). The traps were replaced with fresh 1 N sodium hydroxide solution at each sampling time. All of the soil samples were extracted and processed immediately after they were removed from the flow-through system.

Analytical procedure
The soil samples were first extracted with 4 consecutive extractions using 100 mL of acetonitrile, acetonitrile/methanol (7/3; v/v), acetonitrile/water (7/3; v/v), and methanol/water (7/3; v/v). The extractions were performed by shaking the soil/solvent mixture for 30 minutes at 300 strokes per minute at room temperature, followed by centrifugation for 15 minutes at 3600 rpm. Aliquots of the extracts were assayed by LSC. The organic solvent extracts were pooled, concentrated and analysed by HPLC. Soils were further extracted with 0.5 N NaOH solutions in order to characterize the bound residue portion. The fulvic fraction was subjected to HPLC analyses. The soils were then air-dried, and the non-extractable residue (NER) or humins was determined by oxidative combustion analysis.

Aliquots of organic solvent pooled extracts for each sample were concentrated by a rotary evaporator at room temperature prior to HPLC analysis. The NaOH extracts were fractionated into fulvic and humic fractions by adjusting the *p*H of the extract solutions to approximately 2 with HCl. The fulvic acid (supernatant) was separated from the humic acid (precipitate) by shaking vigorously by hand and allowing the samples to sit at room temperature for approximately 30 minutes. This was followed by centrifugation at ~ 3000 rpm for 20 minutes. The fulvic acid fraction was directly subjected to analysis by HPLC.

Samples were processed immediately after collecting by extracting with organic solvents and analysed as soon as they were worked up. If this was not feasible, the extracts were stored in the freezer concentrated before analysis. For the NaOH extraction, soil samples after extracting with organic solvents were stored in freezer for up to ~ 2 months. Analysis of the NaOH extracts from 14 DAT samples indicated that triticonazole is still intact during the storage.

Radioactivity was quantified by liquid scintillation counting. Triplicate aliquots of the extracts were added to HIONIC Fluor scintillation cocktail (Packard) for counting.

Non-extracted radioactivity (humins) was quantified by oxidative combustion analysis. The dry samples were ground into homogeneous soil samples before weighing and combustion. The oxidizer automatically prepared

the samples for radioassay by liquid scintillation counting with Harvey Cocktail scintillant (R.J. Harvey Instrument Corp).

The reference standards were chromatographed by HPLC to confirm the identity of the metabolites by retention time matching. The HPLC conditions were exactly the same (method 1) with those described above.

For LC/MS characterization, the pooled extracts from kinetic samples or extracts from high dose samples (using the same procedures of the kinetic samples). The extracts were pooled, concentrated by rotary evaporator and reconstituted in small volume of 50% ACN in water before subjected to LC/MS characterization. The peaks corresponding to metabolites (identified by radiodetector) were characterized by LC/MS as described in the Appendix C of the Analytics Reports.

Details on the HPLC setup are provided in the study report.

Findings:

Mass balance
The total recoveries of radioactivity from soils treated with [phenyl-U-^{14}C]-triticonazole and [triazole-3(5)-^{14}C]-triticonazole are presented in the tables below.

Results showed that only two metabolites, RPA 404766 (Cis-diol, at t_R of ~ 25.5 min.) and RPA 406341 (Trans-diol, at t_R of ~ 28.5 min), were greater than 5 % AR, with maximum occurrences of 9.11 and 8.38 % AR (in single replicates). Some minor degradation products were also found, each representing less than 5 % AR.

Table B.8.1.1.1-28 Material balance of [triazole-3(5)-^{14}C]-triticonazole in a sand soil (California) under aerobic conditions

Rep 1	**0 DAT**	**14 DAT**	**30 DAT**	**63 DAT**	**91 DAT**	**120 DAT**	**184 DAT**	**274 DAT**	**366 DAT**
CO_2	NA	0.05	0.12	0.48	0.77	1.03	1.44	1.86	2.34
Extract 1	85.07	77.48	75.18	71.31	69.23	65.76	60.39	61.18	53.27
Extract 2	12.74	12.93	12.86	14.39	14.63	13.90	13.82	12.72	14.29
Extract 3	1.79	4.49	5.25	6.87	7.73	8.54	6.31	12.24	12.02
Extract 4	0.24	1.18	1.54	2.13	2.74	2.57	2.64	2.87	3.92
Total Org. Ext.	99.84	96.08	94.83	94.70	94.33	90.77	83.16	89.01	83.50
NaOH Ext	NP	1.50	1.88	2.20	2.64	3.25	4.14	4.71	6.51
Humins	0.16	1.75	2.64	3.69	4.15	5.01	7.38	10.38	10.40
Total Recovery	**100.00**	**99.38**	**99.47**	**101.07**	**101.89**	**100.06**	**96.12**	**105.96**	**102.75**
Rep 2									
CO_2	NA	0.05	0.12	0.48	0.77	1.03	1.44	1.86	2.34
Extract 1	85.14	78.23	76.00	71.77	72.22	65.46	58.88	60.37	49.78
Extract 2	13.45	12.74	12.77	14.58	14.55	13.35	13.41	13.91	14.44
Extract 3	1.96	4.35	5.07	7.06	7.63	8.47	6.33	11.95	13.59
Extract 4	0.26	1.16	1.53	2.21	2.71	2.69	2.63	3.11	4.15
Total Org. Ext.	100.81	96.48	95.37	95.62	97.11	89.97	81.25	89.34	81.96
NaOH Ext	NP	1.46	1.83	2.35	2.63	3.30	4.48	4.69	7.04
Humins	0.15	1.70	2.65	3.11	4.41	5.14	7.90	10.08	11.05
Total Recovery	**100.96**	**99.69**	**99.97**	**101.56**	**104.92**	**99.44**	**95.07**	**105.97**	**102.39**

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
Extract 1 = Acetonitrile
Extract 2 = Acetonitrile/methanol (7:3)
Extract 3 = Acetonitrile/water (7:3)
Extract 4 = Methanol/water (7:3)
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-29 Material balance of [triazole-3(5)-^{14}C]-triticonazole in a loam soil (New Jersey) under aerobic conditions

Rep 1	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
CO_2	NA	0.02	0.03	0.13	0.23	0.35	0.59	1.27	1.63
Extract 1	80.24	67.86	63.41	55.66	50.68	47.93	42.55	40.16	31.85
Extract 2	15.47	15.74	14.65	14.25	14.39	12.84	12.63	11.31	9.66
Extract 3	3.40	5.51	5.54	6.34	6.62	6.23	6.17	6.67	5.90
Extract 4	0.62	1.90	2.48	3.36	2.89	3.44	3.05	3.48	4.16
Total Org. Ext.	99.73	91.01	86.08	79.61	74.58	70.44	64.40	61.61	51.57
NaOH Ext	NP	3.26	4.70	7.86	11.11	12.45	14.94	17.13	19.94
Humins	0.26	4.66	7.21	11.38	13.56	15.87	20.97	26.42	31.67
Total Recovery	**99.99**	**98.95**	**98.02**	**98.98**	**99.48**	**99.11**	**100.90**	**106.44**	**104.81**
Rep 2									
CO_2	NA	0.02	0.03	0.13	0.23	0.35	0.59	1.27	1.63
Extract 1	80.62	68.74	63.14	58.31	53.18	48.31	36.77	39.53	32.70
Extract 2	15.92	15.53	15.07	14.56	14.25	13.25	11.72	11.37	9.51
Extract 3	3.49	5.24	5.51	6.09	6.41	6.13	6.38	6.68	6.03
Extract 4	0.63	1.79	2.43	3.26	2.94	3.41	3.02	3.39	4.42
Total Org. Ext.	100.66	91.30	86.15	82.22	76.78	71.10	57.89	60.97	52.66
NaOH Ext	NP	3.01	4.50	7.34	10.35	11.55	17.94	17.20	19.64
Humins	0.27	4.41	7.01	11.18	13.15	14.66	23.73	26.72	29.84
Total Recovery	**100.93**	**98.74**	**97.69**	**100.87**	**100.51**	**97.66**	**100.15**	**106.16**	**103.77**

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
Extract 1 = Acetonitrile
Extract 2 = Acetonitrile/methanol (7:3)
Extract 3 = Acetonitrile/water (7:3)
Extract 4 = Methanol/water (7:3)
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-30 Material balance of [phenyl-U-^{14}C]-triticonazole in a loam soil (New Jersey) under aerobic conditions

Rep 1	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
CO_2	NA	0.44	1.43	3.48	5.19	6.97	9.37	13.13	16.25
Extract 1	79.78	66.92	60.07	55.33	49.34	47.53	37.77	35.50	31.42
Extract 2	15.57	15.32	14.82	14.30	13.18	12.79	11.26	10.21	9.01
Extract 3	3.51	5.10	5.22	5.65	5.48	5.14	7.91	5.23	4.60
Extract 4	0.66	1.77	2.43	2.95	2.22	2.79	2.39	3.03	3.60
Total Org. Ext.	99.52	89.11	82.54	78.23	70.22	68.25	59.33	53.97	48.63
NaOH Ext	NP	3.02	4.05	5.27	8.06	7.24	8.86	8.68	8.92
Humins	0.48	4.54	7.71	10.32	13.03	13.51	19.01	21.39	22.91
Total Recovery	**100.00**	**97.11**	**95.73**	**97.30**	**96.50**	**95.97**	**96.57**	**97.17**	**96.71**
Rep 2									
CO_2	NA	0.44	1.43	3.48	5.19	6.97	9.37	13.13	16.25
Extract 1	76.79	66.86	60.31	53.60	52.18	48.01	39.86	35.92	30.23
Extract 2	15.34	15.41	14.47	13.76	13.56	13.04	11.73	10.56	8.79
Extract 3	3.58	5.13	5.16	5.48	5.50	5.24	7.97	5.26	4.44
Extract 4	0.66	1.71	2.26	2.85	2.16	2.98	2.41	3.02	3.56
Total Org. Ext.	96.37	89.11	82.20	75.69	73.40	69.27	61.97	54.76	47.03
NaOH Ext	NP	2.96	3.89	5.50	7.75	7.14	8.66	8.68	8.48
Humins	0.35	4.47	7.51	10.72	12.87	14.01	17.79	22.24	22.39
Total Recovery	**96.72**	**96.98**	**95.03**	**95.39**	**99.21**	**97.39**	**97.79**	**98.81**	**94.15**

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
Extract 1 = Acetonitrile
Extract 2 = Acetonitrile/methanol (7:3)
Extract 3 = Acetonitrile/water (7:3)
Extract 4 = Methanol/water (7:3)
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-31 Material balance of [triazole-3(5)-^{14}C]-triticonazole in a sand soil (Wisconsin) under aerobic conditions

Rep 1	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
CO_2	NA	0.02	0.03	0.05	0.08	0.11	0.15	0.31	0.45
Extract 1	85.53	72.06	66.40	59.99	59.60	52.24	40.85	40.41	39.49
Extract 2	12.21	13.50	13.67	14.05	14.20	14.53	13.39	13.59	11.52
Extract 3	1.86	4.37	5.05	7.07	6.39	7.25	9.21	11.02	9.06
Extract 4	0.24	1.61	2.30	3.57	3.37	3.76	3.94	4.36	4.70
Total Org. Ext.	99.84	91.54	87.42	84.68	83.56	77.78	67.39	69.38	64.77
NaOH Ext	NP	3.40	4.60	7.55	10.35	11.20	16.66	18.15	18.89
Humins	0.16	3.13	5.27	7.07	8.53	11.66	15.53	17.69	19.26
Total Recovery	**100.00**	**98.09**	**97.32**	**99.35**	**102.52**	**100.75**	**99.73**	**105.53**	**103.37**
Rep 2									
CO_2	NA	0.02	0.03	0.05	0.08	0.11	0.15	0.31	0.45
Extract 1	85.01	72.14	67.28	63.46	59.58	55.47	47.92	46.55	39.11
Extract 2	12.07	13.38	13.44	13.75	13.86	14.09	13.68	12.64	10.67
Extract 3	1.81	4.71	4.67	5.91	6.32	6.23	6.66	7.99	7.47
Extract 4	0.24	1.47	2.15	3.16	3.63	3.37	3.05	3.45	4.40
Total Org. Ext.	99.13	91.70	87.54	86.28	83.39	79.16	71.31	70.64	61.65
NaOH Ext	NP	3.28	4.42	7.02	10.51	11.09	15.76	17.94	19.40
Humins	0.13	3.00	4.98	6.91	8.36	11.15	13.59	18.31	20.08
Total Recovery	**99.26**	**98.00**	**96.97**	**100.26**	**102.34**	**101.51**	**100.81**	**107.20**	**101.58**

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
Extract 1 = Acetonitrile
Extract 2 = Acetonitrile/methanol (7:3)
Extract 3 = Acetonitrile/water (7:3)
Extract 4 = Methanol/water (7:3)
All values found in this table were rounded to two decimal point

Characterisation and identification of residues in extracts

The amounts of triticonazole and its metabolites recovered at each time point are shown in the tables below as percentages of the total applied radioactivity.

Table B.8.1.1.1-32 Biotransformation of [triazole-3(5)-^{14}C]-triticonazole in organic solvent extracts of a sand soil (California) under aerobic conditions – Replicate 1 (% AR, numbers shaded in grey exceed 5 % AR)

Rep 1	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
Triazole (5.5 min)	ND	ND	ND	ND	ND	ND	ND	0.69	2.66
Triazole acetic (5.7min)	ND	ND	ND	ND	ND	0.50	1.00	5.27	3.00
Region 3 (5.9 min)	ND	ND	ND	ND	ND	ND	ND	0.99	1.84
Region 4 (6 min)	ND	ND	ND	ND	ND	ND	0.93	0.61	1.36
RPA 404766 (Cis-diol) (25.5 min)	ND	1.15	1.99	2.50	4.26	6.29	6.44	8.38	6.79
Region 6 (27 min)	3.41	ND	ND	ND	ND	0.54	0.57	1.32	0.83
RPA 406341 (Trans-diol) (28.5 min)	ND	0.63	0.68	2.30	4.08	4.41	6.28	8.28	8.38
Region 8 (28.7 min)	ND	ND	ND	ND	ND	ND	1.42	1.17	2.62
Region 9 (29 min)	ND	ND	ND	ND	1.25	1.78	1.07	ND	ND
Region 10 (29.8 min)	ND	ND	ND	ND	ND	0.34	ND	0.70	0.41
Region 11 (30.5 min)	ND	ND	ND	ND	ND	0.26	0.72	1.71	1.77
Region 12 (31.5 min)	ND	ND	ND	ND	ND	0.54	1.36	1.68	2.10
Region 13 (31.8 min)	ND	ND	ND	ND	1.08	0.68	0.72	1.46	0.73
Region 14 (32.7 min)	ND	ND	ND	ND	ND	ND	ND	1.17	0.85
Region 15 (32.8 min)	ND	ND	0.46	1.14	1.54	1.29	1.76	1.05	0.75
Triticonazole (34 min)	95.65	93.51	90.75	87.99	80.94	72.52	59.23	52.24	46.17
Region 16 (36 min)	0.79	0.78	ND	ND	0.58	0.95	1.66	2.29	2.56
Region 17 (36.8 min)	ND	ND	0.93	0.78	0.59	0.32	ND	ND	ND
Sub Total	99.85	96.07	94.81	94.71	94.32	90.42	83.16	89.01	82.82
Others	0.00	0.01	0.02	0.00	0.01	0.35	0.00	0.00	0.68
Total Org. Ext.	99.84	96.08	94.83	94.70	94.33	90.77	83.16	89.01	83.50
NaOH Ext	NA	1.50	1.88	2.20	2.64	3.25	4.14	4.71	6.51
CO_2	NA	0.05	0.12	0.48	0.77	1.03	1.44	1.86	2.34
Humins	0.16	1.75	2.64	3.69	4.15	5.01	7.38	10.38	10.40

Total	100.01	99.38	99.47	101.08	101.89	100.06	96.12	105.96	102.75

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-33 Biotransformation of [triazole-3(5)-^{14}C]-triticonazole in organic solvent extracts of a sand soil (California) under aerobic conditions – Replicate 2 (% AR, numbers shaded in grey exceed 5 % AR)

Rep 2	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
Triazole (5.5 min)	ND	ND	ND	ND	ND	ND	ND	2.96	2.94
Triazole acetic (5.7 min)	ND	ND	ND	ND	ND	0.52	1.06	2.15	3.39
Region 3 (5.9 min)	ND	ND	ND	ND	ND	ND	ND	0.93	1.96
Region 4 (6 min)	ND	ND	ND	ND	ND	ND	ND	0.45	0.76
RPA 404766 (Cis-diol) (25.5 min)	ND	0.81	1.45	2.89	4.66	6.51	6.33	9.11	7.84
Region 6 (27 min)	ND	ND	ND	ND	ND	0.44	0.54	1.29	1.48
RPA 406341 (Trans-diol) (28.5 min)	ND	0.66	1.08	2.71	4.28	4.98	3.45	8.02	8.19
Region 8 (28.7 min)	ND	ND	ND	ND	ND	ND	4.43	1.53	1.61
Region 9 (29 min)	ND	ND	ND	ND	0.84	2.29	1.18	ND	ND
Region 10 (29.8 min)	ND	ND	ND	ND	0.11	0.65	0.71	0.49	0.63
Region 11 (30.5 min)	ND	ND	ND	ND	ND	ND	ND	1.47	1.92
Region 12 (31.5 min)	ND	ND	ND	ND	ND	1.03	0.98	1.85	2.89
Region 13 (31.8 min)	ND	ND	ND	ND	1.11	0.52	1.09	0.94	ND
Region 14 (32.7 min)	ND	ND	ND	ND	ND	ND	ND	1.12	ND
Region 15 (32.8 min)	ND	ND	0.49	0.78	1.36	2.22	1.66	0.91	1.70
Triticonazole (34 min)	99.81	93.91	91.27	86.25	82.97	68.34	57.12	54.48	45.13
Region 16 (36 min)	1.00	1.10	ND	ND	1.20	0.98	2.71	1.63	1.52
Region 17 (36.8 min)	ND	ND	1.08	0.98	0.67	ND	ND	ND	ND
Sub Total	100.81	96.48	95.37	93.61	97.20	88.48	81.26	89.33	81.96
Others	0.00	0.00	0.00	2.01	0.00	1.49	0.00	0.01	0.00
Total Org. Ext.	100.81	96.48	95.37	95.62	97.11	89.97	81.25	89.34	81.96
NaOH Ext	NA	1.46	1.83	2.35	2.62	3.30	4.48	4.69	7.04
CO_2	NA	0.05	0.12	0.48	0.77	1.03	1.44	1.86	2.34
Humins	0.15	1.70	2.65	3.11	4.41	5.14	7.90	10.08	11.05
Total	100.96	99.69	99.97	101.56	105.00	99.44	95.08	105.97	102.39

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-34 Biotransformation of [triazole-3(5)-^{14}C]-triticonazole in organic solvent extracts of a loam soil (New Jersey) under aerobic conditions – Replicate 1 (% AR, numbers shaded in grey exceed 5 % AR)

Rep 1	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
Region 1 (5.3 min)	ND	ND	ND	ND	ND	ND	ND	ND	3.92
Triazole (5.5 min)	ND	ND	0.88	2.94	2.23	3.13	3.28	3.39	2.39
Triazole acetic (5.7 min)	ND	ND	0.32	ND	2.48	1.89	4.28	2.53	1.07
Region 4 (5.9 min)	ND	ND	0.20	1.29	0.51	0.70	2.29	0.59	0.65
Region 5 (6 min)	ND	ND	ND	ND	ND	ND	0.72	0.63	0.41
RPA 404766 (Cis-diol) (25.5 min)	ND	3.17	6.09	6.70	5.73	5.93	4.84	5.12	3.96
Region 7 (27 min)	ND	ND	0.56	0.70	0.80	1.23	0.53	0.98	1.01
RPA 406341 (Trans-diol) (28.5 min)	ND	2.25	3.67	4.65	4.79	5.55	3.47	4.81	3.23
Region 9 (28.7 min)	ND	0.97	1.73	1.65	2.00	1.23	1.57	1.24	1.32
Region 10 (29 min)	ND	ND	ND	0.31	0.40	0.80	1.48	ND	ND
Region 11 (29.8 min)	ND	ND	0.29	ND	0.41	0.79	0.48	0.39	0.41
Region 12 (30 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Region 13 (30.5 min)	ND	ND	ND	ND	0.95	2.43	2.12	1.23	1.82
Region 14 (30.7 min)	ND	ND	0.73	0.88	0.86	0.62	2.47	2.64	3.30
Region 15 (31.6 min)	ND	ND	0.39	1.18	1.51	1.68	1.42	2.13	2.50
Region 16 (31.8 min)	ND	ND	ND	ND	ND	ND	ND	0.93	0.45
Region 17 (32 min)	ND	ND	0.99	ND	1.33	0.27	ND	1.21	0.25
Region 18 (32.7 min)	ND	1.43	1.52	1.99	1.42	1.88	1.15	0.76	0.24
Region 19 (32.8 min)	ND	ND	ND	ND	ND	ND	ND	ND	0.81

Region 20 (33 min)	ND	ND	ND	ND	0.40	0.49	0.62	ND	ND
Triticonazole (34 min)	98.98	81.86	66.88	54.60	46.32	39.60	31.67	30.71	21.78
Region 21 (35.9 min)	0.76	0.76	0.77	1.27	1.10	2.23	1.55	1.06	0.90
Region 22 (36 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Region 23 (36.5 min)	ND	0.57	0.47	0.97	1.34	ND	0.44	1.23	1.14
Region 24 (36.8 min)	ND	ND	0.58	0.47	ND	ND	ND	ND	ND
Sub Total	99.74	91.01	86.07	79.60	74.58	70.45	64.38	61.58	51.56
Others	0.00	0.00	0.01	0.01	0.00	0.00	0.02	0.03	0.01
Total Org. Ext.	99.73	91.01	86.08	79.61	74.58	70.44	64.40	61.61	51.57
NaOH Ext	NA	3.26	4.70	7.86	11.11	12.45	14.94	17.13	19.94
CO2	NA	0.02	0.03	0.13	0.23	0.35	0.59	1.27	1.63
Humins	0.26	4.66	7.21	11.38	13.56	15.86	20.97	26.42	31.67
Total	100.00	98.95	98.02	98.98	99.48	99.11	100.90	106.43	104.81

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-35 Biotransformation of [triazole-3(5)-^{14}C]-triticonazole in organic solvent extracts of a loam soil (New Jersey) under aerobic conditions – Replicate 2 (% AR, numbers shaded in grey exceed 5 % AR)

Rep 2	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
Region 1 (5.3 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Triazole (5.5 min)	ND	ND	0.74	2.68	3.37	2.05	1.84	1.04	1.91
Triazole acetic (5.7 min)	ND	ND	0.47	ND	1.88	2.70	2.15	2.51	4.31
Region 4 (5.9 min)	ND	ND	0.34	1.11	0.47	0.76	1.09	3.04	1.41
Region 5 (6 min)	ND	ND	ND	ND	ND	ND	0.80	0.50	0.38
RPA 404766 (Cis-diol) (25.5 min)	ND	3.73	5.13	6.59	6.70	6.38	4.98	5.39	3.58
Region 7 (27 min)	ND	ND	0.46	0.87	1.19	1.13	1.01	0.45	0.57
RPA 406341 (Trans-diol) (28.5 min)	ND	1.92	3.69	4.22	4.58	3.41	3.62	5.04	4.24
Region 9 (28.7 min)	ND	0.96	0.99	1.91	1.35	2.08	2.47	1.48	1.79
Region 10 (29 min)	ND	ND	ND	0.57	1.26	1.20	0.55	0.57	ND
Region 11 (29.8 min)	ND	ND	0.39	ND	ND	0.45	0.37	1.86	0.52
Region 12 (30 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Region 13 (30.5 min)	ND	ND	0.36	1.04	2.01	1.65	2.94	2.71	2.13
Region 14 (30.7 min)	ND	ND	ND	ND	0.41	1.00	0.51	ND	2.86
Region 15 (31.6 min)	ND	ND	ND	1.18	1.72	1.16	1.60	2.90	2.01
Region 16 (31.8 min)	ND	ND	ND	ND	ND	ND	ND	ND	0.34
Region 17 (32 min)	ND	ND	0.49	0.98	0.69	0.55	0.86	0.58	0.46
Region 18 (32.7 min)	ND	1.58	1.27	1.57	1.62	1.02	0.49	1.37	0.48
Region 19 (32.8 min)	ND	ND	0.60	ND	0.56	1.13	0.88	0.27	0.50
Region 20 (33 min)	ND	ND	ND	ND	ND	ND	ND	ND	0.37
Triticonazole (34 min)	99.85	81.17	69.72	57.19	46.80	42.06	29.10	27.80	22.25
Region 21 (35.9 min)	0.82	1.15	0.84	1.40	1.60	1.78	1.49	0.87	0.97
Region 22 (36 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Region 23 (36.5 min)	ND	0.78	0.22	0.68	0.57	0.60	1.15	2.27	0.61
Region 24 (36.8 min)	ND	ND	0.45	0.24	ND	ND	ND	ND	ND
Sub Total	100.67	91.29	86.16	82.23	76.78	71.11	57.90	60.65	51.69
Others	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.32	0.97
Total Org. Ext.	100.66	91.30	86.15	82.22	76.78	71.10	57.89	60.97	52.66
NaOH Ext	NA	3.01	4.50	7.34	10.35	11.55	17.94	17.20	19.64
CO2	NA	0.02	0.03	0.13	0.23	0.35	0.59	1.27	1.63
Humins	0.27	4.41	7.01	11.18	13.15	14.66	23.73	26.72	29.84
Total	100.94	98.74	97.70	100.88	100.51	97.67	100.16	106.16	103.77

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-36 **Biotransformation of [phenyl-U-^{14}C]-triticonazole in organic solvent extracts of a loam soil (New Jersey) under aerobic conditions – Replicate 1 (% AR, numbers shaded in grey exceed 5 % AR)**

Rep 1	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
RPA 404766 (Cis-diol) (25.5 min)	ND	3.44	5.65	7.17	6.33	6.66	5.74	5.34	4.29
Region 7 (27 min)	ND	ND	0.56	1.06	1.44	0.87	1.13	0.96	0.93
RPA 406341 (Trans-diol) (28.5 min)	ND	2.42	3.27	5.96	5.22	5.73	3.62	4.83	4.18
Region 4 (28.7 min)	ND	ND	ND	ND	ND	ND	ND	1.25	1.45
Region 5 (29 min)	ND	0.91	1.82	1.67	1.95	1.69	2.81	0.37	0.60
Region 6 (29.8 min)	ND	ND	ND	ND	ND	ND	ND	0.37	ND
Region 7 (30 min)	ND	ND	ND	ND	0.18	0.55	0.54	2.50	1.70
Region 8 (30.5 min)	ND	0.30	ND	1.06	1.88	1.67	2.54	2.82	3.49
Region 9 (31.5 min)	ND	ND	ND	ND	ND	2.21	1.95	2.87	2.34
Region 10 (31.8 min)	ND	ND	0.88	1.17	1.33	ND	1.28	0.63	ND
Region 11 (32 min)	ND	ND	ND	ND	0.79	1.31	ND	0.76	1.09
Region 12 (32.7 min)	ND	1.35	1.71	2.14	1.45	1.44	1.48	0.67	1.51
Region 13 (33 min)	ND	ND	ND	ND	0.20	0.51	0.55	ND	0.32
Triticonazole (34 min)	98.77	79.56	67.10	56.01	46.54	42.76	34.96	28.04	23.75
Region 14 (35.9 min)	0.75	0.50	1.54	2.00	1.64	2.09	1.57	1.18	1.37
Region 15 (36 min)	ND	ND	ND	ND	ND	ND	ND	1.38	1.22
Region 16 (36.3 min)	ND	0.63	ND	ND	0.91	0.36	1.16	ND	ND
Region 17 (36.8 min)	ND	ND	ND	ND	0.38	0.40	ND	ND	ND
Sub Total	99.52	89.11	82.54	78.23	70.23	68.24	59.34	53.98	48.24
Others	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.37
Total Org. Ext.	99.52	89.11	82.54	78.23	70.22	68.25	59.33	53.97	48.63
NaOH Ext	NA	3.02	4.05	5.27	8.06	7.24	8.86	8.68	8.92
CO2	NA	0.44	1.43	3.48	5.29	6.97	9.37	13.13	16.25
Humins	0.48	4.54	7.71	10.32	13.03	13.51	19.01	21.39	22.91
Total	100.00	97.11	95.73	97.30	96.61	95.97	96.58	97.18	96.69

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-37 **Biotransformation of [phenyl-U-^{14}C]-triticonazole in organic solvent extracts of a loam soil (New Jersey) under aerobic conditions – Replicate 2 (% AR, numbers shaded in grey exceed 5 % AR)**

Rep 2	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
RPA 404766 (Cis-diol) (25.5 min)	ND	4.04	4.74	7.55	7.48	7.32	6.54	5.08	4.96
Region 2 (27 min)	ND	ND	ND	0.89	0.90	1.07	1.05	1.08	1.11
RPA 406341 (Trans-diol) (28.5 min)	ND	2.41	3.91	5.12	5.48	5.11	4.63	4.86	4.04
Region 4 (28.7 min)	ND	ND	ND	1.59	2.47	2.92	2.30	1.80	1.28
Region 5 (29 min)	ND	1.31	2.02	ND	ND	ND	0.84	0.36	ND
Region 6 (29.8 min)	ND	ND	ND	ND	0.50	0.43	0.60	0.41	0.64
Region 7 (30 min)	ND	ND	ND	ND	ND	ND	ND	2.15	1.98
Region 8 (30.5 min)	ND	ND	ND	1.19	1.83	2.09	3.25	2.25	2.50
Region 9 (31.5 min)	ND	ND	ND	ND	ND	ND	1.72	2.32	2.03
Region 10 (31.8 min)	ND	ND	ND	ND	1.98	1.99	1.52	1.24	ND
Region 11 (32 min)	ND	ND	0.95	1.35	0.86	0.94	ND	1.37	0.45
Region 12 (32.7 min)	ND	1.55	1.64	1.91	1.83	1.36	0.55	0.73	1.08
Region 13 (33 min)	ND	ND	ND	ND	0.51	0.69	1.13	ND	0.43
Triticonazole (34 min)	95.58	78.45	67.78	54.37	46.39	42.21	35.35	28.33	24.20
Region 14 (35.9 min)	0.80	0.78	1.16	1.72	2.11	1.39	1.95	1.45	0.79
Region 15 (36 min)	ND	ND	ND	ND	0.70	1.15	0.54	1.35	1.53
Region 16 (36.3 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Region 17 (36.8 min)	ND	0.57	ND	ND	0.40	0.60	ND	ND	ND
Sub Total	96.38	89.10	82.21	75.68	73.42	69.26	61.97	54.77	47.03
Others	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.00	0.00
Total Org. Ext.	96.37	89.11	82.20	75.69	73.40	69.27	61.97	54.76	47.03
NaOH Ext	NA	2.96	3.89	5.50	7.75	7.14	8.66	8.68	8.48
CO2	NA	0.44	1.43	3.48	5.29	6.97	9.37	13.13	16.25
Humins	0.35	4.47	7.51	10.72	12.87	14.01	17.79	22.24	22.39

Total	96.73	96.98	95.04	95.39	99.33	97.39	97.79	98.82	94.15

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-38 Biotransformation of [triazole-3(5)-^{14}C]-triticonazole in organic solvent extracts of a sand soil (Wisconsin) under aerobic conditions – Replicate 1 (% AR, numbers shaded in grey exceed 5 % AR)

Rep 1	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
Triazole (5.5 min)	ND	ND	ND	ND	ND	0.71	0.89	0.16	2.08
Triazole acetic (5.7 min)	ND	ND	ND	0.54	1.05	0.68	0.86	0.74	1.09
Region 3 (5.9 min)	ND	ND	ND	0.37	0.41	0.33	ND	0.34	0.76
RPA 404766 (Cis-diol) (25.5 min)	ND	3.34	5.39	6.97	7.56	6.70	5.43	6.75	5.75
Region 5 (27 min)	ND	ND	0.52	1.09	1.80	1.02	1.64	2.75	3.74
Region 6 (27.4 min)	ND	ND	ND	ND	ND	0.62	0.67	0.35	ND
RPA 406341 (Trans-diol) (28.5 min)	ND	2.94	4.09	5.28	6.05	5.91	5.38	5.32	4.83
Region 8 (28.7 min)	ND	1.04	1.31	2.70	2.92	3.10	3.96	4.98	4.77
Region 9 (29 min)	ND	ND	ND	0.22	0.62	1.05	0.93	1.08	0.98
Region 10 (29.8 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Region 11 (30 min)	ND	ND	ND	ND	ND	ND	1.28	2.07	1.32
Region 12 (30.5 min)	ND	ND	ND	ND	0.41	0.52	0.71	ND	1.37
Region 13 (31.5 min)	ND	ND	ND	ND	ND	0.40	ND	2.39	3.44
Region 14 (31.6 min)	ND	ND	ND	1.00	1.29	1.30	1.39	1.26	1.30
Region 15 (32 min)	ND	ND	ND	ND	0.86	ND	1.66	ND	ND
Region 16 (32.5 min)	ND	1.35	1.67	2.26	3.38	2.07	3.37	4.58	4.12
Region 17 (32.8 min)	ND	ND	ND	1.06	ND	0.93	1.33	0.81	0.48
Triticonazole (34 min)	99.18	81.37	73.35	61.97	55.63	50.92	35.21	32.85	26.73
Region 18 (35.9 min)	ND	0.83	0.69	0.96	1.20	0.69	0.99	1.32	1.18
Region 19 (36 min)	0.67	0.66	0.42	ND	0.38	0.40	0.34	0.76	0.84
Sub Total	99.85	91.53	87.44	84.42	83.56	77.35	66.04	68.51	64.78
Others	0.00	0.01	0.00	0.26	0.00	0.43	1.35	0.87	0.00
Total Org. Ext.	99.84	91.54	87.42	84.68	83.56	77.78	67.39	69.38	64.77
NaOH Ext	NA	3.40	4.60	7.55	10.35	11.20	16.66	18.15	18.89
CO2	NA	0.02	0.03	0.05	0.08	0.11	0.15	0.31	0.45
Humins	0.16	3.13	5.27	7.07	8.53	11.66	15.53	17.69	19.26
Total	100.01	98.09	97.34	99.35	102.52	100.75	99.73	105.53	103.38

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Table B.8.1.1.1-39 Biotransformation of [triazole-3(5)-^{14}C]-triticonazole in organic solvent extracts of a sand soil (Wisconsin) under aerobic conditions – Replicate 2 (% AR, numbers shaded in grey exceed 5 % AR)

Rep 2	0 DAT	14 DAT	30 DAT	63 DAT	91 DAT	120 DAT	184 DAT	274 DAT	366 DAT
Triazole (5.5 min)	ND	ND	ND	ND	ND	ND	0.81	0.14	2.37
Triazole acetic (5.7 min)	ND	ND	ND	0.91	1.63	0.67	1.27	1.33	1.17
Region 3 (5.9 min)	ND	ND	ND	0.35	0.63	0.67	ND	0.66	0.91
RPA 404766 (Cis-diol) (25.5 min)	ND	3.48	4.65	6.44	6.48	7.59	7.01	7.05	4.48
Region 5 (27 min)	ND	ND	ND	1.10	1.73	1.31	1.48	3.25	3.77
Region 6 (27.4 min)	ND	ND	ND	ND	ND	ND	0.73	ND	ND
RPA 406341 (Trans-diol) (28.5 min)	ND	2.28	3.45	5.52	4.81	5.56	4.09	6.09	4.60
Region 8 (28.7 min)	ND	1.19	1.49	1.79	3.48	1.66	3.84	4.55	4.60
Region 9 (29 min)	ND	ND	ND	0.84	0.38	1.66	2.11	1.00	1.35
Region 10 (29.8 min)	ND	ND	ND	ND	0.37	ND	0.53	ND	ND
Region 11 (30 min)	ND	ND	ND	ND	ND	0.16	0.52	1.15	1.93
Region 12 (30.5 min)	ND	ND	ND	ND	0.54	0.82	1.12	0.58	ND
Region 13 (31.5 min)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Region 14 (31.6 min)	ND	ND	ND	0.82	0.81	1.77	2.11	2.54	2.76
Region 15 (32 min)	ND	ND	ND	0.89	0.31	0.95	0.99	1.31	1.25
Region 16 (32.5 min)	ND	1.46	2.09	2.35	2.06	1.80	2.03	3.99	4.68
Region 17 (32.8 min)	ND	0.39	ND	ND	1.22	1.77	2.69	ND	0.64

Triticonazole (34 min)	98.34	81.31	74.29	64.14	56.71	48.94	38.41	33.89	24.45
Region 18 (35.9 min)	ND	0.93	1.01	0.80	1.61	0.58	0.79	1.00	0.96
Region 19 (36 min)	0.79	0.64	0.57	ND	0.28	0.88	0.78	0.92	0.66
Sub Total	99.13	91.68	87.55	85.95	83.05	76.79	71.31	69.45	60.58
Others	0.00	0.02	0.00	0.33	0.35	2.37	0.00	1.19	1.07
Total Org. Ext.	99.13	91.70	87.54	86.28	83.40	79.16	71.31	70.64	61.65
NaOH Ext	NA	3.28	4.42	7.02	10.51	11.09	15.76	17.94	19.40
CO2	NA	0.02	0.03	0.05	0.08	0.11	0.15	0.31	0.45
Humins	0.13	3.00	4.98	6.91	8.36	11.15	13.59	18.31	20.08
Total	99.26	98.00	96.98	100.26	102.35	101.51	100.81	107.20	101.58

NA = Not applicable (no sample analysed) - There were no volatile traps for time zero
NP = Not performed
All values found in this table were rounded to two decimal points

Isomerization

The HPLC method 1 used to analyse triticonazole and its metabolites also separates the *E* and *Z* isomers of triticonazole (the *E* isomer, triticonazole, at a retention time of approximately 34 min and the *Z* isomer (RPA 406203) at a retention time of approximately 36 min). As a result, the interconversion of the isomers of triticonazole in soil under aerobic conditions can be followed. Results showed that the *E* isomer was the major component of triticonazole, while the levels of the *Z* isomer (RPA 406203) were less than 2 % in all samples during 1 year of incubation, suggesting that there were no significant conversions of the *E* to the *Z* isomers.

The chiral method, which separates the *R* and *S* stereo isomers of triticonazole, was used to check the distribution of the *R* and *S* isomers of triticonazole in soils at the beginning (0 DAT), middle (91 DAT) and the end (366 DAT) of the incubation. Results showed that the ratios did not significantly change. It can be concluded that both *R* and *S* isomers of the racemic parent are comparably degradable.

Table B.8.1.1.1-40 Stereo isomer ratios of triticonazole from selected soil extract samples throughout the study

DAT	Stereo isomer	California soil [triazole-3(5)-^{14}C]	New Jersey soil [phenyl-U-^{14}C]	New Jersey soil [triazole-3(5)-^{14}C]	Wisconsin soil [triazole-3(5)-^{14}C]
0 DAT	*S* isomer	50.24	49.99	50.66	50.34
	R isomer	49.76	50.01	49.34	49.66
91 DAT	*S* isomer	52.10	51.14	50.19	53.18
	R isomer	47.90	48.86	49.81	46.82
366 DAT	*S* isomer	50.36	58.38	52.60	58.39
	R isomer	49.64	41.62	47.40	41.61

Conclusion:

The study demonstrated that triticonazole steadily degraded in soil under aerobic conditions. Results showed that only two metabolites, RPA 404766 (Cis-diol, at t_R of ~ 25.5 min.) and RPA 406341 (Trans-diol, at t_R of ~ 28.5 min), were greater than 5 % AR, with maximum occurrences of 9.11 % AR (California, DAT 274) and 8.19 % AR (California, DAT 366) (in single replicates). Some minor degradation products were also found, each representing less than 5 % AR.

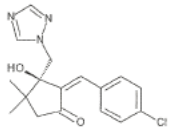
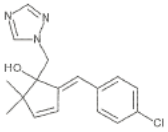
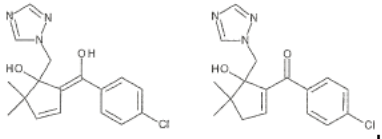
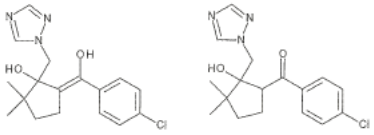
Furthermore, it can be concluded that both the *R* and *S* isomers of the racemic parent are comparably degradable. Unknown metabolites observed in legacy studies were not reproduced.

Comments (RMS AT):

- The study follows OECD guideline 307 and is considered reliable. However, with a nominal dose rate of 580 g ai/ha the study is clearly overdosed considering the intended field application rate of 12.5 g ai/ha only.
- This study, investigating degradation of triticonazole in three US soils, was originally not included in the applicant dossier but was submitted later in the evaluation process in order to support metabolite identification issues. Indeed, the study probably gives the most fundamental insights into the

metabolite profile to be expected from degradation of triticonazole in aerobic soils, particularly as it also covers the full one year incubation period. For some of the more prominent unknown metabolites observed below 5 % AR structures were proposed based on additional mass spectroscopy (see Table below).

Table B.8.1.1.1-41 Tentatively identified metabolites of triticonazole metabolites occurring below 5 % AR in this study.

			
'Ketone metabolite' (MWT 331) (t_R ~ 27 min)	**MWT 315 (t_R ~ 31 min)**	**MWT 331 (t_R ~ 32 min)**	**MWT 333 (t_R ~ 36 min)**

- The RMS AT considers it worthwhile to notice that the common triazole fungicide metabolites 1,2,4-triazole and 1,2,4-triazole-1-ylacetic acid have been identified in this study at low concentrations (below 5 % AR, triazole label only).
- The study also indicates that there is neither transformation from the *Z* (i.e. triticonazole) to the *E* isomer (RPA 406203), nor a significant change in the *R*/*S* isomerization of triticonazole. This leads to the conclusion that the *R*/*S* isomers of triticonazole are comparably degradable.
- The study was kinetically re-assessed by the RMS AT (refer to Kreschnak (2015) in chapter B.8.1.2.1.1, aerobic degradation of the active substance).

Reference:	**Aerobic soil metabolism of ^{14}C-BAS 595 F**
Author(s), year:	Ta, C., Strobush, A., 2015
Report/Doc. number:	2014/7000472
Guideline(s):	EPA 835.4100, OECD 307 (2002), SETAC (1995)
GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Test material

[Phenyl-U-^{14}C]-triticonazole (BAS 595 F)

Reg.No.	4378513
Lot/Batch number	866-1401
Molecular Weight	317.82 g/mol (non-labelled)
Site of radiocarbon labeling:	phenyl-U-^{14}C
Radiochemical purity:	99.5 %
Specific activity of ai:	357000 dpm/µg (5.95 MBq/mg)

[Triazole-3(5)-^{14}C]-triticonazole (BAS 595 F)

Reg.No.	4378513
Lot/Batch number	867-1301
Molecular Weight	317.82 g/mol (non-labelled)
Site of radiocarbon labeling:	triazole-3(5)-^{14}C
Radiochemical purity:	99.3 %
Specific activity of ai:	391200 dpm/µg (6.52 MBq/mg)

Soil

The soil was a loamy sand (Li 10) from Germany, representative of the intended use areas. The soil was collected from the field, 2-mm mesh-sieved and stored in the refrigerator. Soil moisture was adjusted to approximately 50 % MWHC prior to the application of the test solutions and maintained throughout the incubation period. Soil characterization is presented in the table below.

Table B.8.1.1.1-42 Properties of the test soil

Name	Li 10
USDA Textural class	Loamy sand
Sand [%]	80
Silt [%]	12
Clay [%]	8
Cation Exchange Capacity [meq/100 g]	6.2
Max. Water Hold. Capacity [g/100 g dry soil]	22.2
Total Organic Matter [%]	1.4
Total Organic Carbon [%]	0.81[(a)]
pH (water)	6.7
pH ($CaCl_2$)	6.3
Microbial Biomass Carbon at 0 DAT [µg/g dry soil]	281
Microbial Biomass Carbon at 153 DAT [µg/g dry soil]	313
Bulk Density [g/cc]	1.37

(a) Total organic carbon percent = percent organic matter / 1.724
DAT = days after treatment

Test system
Soil aliquots (50 g of dry weight) were placed in 250-mL polypropylene bottles and treated with the test item at a rate of 0.2 mg/kg soil, corresponding to 4-times the proposed maximum field application rate of 12.5 g a.i./ha. This elevated application rate will allow for the identification and quantitation of the parent and metabolites. The treated soil samples were connected to a flow-through test system and incubated in the dark at 20 ± 2°C for 120 days. Moisturized and CO_2-free air was passed over the soil in order to maintain the aerobic conditions. The evolved $^{14}CO_2$ was trapped in NaOH solutions (1 N).

Sampling
Duplicate samples were collected at 0, 3, 8, 14, 30, 59, 91, and 120 DAT. The traps were replaced with fresh aqueous sodium hydroxide solutions (1N) at each sampling time. The soil samples were extracted and processed immediately after sampling.

Analytical procedure
Each soil sample was sequentially extracted with 100 mL of acetonitrile, acetonitrile/methanol (7:3), acetonitrile/water (7:3) and methanol/water (7:3) by shaking for 30 minutes at 300 rpm and then, centrifugation for 15 minutes at 4000 rpm. Each extract was brought to a volume of 100 mL, assayed by LSC. Then all extracts were combined. An aliquot of each pooled organic solvent extracts was concentrated, diluted with acetonitrile and analyzed by LSC and gradient HPLC. Identification of the transformation products was performed by LC-MS/MS and/or retention time matching with standards by HPLC. Furthermore, chiral reverse phase HPLC analysis for the isomeric identification and separation of triticonazole and its metabolites. Reference substances used: R-triticonazole, RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406780, RPA 407922, 1,2,4-triazole, 1,2,4-triazol-1-ylacetic acid.

The extracted soil samples were air-dried, and the amount of non-extractable residues (NER) was determined by oxidative combustion analysis. The extracted soil samples at 59 DAT and 120 DAT were further characterized for fulvic acid, humic acid and humin contents using an extraction procedure with NaOH (0.5 N) and precipitation of humic acids by HCl. The respective solvents were analyzed by LSC. Humins were determined by oxidative combustion analysis.

Findings:

Mass balance
The total recoveries of radioactivity from soils treated with [phenyl-U-^{14}C]-triticonazole and [triazole-3(5)-^{14}C]-triticonazole are presented in the tables below.

Table B.8.1.1.1-43 Material Balance of [phenyl-U-^{14}C]-triticonazole in Li 10 Soil (% AR)

DAT	Extracts				ERR	NER	Volatiles	Material
	1	2	3	4			NaOH	Balance
0 rep 1	83.10	14.00	2.39	0.41	99.91	0.09	NA	100.00
0 rep 2	84.36	14.05	2.34	0.43	101.19	0.10	NA	101.28
0 mean	**83.73**	**14.03**	**2.37**	**0.42**	**100.55**	**0.09**	**NA**	**100.64**
3 rep 1	80.44	14.81	4.00	0.97	100.22	1.70	0.10	102.01
3 rep 2	78.14	14.02	3.94	0.94	97.05	1.80	0.11	98.96
3 mean	**79.29**	**14.42**	**3.97**	**0.95**	**98.63**	**1.75**	**0.11**	**100.49**
8 rep 1	75.37	14.77	3.98	1.01	95.14	2.29	0.21	97.63
8 rep 2	75.73	14.90	4.49	1.21	96.33	2.94	0.23	99.50
8 mean	**75.55**	**14.84**	**4.24**	**1.11**	**95.73**	**2.61**	**0.22**	**98.57**
14 rep 1	74.92	13.93	5.11	1.38	95.34	4.20	0.38	99.92
14 rep 2	74.83	13.85	4.95	1.31	94.93	3.98	0.41	99.32
14 mean	**74.88**	**13.89**	**5.03**	**1.34**	**95.14**	**4.09**	**0.40**	**99.62**
30 rep 1	70.80	13.71	5.45	1.68	91.65	6.69	0.83	99.16
30 rep 2	69.60	14.38	5.40	1.63	91.01	6.41	0.83	98.25
30 mean	**70.20**	**14.04**	**5.42**	**1.66**	**91.33**	**6.55**	**0.83**	**98.71**
59 rep 1	67.28	13.93	5.14	1.72	88.08	8.62	1.59	98.29
59 rep 2	66.99	14.36	5.61	1.91	88.87	10.01	1.30	100.18
59 mean	**67.13**	**14.15**	**5.38**	**1.82**	**88.47**	**9.31**	**1.45**	**99.23**
91 rep 1	66.96	14.58	6.22	2.09	89.85	12.00	2.32	104.17
91 rep 2	67.27	15.08	6.84	2.29	91.48	13.22	1.76	106.47
91 mean	**67.12**	**14.83**	**6.53**	**2.19**	**90.66**	**12.61**	**2.04**	**105.32**
120 rep 1	60.55	13.15	6.13	2.17	82.00	13.24	2.85	98.09
120 rep 2	60.33	12.96	6.41	2.42	82.12	14.00	2.22	98.34
120 mean	**60.44**	**13.06**	**6.27**	**2.29**	**82.06**	**13.62**	**2.53**	**98.21**

Extract 1 = Acetonitrile
Extract 2 = Acetonitrile/methanol (7:3)
Extract 3 = Acetonitrile/water (7:3)
Extract 4 = Methanol/water (7:3)
ERR = Extractable radioactive residues
NER = Non extractable residues (by combustion)
NA = Not applicable (no sample analysed)
There were no volatile traps collected for 0 DAT

Table B.8.1.1.1-44 Material Balance of [triazole-3(5)-^{14}C]-triticonazole in Li 10 Soil (% AR)

DAT	Extracts				ERR	NER	Volatiles	Material
	1	2	3	4			NaOH	Balance
0 rep 1	83.04	13.88	2.48	0.46	99.87	0.13	NA	100.00
0 rep 2	81.15	12.85	2.45	0.44	96.89	0.14	NA	97.02
0 mean	**82.09**	**13.37**	**2.47**	**0.45**	**98.38**	**0.13**	**NA**	**98.51**
3 rep 1	79.80	13.97	4.10	0.99	98.86	1.74	0.07	100.66
3 rep 2	74.96	13.64	4.28	1.04	93.92	1.92	0.06	95.91
3 mean	**77.38**	**13.81**	**4.19**	**1.01**	**96.39**	**1.83**	**0.07**	**98.29**
8 rep 1	71.33	14.76	5.23	1.36	92.67	3.39	0.09	96.15
8 rep 2	71.45	14.87	5.36	1.40	93.08	3.61	0.08	96.77
8 mean	**71.39**	**14.82**	**5.30**	**1.38**	**92.88**	**3.50**	**0.09**	**96.47**
14 rep 1	71.35	13.94	5.62	1.55	92.46	4.63	0.11	97.19
14 rep 2	71.38	14.48	5.47	1.56	92.90	4.73	0.10	97.72
14 mean	**71.37**	**14.21**	**5.55**	**1.56**	**92.68**	**4.68**	**0.10**	**97.46**
30 rep 1	65.76	13.46	5.83	1.75	86.80	7.51	0.15	94.45
30 rep 2	70.90	14.15	5.94	1.84	92.82	7.83	0.14	100.79
30 mean	**68.33**	**13.80**	**5.88**	**1.79**	**89.81**	**7.67**	**0.15**	**97.62**
59 rep 1	61.35	13.71	6.06	1.99	83.11	10.82	0.23	94.16
59 rep 2	63.44	13.92	5.99	1.95	85.29	10.54	0.22	96.05
59 mean	**62.39**	**13.82**	**6.02**	**1.97**	**84.20**	**10.68**	**0.23**	**95.10**
91 rep 1	59.02	13.39	6.76	2.24	81.40	13.49	0.33	95.23
91 rep 2	63.04	13.73	6.40	2.14	85.32	13.88	0.34	99.54
91 mean	**61.03**	**13.56**	**6.58**	**2.19**	**83.36**	**13.69**	**0.33**	**97.38**
120 rep 1	56.69	12.24	6.73	2.46	78.12	14.97	0.42	93.51
120 rep 2	57.59	13.29	6.92	2.40	80.19	15.38	0.40	95.97
120 mean	**57.14**	**12.76**	**6.82**	**2.43**	**79.16**	**15.18**	**0.41**	**94.74**

Extract 1 = Acetonitrile
Extract 2 = Acetonitrile/methanol (7:3)

Extract 3 = Acetonitrile/water (7:3)
Extract 4 = Methanol/water (7:3)
ERR= Extractable radioactive residues
NER = Non extractable residues (by combustion)
NA = Not applicable (no sample analysed)
There were no volatile traps collected for 0 DAT

For the 59 DAT samples treated with [phenyl-U-^{14}C]-triticonazole, NER (9.31 % AR) were further characterized for their fulvic (4.73 %), humic (1.54 % AR), and humin (2.76 % AR) content. At 120 DAT, the NER content increased to 13.62 % AR, from which the fulvic, humic and humin components amounted for 6.35, 2.64 and 3.82 % AR, respectively.

Considering 59 DAT samples treated with [triazole-3(5)-^{14}C]-triticonazole, the radioactivity recovered in the NER (10.68 % AR) as fulvic, humic and humin components was 6.19, 1.39 and 2.82 % AR, respectively. At 120 DAT, the NER content increased to 15.18 % AR, from which the fulvic, humic and humin components amounted for 8.84, 2.17 and 3.84 % AR, respectively.

Characterisation and identification of residues in extracts

The amounts of triticonazole and its metabolites recovered at each time point are presented in the Tables below. Results showed that only two metabolites, RPA 404766 (Cis-diol, at t_R of ~ 25.3 min.) and RPA 406341 (Trans-diol, at t_R of ~ 28.5 min), were greater than 5 % AR, with maximum occurrences of 6.99 and 6.17 % AR. Some minor degradation products were also found, each representing less than 5 % AR.

Table B.8.1.1.1-45 HPLC Quantitation of [phenyl-U-^{14}C]-triticonazole residues in Li 10 soil extract (% AR, numbers shaded in grey exceed 5 % AR)

DAT	t_R (min)							
	25.5-25.6 RPA 404766 (Cis-diol)	25.8	27.1-27.3	28.6-28.7 RPA 406341 (Trans-diol)	28.9-29.0[a]	29.1-29.2	29.5-29.8	30.6-30.8
0 rep 1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0 rep 2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0 mean	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
3 rep 1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 rep 2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3 mean	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
8 rep 1	1.66	0.00	0.00	1.71	1.42	0.00	0.00	0.00
8 rep 2	2.39	0.00	0.00	1.56	1.65	0.00	0.00	0.00
8 mean	**2.03**	**0.00**	**0.00**	**1.64**	**1.53**	**0.00**	**0.00**	**0.00**
14 rep 1	2.49	0.00	0.00	2.20	1.41	0.00	0.00	0.00
14 rep 2	4.06	0.00	0.00	2.91	1.92	0.00	0.00	0.00
14 mean	**3.28**	**0.00**	**0.00**	**2.59**	**1.66**	**0.00**	**0.00**	**0.00**
30 rep 1	4.05	0.00	0.42	2.67	1.90	0.00	0.00	0.00
30 rep 2	5.17	0.00	0.49	3.64	2.49	0.00	0.00	0.00
30 mean	**4.61**	**0.00**	**0.46**	**3.15**	**2.20**	**0.00**	**0.00**	**0.00**
59 rep 1	6.10	0.00	1.57	4.35	3.23	0.00	0.00	0.00
59 rep 2	5.39	0.00	1.33	5.51	3.77	0.00	0.00	0.00
59 mean	**5.74**	**0.00**	**1.45**	**4.93**	**3.50**	**0.00**	**0.00**	**0.00**
91 rep 1	6.98	0.00	1.21	5.56	4.08	0.00	0.00	0.35
91 rep 2	7.00	0.00	1.12	6.18	4.87	0.00	0.55	0.63
91 mean	**6.99**	**0.00**	**1.16**	**5.87**	**4.47**	**0.00**	**0.27**	**0.49**
120 rep 1	5.35	0.00	1.26	5.78	3.78	1.07	0.23	0.57
120 rep 2	5.57	0.44	1.68	5.88	4.83	0.69	0.83	0.00
120 mean	**5.46**	**0.22**	**1.47**	**5.83**	**4.30**	**0.88**	**0.53**	**0.29**

DAT	t_R (min)						
	31.6-32.1	32.1-32.3	32.5-32.7[b]	34.3-34.6 Triticonazole	34.9-35.1	34.9-36.2	36.9-37.2
0 rep 1	0.00	0.00	0.00	99.91	0.00	0.00	0.00
0 rep 2	0.00	0.00	0.00	101.19	0.00	0.00	0.00
0 mean	**0.00**	**0.00**	**0.00**	**100.55**	**0.00**	**0.00**	**0.00**
3 rep 1	0.00	0.00	0.00	97.29	1.78	1.78	1.14
3 rep 2	0.00	0.00	0.00	95.06	1.99	1.99	0.00

3 mean	**0.00**	**0.00**	**0.00**	**96.18**	**1.89**	**1.89**	**0.57**
8 rep 1	0.00	0.00	0.00	90.34	0.00	0.00	0.00
8 rep 2	0.00	0.00	0.00	90.73	0.00	0.00	0.00
8 mean	**0.00**	**0.00**	**0.00**	**90.54**	**0.00**	**0.00**	**0.00**
14 rep 1	0.00	0.00	0.00	89.24	0.00	0.00	0.00
14 rep 2	0.00	0.00	0.00	86.04	0.00	0.00	0.00
14 mean	**0.00**	**0.00**	**0.00**	**87.64**	**0.00**	**0.00**	**0.00**
30 rep 1	0.00	0.00	1.83	79.83	0.00	0.62	0.33
30 rep 2	0.64	0.00	2.07	76.51	0.00	0.00	0.00
30 mean	**0.32**	**0.00**	**1.95**	**78.17**	**0.00**	**0.31**	**0.16**
59 rep 1	0.92	0.00	1.82	69.46	0.00	0.63	0.00
59 rep 2	1.44	0.00	2.42	68.16	0.00	0.84	0.00
59 mean	**1.18**	**0.00**	**2.12**	**68.81**	**0.00**	**0.74**	**0.00**
91 rep 1	1.50	1.07	3.25	64.45	0.00	1.40	0.00
91 rep 2	1.12	0.70	3.70	64.39	0.00	1.21	0.00
91 mean	**1.31**	**0.89**	**3.48**	**64.42**	**0.00**	**1.30**	**0.00**
120 rep 1	1.87[(c)]	0.00	2.48	58.28	0.00	1.31	0.00
120 rep 2	1.21[(c)]	1.22	3.53	54.98	0.00	1.28	0.00
120 mean	**1.54**	**0.61**	**3.01**	**56.63**	**0.00**	**1.30**	**0.00**

(a) Tentatively identified as a ketone metabolite with a ketone (O=) moiety in the central part of the molecule (mol mass 331 g/mol)
(b) Tentatively identified as a metabolite oxidized (O=) at the methylene bridge between the chlorophenyl and the substituted 5-membered ring (mol mass 331 g/mol)
(c) Two extremely close peaks were summed

Table B.8.1.1.1-46 HPLC Quantitation of [triazole-3(5)-^{14}C]-triticonazole residues in Li 10 soil extract (% AR, numbers shaded in grey exceed 5 % AR)

	t_R (min)							
DAT	**5.3-5.7**	**25.3-25.6 RPA 404766 (Cis-diol)**	**27.1-27.4**	**28.5-28.7 RPA 406341 (Trans-diol)**	**28.9-29.0[(a)]**	**29.1-29.2**	**29.5-29.8**	**30.6-30.8**
0 rep 1	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0 rep 2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
0 mean	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**	**0.00**
3 rep 1	0.00	0.86	0.00	0.00	0.00	2.04	0.00	0.00
3 rep 2	0.00	1.47	0.00	2.15	0.00	0.00	0.00	0.00
3 mean	**0.00**	**1.16**	**0.00**	**1.08**	**0.00**	**1.02**	**0.00**	**0.00**
8 rep 1	0.00	2.68	0.00	2.11	1.06	0.00	0.00	0.00
8 rep 2	0.00	2.34	0.00	3.36	0.00	0.00	0.00	0.00
8 mean	**0.00**	**2.51**	**0.00**	**2.74**	**0.53**	**0.00**	**0.00**	**0.00**
14 rep 1	0.00	2.90	0.00	2.45	1.51	0.00	0.00	0.00
14 rep 2	0.00	3.18	0.00	2.74	1.54	0.00	0.00	0.00
14 mean	**0.00**	**3.04**	**0.00**	**2.60**	**1.52**	**0.00**	**0.00**	**0.00**
30 rep 1	0.86	4.96	0.82	3.65	3.44	0.00	0.00	0.00
30 rep 2	0.86	5.50	0.66	3.87	2.16	0.00	0.00	0.00
30 mean	**0.86**	**5.23**	**0.74**	**3.76**	**2.80**	**0.00**	**0.00**	**0.00**
59 rep 1	1.48[(c)]	5.73	1.07	4.67	3.57	0.00	0.00	0.00
59 rep 2	1.10[(c)]	5.70	0.60	5.18	2.81	0.00	0.00	0.00
59 mean	**1.29**	**5.71**	**0.83**	**4.92**	**3.19**	**0.00**	**0.00**	**0.00**
91 rep 1	1.83[(c)]	5.71	0.63	5.19	4.38	0.00	0.69	0.00
91 rep 2	1.16	6.25	1.97	5.67	4.49	0.00	0.00	0.00
91 mean	**1.50**	**5.98**	**1.30**	**5.43**	**4.43**	**0.00**	**0.35**	**0.00**
120 rep 1	1.58[(c)]	6.16	1.80	5.86	4.30	0.00	0.36	0.84
120 rep 2	1.39[(c)]	6.33	1.27	6.48	3.70	0.00	0.00	0.90
120 mean	**1.48**	**6.25**	**1.54**	**6.17**	**4.00**	**0.00**	**0.18**	**0.87**

	t_R (min)						
DAT	**31.6-32.1**	**32.1-32.3**	**32.5-32.8[(b)]**	**34.3-34.6 Triticonazole**	**34.9-36.2**	**36.8-37.2**	**Sum Others**
0 rep 1	0.00	0.00	0.00	98.03	0.00	1.83	0.00
0 rep 2	0.00	0.00	0.00	95.55	0.00	1.33	0.00
0 mean	**0.00**	**0.00**	**0.00**	**96.80**	**0.00**	**1.58**	**0.00**
3 rep 1	0.00	0.00	0.00	92.68	0.00	3.28	0.00
3 rep 2	0.00	0.00	0.00	89.09	0.00	1.21	0.00

3 mean	**0.00**	**0.00**	**0.00**	**90.89**	**0.00**	**2.25**	**0.00**
8 rep 1	0.00	0.00	1.12	84.50	0.00	1.20	0.00
8 rep 2	0.00	0.00	0.00	85.71	0.00	1.68	0.00
8 mean	**0.00**	**0.00**	**0.56**	**85.10**	**0.00**	**1.44**	**0.00**
14 rep 1	0.00	0.00	1.28	82.70	0.87	0.75	0.00
14 rep 2	0.00	0.00	1.77	82.12	0.72	0.83	0.00
14 mean	**0.00**	**0.00**	**1.53**	**82.41**	**0.79**	**0.79**	**0.00**
30 rep 1	0.62	0.00	1.45	68.50	1.65	0.86	0.00
30 rep 2	0.61	0.00	1.91	74.41	0.96	1.86	0.00
30 mean	**0.62**	**0.00**	**1.68**	**71.46**	**1.30**	**1.36**	**0.00**
59 rep 1	1.26	0.00	2.57	61.50	0.58	0.67	0.00
59 rep 2	0.87	1.09	3.12	63.06	1.15	0.61	0.00
59 mean	**1.07**	**0.55**	**2.84**	**62.28**	**0.87**	**0.64**	**0.00**
91 rep 1	1.95[(d)]	0.00	3.54	55.55	0.75	0.51	0.64
91 rep 2	1.59	0.00	3.27	58.11	1.01	1.12	0.68
91 mean	**1.77**	**0.00**	**3.40**	**56.83**	**0.88**	**0.82**	**0.66**
120 rep 1	1.52	1.00	3.10	48.50	1.16	0.58	1.36[(a)]
120 rep 2	1.10	1.25	2.51	51.87	1.14	0.74	1.54[(b)]
120 mean	**1.31**	**1.13**	**2.81**	**50.19**	**1.15**	**0.66**	**1.45**

(a) Tentatively identified as a ketone metabolite with a ketone (O=) moiety in the central part of the molecule (mol mass 331 g/mol)
(b) Tentatively identified as a metabolite oxidized (O=) at the methylene bridge between the chlorophenyl and the substituted 5-membered ring (mol mass 331 g/mol)
(c) Sum of three peaks
(d) Two extremely close peaks were summed

Isomerization

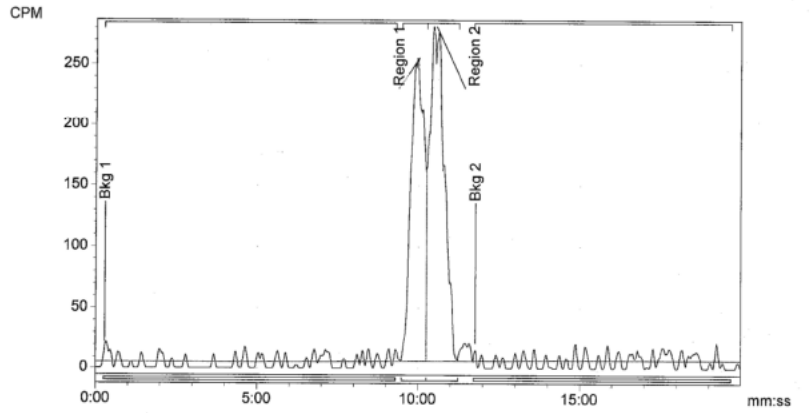
Results of the non-chiral HPLC method showed that the E isomer was the major component of triticonazole, while the levels of the Z isomer (RPA 406203) were not detected in all samples during the incubation, suggesting that there were no significant conversions of the E to the Z isomers.

Additionally, chiral-HPLC analysis of samples taken at the beginning (0 DAT), middle (59 DAT) and the end (120 DAT) of the incubation demonstrated that no significant metabolic preference for the *R* versus *S* stereo isomer occurred during the soil metabolism of the parent compound triticonazole.

Table B.8.1.1.1-47 Isomer ratios of triticonazole from selected soil extract samples throughout the study

DAT	Label	Total % *R* / *S* isomer	*R* / *S* ratio
0	Phenyl	49.62 / 49.59	1.00
	Triazole	49.92 / 48.11	1.04
59	Phenyl	49.70 / 48.82	1.02
	Triazole	48.38 / 46.44	1.04
120	Phenyl	49.80 / 44.46	1.12
	Triazole	47.87 / 46.70	1.03

It can be concluded that both the *R* and *S* stereo isomers of the racemic parent are comparably degradable. The separation of isomers of individual metabolites proved to be extremely difficult due to their low levels and other impurities co-eluted. Only metabolite RPA 406341 (Trans-diol) exhibits an acceptable separation, which demonstrated a similar ratio with the test substance (see figure below). This result suggests that no significant metabolic preference for the *R* versus *S* isomer occurred during the formation of metabolites from triticonazole.



Regions: ^{14}C Detector: ß-RAM

Number	Name	Retention (mm:ss)	Start (mm:ss)	End (mm:ss)	Area (CPM)	%ROI (%)	%Total (%)	Relative Retention
1	Bkg 1	0:17	0:15	9:18				
2	Region 1	10:01	9:29	10:15	6799	43.65	43.01	
3	Region 2	10:33	10:15	11:14	8777	56.35	55.52	
4	Bkg 2	11:46	11:43	19:41				
	2 Peaks				15575	100.00	98.52	

Figure B.8.1.1.1-1: Chiral HPLC radio-chromatogram of isolated metabolite RPA 406341 (Trans-diol)

Transformation of parent compound

In soil and under aerobic conditions, the major degradation pathway of triticonazole is the hydroxylation to produce either hydroxylated derivatives or logical products from the hydroxylated derivatives of the parent compound. Ultimately, triticonazole and its degradation products are mineralized to CO_2 by soil microorganisms.

Additionally, structures were proposed for the degradation products that had the highest maximum occurrences below 5 % AR. As observed amount of these compounds were decreasing from the respective maxima towards the end of the study, further assessment is not necessary. Due to missing mass spectrometrical data in old studies it was not possible to assign these structures to one or the other non-identified peaks between 5 % and 10 % maximum occurrences in old studies.

Conclusion:

The study demonstrated that triticonazole steadily degraded in soil under aerobic conditions. There were only two metabolites, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol), greater than 5 % AR, with maximum occurrences of 6.99 % AR (DAT 91) and 6.17 % AR (DAT 120) in Li 10 soil, respectively. Some minor degradation products were also found, each representing less than 5 % AR. Furthermore, it can be concluded that both the *R* and *S* isomers of the racemic parent are comparably degradable. Unknown metabolites observed in legacy studies were not reproduced.

Comments (RMS AT):

- The study follows OECD guideline 307 with some limited information:
  - No information on the history of the sampled fields is given in the study report
  - No details are given on the storage prior the incubation except that the soil was stored in the refrigerator

  On overall the study is considered reliable.

- One major purpose of this study was to further elucidate metabolites observed in legacy studies between 5 and 10 % AR (see studies above). However, already finished by 120 days, the study obviously failed to generate sufficient amounts of metabolites observed at late stage in the one-year legacy studies. Notice that by study termination roughly 53 % of triticonazole were still present in soil with several of the metabolites still increasing.

- For two of the more prominent unknown metabolites observed below 5 % AR but showing increasing tendency towards study end (i.e. t_R 28.9 - 29.0 min and t_R 32.5 - 32.8 min) structures were proposed based on additional mass spectroscopy: the first being most probably a ketone metabolite with a ketone (O=) moiety in the central part of the molecule (mol mass 331 g/mol), the second one potentially oxidized (O=) at the methylene bridge between the chlorophenyl and the substituted 5-membered ring (mol mass 331 g/mol) (also refer to Ta & Strobush, 2012).

- Another major purpose of this study was to investigate the isomeric behaviour of triticonazole and it metabolites in soil. Except for the parent and RPA 406341 (Trans-diol) separation of isomers was not possible due to the low levels of the metabolites and other impurities co-eluted. However, on basis of the results obtained for RPA 406341 (Trans-diol) the notifier concluded that no significant metabolic preference for the *R* versus *S* isomer occurred during the formation of all other metabolites from triticonazole. The RMS AT notices that non-preferential formation and degradation of metabolites could indeed only be demonstrated for RPA 406341 (Trans-diol). However, on basis of similarities in the molecule structures the RMS AT considers at least RPA 404766 (Cis-diol) showing a similar non-preferential formation and degradation in soil.

- Degradation trigger endpoints were evaluated directly in the study and are summarized in the rate section (B.8.1.2, rate of degradation). Degradation modelling endpoints were re-assessed by Donaldson (2015).

Reference:	**Statement - Exposure assessment for "Met 6" and "Met 7", potential degradation products of BAS 595F triticonazole**
Author(s), year:	Szegedi, K., 2018
Report/Doc. Number:	2018/1091281
Guideline(s):	None
GLP:	Not applicable (statement)
Validity:	Partly (refer to comment section)
Status:	**New submission**

The molar weight of 'Met 6 (MWT 333)' is known: 333 g. Considering this information and that the main metabolism pathway of triticonazole is the formation of hydroxy metabolites it is reasonable to assume that the compound is a hydroxylated derivative of the parent compound triticonazole. In line with the molar weight of other hydroxy-metabolites, the molar weight of 333.8 g/mol belongs to the non-ionized form.

Although the exact position of the hydroxy group is not known, the structure of already identified hydroxy-metabolites can be excluded. With that the number of possible structures can be reduced to the four indicated in the figure below. Due to rotational symmetry structure a) is identical with RPA 407922 and structure b) is identical with RPA 404886. Due to the same reasons structure c) is identical with structure d). This reduces the number of structures to one.

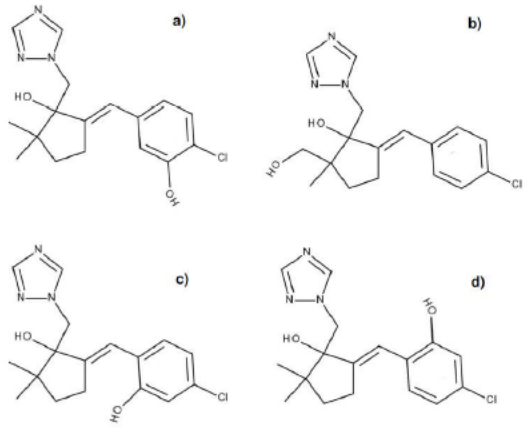


Figure B.8.1.1.1-2: Possible structures of 'Met 6 (MWT 333)'. After exclusion of known structures due to symmetry reasons structure c) (identical with structure d)) remains the only possibility.

The MWT of 315 g of 'Met 7 (MWT 315)' suggests the structure of the parent molecule with an additional unsaturation. According to the results of Ta & Strobush (2012), the only possible position for unsaturation would be only in the cyclopentane ring indicated in the figure below. With that 'Met 7 (MWT 315)' would be the same as the major component of the '404401-NJT-31min' sample in the analysis of Ta & Strobush (2012), with an MWT of 315 g. The relative position of 'Met 7 (MWT 315)' in the HPLC chromatogram in Ayliffe & Austin (1993) is qualitatively similar to the position of the major component of the '404401-NJT-31min' sample in the HPLC chromatogram in the Ta & Strobush (2012): the order of the peaks is similar between the two studies, although not all peaks appear in both studies. In line with the structural formula and the rounding concept of the other metabolites and the parent compound, the molar weight of 315.8 g/mol is proposed for the non-ionized form.

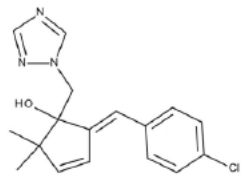


Figure B.8.1.1.1-3: Proposed structure of 'Met 7 (MWT 315)'

Thus, it can be concluded that 'Met 6 (MWT 333)' is triticonazole hydroxylated at the second position of the chlorophenyl ring and 'Met 7 (MWT 315)' is the unsaturated form of triticonazole at the cyclopentane ring.

Comments (RMS AT):

- The RMS AT agrees with the study author, that 'Met 6 (MWT 333)' most probably comprises another mono-hydroxylated derivative of triticonazole. However, as demonstrated in Ta & Strobush (2012), there are other mono-hydroxylated structures of triticonazole possible (and already identified) beside those ones given by the study author above, all having the same mol mass (refer to Ta & Strobush, 2012). Based on findings in Ta & Strobush (2012) other hydroxylated structures (e.g. hydroxylated at the central bond) are indeed considered more reliable, particularly with respect to the HPLC retention times. Notice that triticonazole derivatives hydroxylated at the chlorophenyl ring (e.g. RPA 407922) have never been unambiguously identified in any of the soil degradation studies. On overall, the RMS AT considers the exact structure of 'Met 6 (MWT 333)' still uncertain and asks the applicant for further supporting information.

- In contrast to 'Met 6 (MWT 333)' the RMS AT largely agrees with the proposed structure for 'Met 7 (MWT 315)' as this substance was also identified in Ta & Strobush (2012) with a comparable position in the HPLC chromatogram. Nevertheless, the applicant is asked to further support this tentative identification by chromatographic studies with authentic reference material.

B.8.1.1.2. Anaerobic degradation

Studies submitted for first Annex I inclusion:

- **Goodyear (1994)**, investigating triticonazole in one soil under anaerobic conditions

No new studies were submitted.

Reference:	**(^{14}C)-RPA 400727: Anaerobic soil metabolism**
Author(s), year:	Goodyear, A., 1994 (+ Amendment 1998)
Report/Doc. Number:	R012982, 68/136, 200491 + Addendum R012983
Guideline(s):	US-EPA, N, 162-2
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The degradation of [phenyl-U-^{14}C]-triticonazole (called RPA 400727 in the report) in a Manningtree sandy loam soil incubated under anaerobic conditions has been investigated over a 100 day period. The active substance was applied at a rate equivalent to 360 g ai/ha. Soil moistures were adjusted to 75 % of their 33 kPa (0.33 Bar) water holding capacity and samples were maintained in the dark at 25 ± 1 °C. The soil samples were incubated for a 30 days period after which the soils were flooded with deionised water to a depth of 3 cm and an incubation chamber purged with nitrogen. Anaerobic conditions were established two days after flooding.

Duplicate units were removed for analysis following application and immediately prior to flooding. Samples were also removed at intervals of 8, 15, 29, 59 and 100 days following establishment of anaerobic conditions.

Soil samples were Soxhlet extracted with acetonitrile/water (80:20, v/v) and the resulting extracts were analysed by gradient HPLC. Reference substances used: RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406780, RPA 404886, RPA 405826.

At each anaerobic sampling interval the redox potential of the surface water was measured.

Table B.8.1.1.2-48 Soil Characteristics

soil	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H (KCl)	CEC (meq/100g)	Biomass (start) µg C/g soil	Biomass (end) µg C/g soil
Manningtree sandy loam	69	23	8	0.5	7.6	1.9	163	151

Findings:

Overall mean recoveries of the applied radioactivity ranged from 98.5 % at day 0 to 93.2 % after 100 days incubation under anaerobic conditions. The individual recoveries for each incubate sampled were > 92 % AR, with the exception of a single replicate sampled after 29 days incubation under anaerobic conditions, where a recovery of 85.6 % was obtained.

There was a one time stepped decrease in the amount of parent extractable following the onset of anaerobic conditions with a concomitant increase in the amount of unextractable soil bound residue. Following this change there was very little discernible degradation of parent under anaerobic conditions.

The unextractable soil bound residue reached 17.0 % of applied radioactivity and trapped ^{14}C carbon dioxide amounted to 0.8 % of applied radioactivity, 100 days after application. No other volatiles were detected.

Table B.8.1.1.2-49 Recovery of applied radioactivity (% AR, HPLC, mean of duplicate samples)

DAT	Water	Soil extract	NER	CO_2	Total	Triticonazole Soil extracts	Triticonazole Surface water
0 - aerobic phase	not applicable	98.5	not detected	n.a.	98.5	97.4	n.a.
30 - pre-flooding	not applicable	96.2	2.1	1.6	99.9	93.1	n.a.
8 - anaerobic	13.3	59.5	23.1	0.2	96.1	57.4	11.1
15	13.1	60.9	20.8	0.1	94.9	59.0	11.2
29	10.6	53.0	25.2	0.1	88.9	51.1	9.3

59	8.6	72.9	12.5	0.1	94.1	72.2	7.0
100	8.2	67.2	17.0	0.8	93.2	63.8	6.6

Metabolites RPA 406341 (Trans-diol), RPA 404766 (Cis-diol) and RPA 405826 were found in amounts ≤ 1.8 % AR on individual basis. Unknown metabolite fractions were below 1.5 % AR in total. Volatile material except CO_2 was not detected.

The data obtained from soil extracts and surface water showed that very little degradation of the parent occurred and that the percentage of the active ingredient remaining was influenced by the extraction efficiency from the soil. The radioactivity extracted from the soil at each sampling occasion showed a similar profile of the parent and its metabolites, and a greater extraction efficiency was obtained from the later intervals than those earlier in the incubation period. As a result a valid half-life could not be calculated.

The degradation of the parent substance was slow during the aerobic phase of the experiment with only 2 % AR present in each of the soil bound residue and volatile product fractions. Following establishment of anaerobic conditions and subsequent incubation for 8 days the distribution of radioactivity showed a much higher level of soil bound residue and release into the surface water (ca. 23 % and 13 % AR respectively). This distribution remained approximately constant up to 29 days anaerobic conditions, thereafter decreasing gradually to ca 17 % and 8 % AR respectively.

Conclusions:

Triticonazole did not degrade significantly under anaerobic conditions. The lack of degradation prevented a formal *DT50* value from being derived from the study.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some minor deviations:
  - With an application rate of 360 g ai/ha the study is clearly overdosed considered the intended application rate of 12.5 g/ha
  - Only phenyl labelled triticonazole was investigated. However, in view of the results obtained with the phenyl label no new results are expected applying the triazole label.
  - No information is given ion the field history.

  On overall, the study is still considered reliable.

B.8.1.1.3. Soil photolysis

Studies submitted for first Annex I inclusion:

- **Ayliffe & Jones (1998),** investigating triticonazole in one soil under conditions of soil photolysis

No new studies were submitted.

Reference:	**Fungicides: Triticonazole: Soil Photolysis**
Author(s), year:	Ayliffe, J. M., Jones, M. K., 1995 (amended in 1998)
Report/Doc. Number:	C017700, P95/065, 201021
Guideline(s):	US-EPA N, 161-3 (1982)
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

A study to investigate the photolytic degradation of [phenyl-U-^{14}C]-triticonazole following surface application to a sandy loam soil has been performed. Soil samples at 75 % of the 1/3 bar moisture holding capacity were surface treated and aerobically incubated at 20 ± 1 °C for 30 days. The dosing was equivalent to 375 g ai/ha for the non-irradiated soils and 397 g ai/ha for the irradiated soils. Irradiated samples were exposed for 14.9 h each day to an artificial light source equivalent to natural summer sunlight at 50° N (xenon lamp, Heraeus Suntest).

Analytics: gradient HPLC for metabolite profiling and metabolite confirmation, TLC. Reference substances used: RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406203 (Z-isomer), RPA 406780, RPA 404886, RPA 407922.

Table B.8.1.1.3-50 Soil Characteristics

soil	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/100g)	Biomass (µg C/g soil)
Manningtree, sandy loam	58.1	31.4	9.5	2.2	5.1	6.7	347[(a)], 182[(b)]

(a) Non-irradiated soil samples
(b) Irradiated soil samples (determined after further storage time)

Findings:

Table B.8.1.1.3-51 Distribution of radioactivity in irradiated soil (% of AR, HPLC, mean of replicates, numbers shaded in grey exceed 5 % AR)

DAT	Extract	Bound residues	CO_2	Total	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)	RPA 406203 (Z-isomer)
0	95.4	0.0	na	95.5	93.3	nd	nd	nd
3	95.0	0.5	0.1	95.6	91.3	0.3	0.7	1.3
7	95.6	1.3	0.2	97.0	86.9	1.1	2.2	3.6
14	91.8	1.7	0.3	93.8	79.7	1.2	2.6	6.4
21	90.9	2.7	0.8	94.3	75.2	3.3	2.8	7.6
30	88.1	4.1	1.3	93.5	68.2	3.1	3.5	11.0

Table B.8.1.1.3-52 Distribution of radioactivity in non-irradiated soil (% of AR, HPLC, mean of replicates, numbers shaded in grey exceed 5 % AR)

DAT	Extract	Bound residues	CO_2	Total	Triticonazole	RPA 404766 (Cis-diol)	RPA 406341 (Trans-diol)
0	97.4	0.0	na	97.4	94.7	nd	nd
3	97.4	0.4	0.1	97.9	93.4	0.3	0.8
7	93.7	0.5	0.1	94.4	87.2	0.6	2.0
14	97.6	1.0	0.2	98.9	87.7	2.9	2.9
21	95.0	1.4	0.4	96.8	85.2	2.3	3.8
30	95.3	1.7	0.5	97.4	86.3	2.1	4.0

Small amounts of unknown compounds were found up to max. 2.2 % AR (irradiated samples) and up to 3.8 % AR (non-irradiated samples). Amounts of other volatiles than CO_2 were negligible (0.01 % AR). In the irradiated soil samples RPA 406203 (Z-isomer) was found as a major metabolite which amounted up to 11.0 % AR at the end of the study (30 days). Two minor metabolites, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol), were found in both the irradiated and non-irradiated samples with maximum amounts of about 4 and 3 %, respectively. The mean unextracted residue was fractionally higher in the irradiated than in the non-irradiated soil and increased gradually with time. Also CO_2 production was slightly higher in irradiated samples - despite the relative low biomass for the irradiated soil.

Degradation of the parent compound was faster in the irradiated soil samples. Half-lives were in excess of 30 days.

Conclusions:

Triticonazole degraded faster in irradiated soil than in the dark samples. Half-lives were in excess of 30 days. Under light conditions the main pathway of decline is by the trans-cis isomerisation of triticonazole to RPA 406203 (Z-isomer). There is no indication that this metabolite further degrades in the soil as the levels of the minor metabolites were similar for both irradiated and non-irradiated soils.

As the supported use of triticonazole is seed treatment only photolytic degradation on soil is not relevant.

Comments (RMS AT):

- The study broadly follows the draft OECD guideline on phototransformation of chemicals on soil surfaces (2002) with some deviations:
    - With an application rate of 375 g ai/ha the study is clearly overdosed considered the intended application rate of 12.5 g/ha
    - Only phenyl labelled triticonazole was investigated. However, in view of the results obtained with the phenyl label no new results are expected applying the triazole label.

  On overall, the study is still considered reliable.

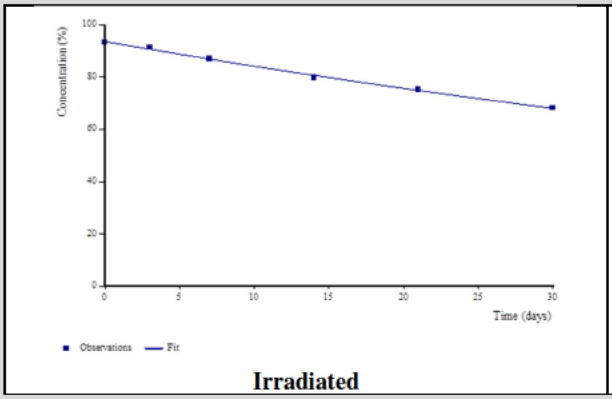
- As observed in aquatic photolysis studies, transformation of triticonazole to RPA 406203 (Z-isomer) under conditions of irradiation is considered to be reversible approaching equilibrium with time. In this respect it is obvious that amounts of RPA 406203 (Z-isomer) further increase if the study would have been conducted for longer time. However, in view of the intended use of triticonazole as a seed treatment the impact of soil photolysis is considered negligible at all.

- Dissipation of triticonazole was re-assessed by the RMS AT in line with pertinent guidance applying CAKE 3.3 (see below).

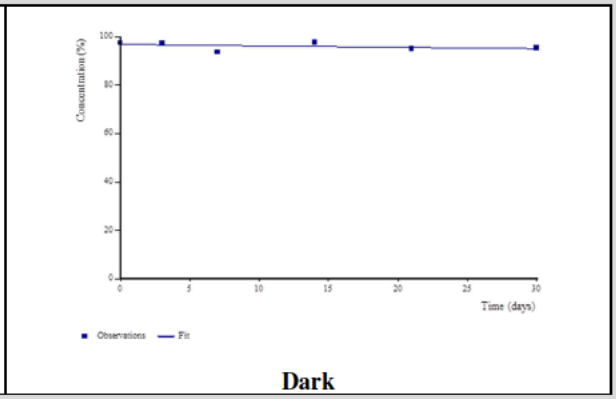
Table B.8.1.1.3-53 Dissipation of triticonazole under conditions of soil photolysis - RMS AT assessment

Test system	Kinetic model	*DT50* (d)	*DT90* (d)	χ^2 err. (%)
Irradiated	SFO	65.3	217	0.5
Dark	SFO	> 1000	> 1000	1.1
Net	SFO	65.3	217	-

Table B.8.1.1.3-54 Dissipation of triticonazole under conditions of soil photolysis (fits) - RMS AT assessment



Irradiated



Dark

B.8.1.1.4. Summary on route of degradation in soil (compiled by the RMS AT)

Legacy studies on the **aerobic degradation** of triticonazole in soil conducted at 22, 25 and 10 °C for one year and two recent degradation study conducted at 20 °C for 120 days and for one year, respectively, showed that the main degradation pathway of triticonazole is hydroxylation releasing the two major mono-hydroxylated transformation products **RPA 406341 (Trans-diol)** (max. 20.2 % AR at 22 °C) and **RPA 404766 (Cis-diol)** (max. 13.9 % AR at 10 °C). These two metabolites were consistently observed in all soils.

Beside these two major degradation products several unknown metabolites, amongst them most probably other mono- and di-hydroxylated as well as oxidized (keto) derivatives of triticonazole, with indicative mol weights (MWT) of 315, 331, 333, 347 and 349 have been detected partly above 5 % AR (and partly > 10 % AR) but could not be unambiguously identified. Notice that in case of the legacy studies (conducted around 1993 - 1996) only metabolites above 10 % AR had to be investigated further. The RMS AT notes that all these unidentified metabolites were observed at late stage of the one-year incubation experiments (above 5 % AR at 140 DAT earliest), with maximum amounts at study termination in several cases. It is also noted that highest amounts of unknown and unidentified metabolite fraction were generally observed in the earliest studies (Ayliffe & Austin, 1993, Ayliffe & McMillan-Staff, 1994, and Ayliffe & Godward, 1993) when HPLC techniques were less advanced in comparison to studies conducted later. In this respect, it cannot be excluded that some of these metabolite fractions actually comprise more than one substance. A summary on unknown metabolite fractions observed above 5 % AR is given in the table below.

Table B.8.1.1.4-55 Unknown metabolite fractions observed above 5 % AR in aerobic soil degradation experiments with triticonazole

Study temp. (°C)	Metabolite coding	Proposed MWT	Soil	Max. occ. (% AR)	Day of max. occ. (DAT)	1st day > 5 % AR	> 5 % AR at two consecutive sampling points	Ref.
22	'Met 5'[(a)]	349	UK clay loam	6.8	363[(b)]	168	Yes	Ayliffe & Austin (1993)
	'Met 6'	333	UK clay loam	12.8	266	140	Yes	
	'Met 7'	315	UK sandy loam	6.5	266	224	Yes	
	'Met 7'	333	UK loamy sand	6.2	363[(b)]	363[(b)]	No	Ayliffe & Godward (1993)
	'Met 8'	315	UK loamy sand	5.3	245	245	No	
10	'Met 6'[(a)]	349	UK sandy loam	10.5	363[(b)]	363[(b)]	No	Ayliffe & Godward (1993)
			UK clay loam	11.1	363[(b)]	363[(b)]	No	
			UK loamy sand	6.5	363[(b)]	363[(b)]	No	
	'Met 7'	333	UK sandy loam	6.9	245	245	No	
			UK clay loam	5.3	306	168	No	
	'Met 8'	315	UK clay loam	6.1	363[(b)]	363[(b)]	No	
25	Unknown	Unknown	Manningtree sandy loam, standard	5.9	365[(b)]	Un-known[(c)]	No[(d)]	Simmonds et al. (1996)
	Unknown	Unknown	Manningtree sandy loam, red. rate	5.2	365[(b)]	Un-known[(c)]	No[(d)]	

(a) Considered to actually comprise two substances with a MWT of 333 and 349 at more or less equimolar amounts (refer to text below)
(b) Last day of incubation
(c) The study report does not contain tabulated results on individual metabolite fractions
(d) Confirmed by the RMS AT on basis of GLP raw data

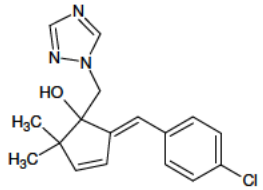
One of these unknown metabolite fractions, called **'Met 6 (MWT 333)'** in Ayliffe & Austin (1993), occurring at max. 12.8 % AR in one soil, was originally claimed being identified as RPA 407922 in Ayliffe & McMillan-Staff (1994). This identification was also accepted for first Annex I approval triggering a number of additional studies with RPA 407922 (amongst them metabolite dosed degradation and sorption studies as well as ecotox studies). However, on basis of information provided by Simmonds & Lowden (2002), applying the same isocratic HPLC methods as used in Ayliffe & Austin (1993) and Ayliffe & McMillan-Staff (1994), and considering further information given in Doble et al. (1996) and Simmonds et al. (1996), the RMS AT now challenges 'Met 6 (MWT 333)' being RPA 407922 (for more information please refer to Ayliffe & McMillan-Staff, 1994, and Simmonds & Lowden, 2002). For that reasons, the applicant was requested by the RMS AT to further underpin their peak assignment. The applicant performed HPLC analysis of the reference substances

RPA 407922 and RPA 406341 (Trans-diol) with the same type of columns and same isocratic and gradient conditions as in Ayliffe & Austin (1993) and Ayliffe & McMillan-Staff (1994). The retention times obtained by the authors could not be reproduced. A complete separation of the two peaks could not be shown unambiguously. Finally, the applicant agreed with the conclusion of the RMS AT that 'Met 6 (MWT 333)' in the chromatogram does not belong to metabolite RPA 407922 but to an unidentified structure. The RMS AT notes that the supporting additional HPLC runs conducted by the applicant have not been submitted to the RMS AT.

On basis of the proposed MWT in Ayliffe & Austin (1993) the applicant concluded that 'Met 6 (MWT 333)' probably represents another mono-hydroxylated triticonazole derivative. Excluding already known mono-hydroxylated derivatives, the applicant came to the conclusion that there is only one possible structure remaining (refer to Szegedi, 2018). The RMS AT agrees with the applicant, that 'Met 6 (MWT 333)' probably comprises another mono-hydroxylated derivative of triticonazole. However, as demonstrated in Ta & Strobush (2012), there are other mono-hydroxylated structures of triticonazole possible (and already identified) beside those ones considered by Szegedi (2018), all having the same mol mass of 333.8 g/mol (refer to Ta & Strobush, 2012). Based on findings in Ta & Strobush (2012) other structures are indeed considered more reliable. Notice that triticonazole derivatives hydroxylated at the chlorophenyl ring (e.g. RPA 407922) have never been unambiguously identified in any of the soil degradation studies. On overall, the RMS AT considers the exact structure of 'Met 6 (MWT 333)' still uncertain.

The applicant further concluded that **'Met 7 (MWT 315)'**, observed above 5 % AR in Ayliffe & Austin (1993) as well, probably represents a triticonazole derivative with an additional unsaturation in the cyclopentane ring (Figure B.8.1.1.4-3). The same structure was observed and tentatively identified in a recent study (Ta & Strobush, 2012) with a similar position in the HPLC chromatogram (below 5 % AR). In general, the RMS AT considers the structure proposal for 'Met 7 (MWT 315)', albeit not fully verified by authentic reference material, scientifically valid and reliable. Nevertheless, the applicant is asked to further support this identification by chromatographic studies with authentic reference material.

Figure B.8.1.1.4-1: Proposed structures of the metabolite fraction 'Met 7 (MWT (315)' observed > 5 % AR at two consecutive sampling points in Ayliffe & Austin (1993)



(*R/S*-isomers)

'Met 7 (MWT 315)'

On basis of additional work done by Simmonds & Lowden (2002) with one additional soil, metabolite fraction 'Met 5 (MWT 349)' observed in Ayliffe & Austin (1993) above 5 % at two consecutive sampling points appears to actually comprise two unidentified compounds at more or less equimolar amounts, one with a mol mass of 333 g/mol and one with a mol mass of 349 g/mol, probably unknown mono- and di-hydroxylated derivatives of triticonazole.

The applicant claims that all unknown degradation products were observed in legacy studies beyond 120 DAT, which would be the study duration according to the respective OECD guidance. Accordingly, considering current guidance documents, no exposure or risk assessment would be necessary for the previously not identified and not reproducible degradation product. The RMS AT notes that OECD guideline 307 indeed recommends continuing the incubation for longer periods (e.g. 6 or 12 months) *where necessary* to characterise the decline of the test substance and the formation and decline of major transformation products. In view of the limited degradation of triticonazole in aerobic laboratory soil incubation experiments accompanied by late formation of degradation products the RMS AT does not agree with the applicant and considers the entire one-year incubation period representative for triggering additional work on metabolites in line with Regulation (EU) No 283/2013. Notice that on basis of soil microbial biomass measurements at the start and end of incubation none of these soils is considered being microbially exhausted during the incubation. The RMS AT also notes that OECD guideline 307 recommends additional incubation experiments at 10 °C if the chemical is applied or released in colder climates (e.g. in northern countries, during autumn/winter periods). As triticonazole is intended to be used as

seed treatment in spring and winter cereals, the RMS AT indeed considers studies conducted at 10 °C equally representative for triggering additional work on metabolites.

The RMS AT considers it worthwhile to notice that the common triazole fungicide metabolites 1,2,4-triazole and 1,2,4-triazole-1-ylacetic acid have only been found at low concentrations (< 5 % AR) in soil degradation experiments investigating triazole labelled parent.

Under aerobic conditions mineralisation to CO_2 is rather limited with 0.1 - 8.1 % AR around 120 DAT, formation of non-extractable residues (NER) is limited as well with 4.5 - 27.3 % AR around 120 DAT.

Degradation of triticonazole under **anaerobic conditions** was not significant and did only lead to minor metabolites as well as to the formation of non-extractable residues (max. 25.2 % AR). Formation of CO_2 was insignificant at all. Notice that anaerobic soil incubation was conducted with phenyl labelled parent only. In view of the results obtained, it is unlikely that applying the triazole label would lead to any new results.

Photolysis on soil surface contributes to the dissipation of triticonazole in soil (if exposed to light), resulting mainly in the formation of **RPA 406203**, the Z-isomer of triticonazole. The reaction from triticonazole (E-isomer) to RPA 406203 (Z-isomer) is considered fully reversible, finally leading to equilibrium of both substances with time. Formation of CO_2 (1.3 % AR after 30 days) and NER (4.1 % AR after 30 days) was limited under conditions of soil photolysis. It is noted that soil photolysis was conducted with phenyl labelled parent only. However, in view of the intended use as seed treatment, triticonazole is not expected to be exposed to light and, therefore, soil photolysis is not considered to be relevant in soil at all.

Figure B.8.1.1.4-2: Proposed route of degradation of triticonazole in soil (notice that all these structures represent racemic mixtures of two isomers with the isomer underlined indicating the isomer structure actually shown in this figure)

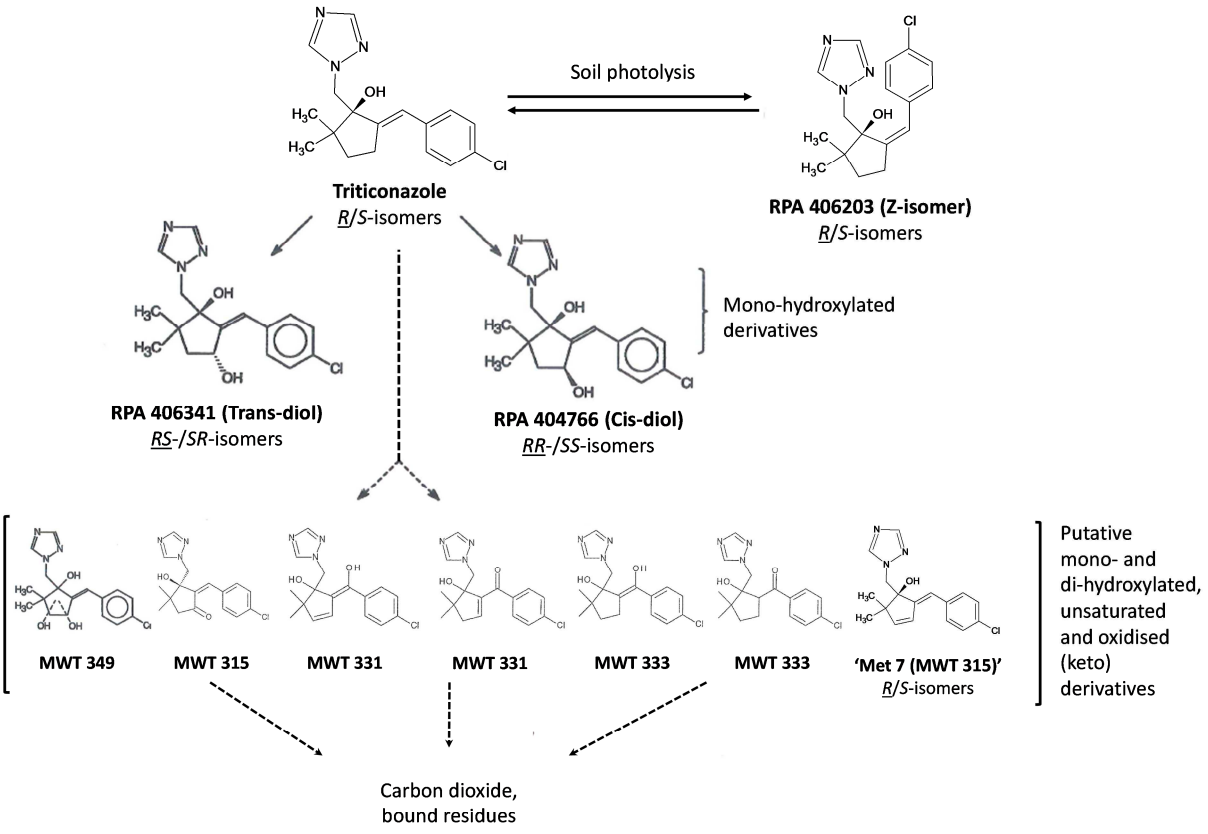


Table B.8.1.1.4-56: Summary on maximum occurrence (% AR) of identified and non-identified (unknown) metabolites in laboratory soil route studies conducted with triticonazole (metabolites shaded in grey require an exposure assessment in soil, groundwater and surface water)

Compound	Aerobic (10 °C)	Aerobic (20 - 25 °C)	Anaerobic	Soil photolysis
RPA 406341 (Trans-diol)	16.1	20.2	1.8[a]	3.5
RPA 404766 (Cis-diol)	13.9	9.9	2.0	3.3
RPA 406203 (Z-isomer)[b]	4.4	4.1	-	11.0
Metabolite fraction 'Met 6 (MWT 333)'[c]	6.9[e]	12.8	-	-
Metabolite fraction 'Met 7 (MWT 315)'[d]	6.1[e]	6.5	-	-

(a) At onset of anaerobic phase (30 DAT)
(b) RPA 406203 (Z-isomer) has to be included in the exposure assessment only in case of spray applications (if there is exposure to irradiation at the soil surface)
(c) 'Met 6' in Ayliffe & Austin (1993), equivalent to 'Met 7' in Ayliffe & Godward (1993)
(d) 'Met 7' in Ayliffe & Austin (1993), equivalent to 'Met 8' in Ayliffe & Godward (1993)
(e) Not above 5 % AR at two consecutive sampling points

Isomeric composition of triticonazole and its metabolites

Triticonazole is a racemic mixture of the two enantiomers (*R*)-(5*E*)-5-(4-chlorobenzylidene)-2,2-dimethyl-1-(1*H*-1,2,4-triazol-1-ylmethyl)cyclopentanol and (*S*)-(5*E*)-5-(4-chlorobenzylidene)-2,2-dimethyl-1-(1*H*-1,2,4-triazol-1-ylmethyl)cyclopentanol. Chiral analysis of representative soil extracts (up to 365 DAT) shows that both the *R* and *S* isomers of the racemic parent are comparably degradable. There is no indication for a significant shift in the *R*/*S* ratio during degradation in aerobic soils.

Metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) are diastereomers which are hydroxylated at the same position in the cyclopentane ring. Metabolite RPA 406341 (Trans-diol) includes the two enantiomers for which the hydroxyl group has the opposite orientation as the second hydroxyl group in the cyclopentane ring (*RS*, *RS* isomers). Metabolite RPA 404766 (Cis-diol) includes the two enantiomers for which both hydroxyl groups have the same orientation (*RR*, *SS* isomers). Chiral analysis of RPA 406341 (Trans-diol) in representative soil extracts show that an enantioselective degradation of the metabolites is unlikely to occur.

Sorption and soil metabolism data show different behaviour of the two major soil metabolites. This observation is in line with physicochemical principles and expectations based on different steric forces around these molecules.

B.8.1.2. Rate of degradation

B.8.1.2.1. Laboratory studies

B.8.1.2.1.1. Aerobic degradation of the active substance

Studies submitted for first Annex I inclusion:

- **Ayliffe & Austin (1993)**, investigating phenyl labelled triticonazole in three soils at 22 °C
- **Ayliffe & McMillan-Staff (1994)**, investigating phenyl labelled triticonazole in one soil at 22 °C
- **Ayliffe & Godward (1993)**, investigating phenyl labelled triticonazole in three soils at 10 °C and in one soil at 10 and 22 °C
- **Doble et al. (1996)**, investigating triazole labelled triticonazole in one soil at 25 °C
- **Simmonds et al. (1996)**, investigating phenyl labelled triticonazole in one soil at contrasting incubation conditions

New studies submitted:

- **Ta & Strobush (2012)**, investigating phenyl and triazole labelled triticonazole in three US soils at 20 °C
- **Ta & Strobush (2015)**, investigating phenyl and triazole labelled triticonazole in one soil at 20 °C
- **Grella et al. (2014)**, investigating non-labelled triticonazole in three soils at 20 °C

Studies on route *and* rate (Ayliffe & Austin, 1993; Ayliffe & McMillan-Staff, 1994; Ayliffe & Godward, 1993; Doble et al., 1996; Simmonds et al., 1996; Ta & Strobush, 2012; and Ta & Strobush, 2015) have already been discussed in section B.8.1.1.1 (refer to route of degradation in soil).

New kinetic assessment studies submitted:

- **Jarvis & Montesano (2014a)**, investigating modelling endpoints of triticonazole in Ayliffe & Austin (1993), Ayliffe & McMillan-Staff (1994), Ayliffe & Godward (1993), Doble et al. (1996) and Simmonds et al. (1996)
- **Szegedi (2016)**, investigating trigger and modelling endpoints in one single soil (10 °C) in Ayliffe & Godward (1993)
- **Donaldson (2015)**, investigating modelling endpoints in Ta & Strobush (2015)
- **Kreschnak (2015)**, summarizing all modelling and trigger endpoints of triticonazole

Notice that kinetic assessment studies submitted for first Annex I inclusion are considered to be superseded by the new submission.

Reference:	**Rate of degradation of BAS 595 F in soils**
Author(s), year:	Grella, B., Ta, C., Strobush, A., 2014
Report/Doc. Number:	2014/7000471
Guideline(s):	EPA 835.4100, OECD 307 (2002), SETAC (1995)
GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Test material	BAS 595 F
Common name	Triticonazole
Reg. No.	4378513
Batch number:	L76-154
CAS number:	131983-72-7
Molecular Weight	317.82 g/mol
Purity	98.6 ± 1.0 %

Soils
The soils were representative of the intended use areas. The soil samples were collected from their respective fields (top 8-inch layer), sieved through a 2-mm mesh-sieve and stored in the refrigerator. Soil characterization is presented in the table below.

Table B.8.1.2.1.1-1 Properties of the soils

Name		LUFA 2.2	LUFA 2.3	LUFA 5M
USDA textural class		Loamy Sand	Sandy Loam	Sandy Loam
	Sand [%]	82	68	60
	Silt [%]	12	22	26
	Clay [%]	6	10	14
Cation exchange capacity [meq/ 100 g]		8.1	9.4	10.4
Max. water holding capacity [%]		25.7	35.2	33.5
Moisture at 1/3 Bar [%]		10.7	12.6	14.7
Moisture at 15 Bar [%]		6.5	6.0	6.4
Total organic carbon [%]		2.8	1.7	1.7
*p*H (1:1 soil: water ratio)		5.8	7.2	7.7
*p*H (0.01 M $CaCl_2$)		5.5	6.9	7.4
Microbial biomass carbon at 0 DAT [µg/g dry soil]		430	311	353
Microbial biomass carbon at 120 DAT [µg/g dry soil]		399	415	449
N total [%]		0.14	0.09	0.09
Olsen phosphorous [mg/L]		7	80	48

Experimental conditions
Soil aliquots (50 g of dry weight) were placed in 250-mL polypropylene centrifuge bottles and treated with the test item at a rate of 0.2 mg/kg soil, corresponding to 4-times the proposed maximum field application rate of 12.5 g a.i./ha. The treated soils were connected to a flow-through test system and incubated in the dark at 20 ± 2 °C for 120 days. Moisturized and CO_2-free air was passed over the soil in order to maintain the aerobic conditions. Soil moisture was adjusted to approximately 50 % MWHC prior to the application of the test solutions and maintained throughout the incubation period.

Sampling
Duplicate samples were collected at 0, 3, 7, 14, 30, 59, 91, and 120 DAT. Within every set of samples belonging to a certain sampling date, at least one sample per soil was incubated without the test item (control samples). The control samples were used for microbial biomass determination and for verification of the analytical method.

Description of analytical procedures
The sample analysis was performed according to the validated method No. 0051 with the exception of the LC-MS conditions. The LC-MS method is described in section CA 4.2.1. Each soil sample was sequentially extracted once with ammonium hydroxide (0.1 M) and twice with acetone. The solvent from the combined extracts was evaporated until 10-15 mL remained and the volume was adjusted to 20 mL by the addition of water. The samples were centrifuged (3000 rpm, 10 min.) and then further extracted by solid phase extraction (SPE), and then the samples were analysed by LC-MS.

The analytical method was verified by using spiked samples of the soils at every sampling date. At the day of the workup, control spiked samples (instrumental recoveries) were prepared by removing 1 mL of the control extract and spiking it with 10 µL of the 10 µg/mL fortification solution. Additionally, prior to workup, fortification samples were made by treating the soil control samples with 0.1 mL of the 10 µg/mL fortification solution (LOQ) or with 0.1 mL of the 100 µg/mL fortification solution (10 × LOQ). The LOQ was set at 20 µg/kg of soil.

Determination of degradation Kinetics
The guidance of FOCUS (2006) was used as the basis for conducting the kinetic analysis, statistical assessment, and selection of the best fit kinetic model for each soil (trigger endpoints). Optimization of model parameters, including estimation of parameter standard errors, was performed using the software KINGUII.

Findings:

Time course of the rate of degradation of triticonazole in the treated soils is presented in the table below.

Table B.8.1.2.1.1-2 Degradation of triticonazole in soil

DAT	Soil LUFA 2.2		Soil LUFA 2.3		Soil LUFA 5M	
	Triticonazole (mg/kg)	Triticonazole (% applied)	Triticonazole (mg/kg)	Triticonazole (% applied)	Triticonazole (mg/kg)	Triticonazole (% applied)
0 rep 1	0.161	84.9	0.176	99.3	0.163	86.6
0 rep 2	0.219	115.1	0.178	100.7	0.213	113.4
0 mean	**0.190**	**100.0**	**0.177**	**100.0**	**0.188**	**100.0**
3 rep 1	0.151	79.5	0.145	81.8	0.195	103.6
3 rep 2	0.155	81.8	0.145	81.9	0.207	110.4
3 mean	**0.153**	**80.7**	**0.145**	**81.8**	**0.201**	**107.0**
7 rep 1	0.142	74.6	0.155	87.5	0.151	80.3
7 rep 2	0.158	83.3	0.151	85.3	0.143	76.3
7 mean	**0.150**	**79.0**	**0.153**	**86.4**	**0.147**	**78.3**
14 rep 1	0.165	86.9	0.149	84.1	0.156	82.9
14 rep 2	0.150	78.7	0.143	81.0	0.152	80.9
14 mean	**0.157**	**82.8**	**0.146**	**82.6**	**0.154**	**81.9**
30 rep 1	0.158	82.9	0.130	73.4	0.135	71.7
30 rep 2	0.162	85.4	0.143	80.6	0.134	71.5
30 mean	**0.160**	**84.1**	**0.136**	**77.0**	**0.134**	**71.6**
59 rep 1	0.118	62.0	0.098	55.3	0.116	61.8
59 rep 2	0.127	66.6	0.099	56.1	0.121	64.2
59 mean	**0.122**	**64.3**	**0.099**	**55.7**	**0.118**	**63.0**
91 rep 1	0.138	72.4	0.098	55.2	0.104	55.5
91 rep 2	0.140	73.9	0.087	48.9	0.113	60.1
91 mean	**0.139**	**73.1**	**0.092**	**52.1**	**0.109**	**57.8**
120 rep 1	0.133	70.1	0.085	48.2	0.097	51.9
120 rep 2	0.136	71.3	0.089	50.4	0.105	56.0
120 mean	**0.134**	**70.7**	**0.087**	**49.3**	**0.101**	**53.9**

Triticonazole (% applied) was calculated by setting 100 % to the mean of the day 0 values
Data for 59-DAT and 120-DAT in soil LUFA 2.2 for both rep1 and rep2 are an average of two analyses
Data for 91-DAT rep 1 and rep 2 in soil LUFA 2.2 are an average of three analyses each

The amount of triticonazole decreased at different rates in the three soils examined. The fastest decrease was seen for LUFA 2.3, where triticonazole decreased to 49.3 % at day 120. In soil LUFA 5M, the amount of triticonazole at day 120 (53.9 %) was close to that of LUFA 2.3. A slower decrease was seen for soil LUFA 2.2 (70.7 % at day 120).

Conclusion:

The rate of the degradation of triticonazole varied in the three soils examined under aerobic conditions. *DT50* values of 317, 125 and 149 days were found in soils LUFA 2.2, LUFA 2.3 and LUFA 5M, respectively.

Comments (RMS AT):

- The study follows OECD guideline 307 and is considered reliable.
- Trigger endpoint assessment was done in this study following pertinent guidance (FOCUS kinetics, 2006), but no details on statistics were reported in the applicant study summary above. Modelling endpoints were additionally assessed by Kreschnak (2015).
- A complete RMS AT synopsis on triticonazole laboratory degradation rates is given in Kreschnak (2015) in chapter B.8.1.2.1.1 (aerobic degradation of the active substance).

Reference:	**Recalculation of Triticonazole laboratory soil degradation kinetics according to FOCUS (2006) guidance**
Author(s), year:	Jarvis, T., Montesano, V., 2014a
Report/Doc. Number:	2014/1083342
Guideline(s):	FOCUS (2006): Guidance Document on Estimating Persistence and Degradation

	Kinetics from Environmental Fate Studies on Pesticides in EU Registration , SANCO/10058/2005, version 2.0, 434 pp.
GLP:	Not applicable (modelling study)
Validity:	None reliable (refer to comment section)
Status:	**New submission**

Material and methods:

Five studies were considered in which the parent triticonazole was applied (Ayliffe & Godward, 1993; Ayliffe & Austin, 1993; Ayliffe & McMillan-Staff, 1994; Doble et al., 1996; and Simmonds et al., 1996). Additionally, three metabolite dosed laboratory soil degradation studies (McGhee, 2000; Unsworth & Clarke, 2000; and Crowe, 2002) were evaluated *[RMS AT: results for the metabolites are given in B.8.1.2.1.2, aerobic degradation of metabolites, breakdown and reaction products]*. Analytical results of triticonazole and its metabolites in soil (in percentage of applied) were obtained from the laboratory soil degradation studies and used as input for the kinetic evaluation. The simulation modelling was performed using KinGui Version 2.

Degradation rates of triticonazole and its metabolites and, furthermore, the formation fractions of the metabolites were derived. When necessary, the *DT50* values were normalised to 20 °C (using a Q_{10} of 2.58) and *p*F2.

Results and discussion:

The evaluation of the parent degradation studies showed a noticeable deviation from SFO kinetics during the latter stages of the incubations. However, due to generally slow degradation of triticonazole in the investigated lab studies, the low formation of metabolites and long study durations (365 d), SFO was considered acceptable for modelling purposes. No separate trigger endpoints were derived as field dissipation studies are triggered regardless which kinetic model is used. Results are presented in the table below.

Table B.8.1.2.1.1-3 Triticonazole: Aerobic soil degradation modelling endpoints

Study	Soil	Incubation conditions		Kinetic Model	*DT50* study cond. (d)	*DT90* study cond. (d)	*DT50* at 20 °C, *p*F2 (d)
		Temp. (°C)	Moisture				
Ayliffe & Austin (1993)	Sandy loam	22	75 % of 33 kPa	SFO	253	840	176
	Clay loam	22	75 % of 33 kPa	SFO	136	452	145
Ayliffe & McMillan-Staff (1994)	Loamy sand	22	75 % of 33 kPa	SFO	187	620	206
Ayliffe & Godward (1993)	Loamy sand	22	75 % of 33 kPa	SFO	249	828	299
	Sandy loam	10	75 % of 33 kPa	SFO	347	>1000	79.8
	Clay loam	10	75 % of 33 kPa	SFO	183	607	61.4
	Loamy sand	10	75 % of 33 kPa	SFO	599	>1000	234
Doble et al. (1996)	Clay	25	75 % of 33 kPa	SFO	492	>1000	401
Simmonds et al. (1996)	Sandy loam (standard)	25	50 % FC	SFO	167	555	166
	Sandy loam (reduced rate)	25	50 % FC	SFO	187	620	186
	Sandy loam	25	20 % FC	SFO	215	714	344
	Sandy loam	10	50 % FC	SFO	413	>1000	100

Conclusion:

The rates of the degradation of triticonazole and its metabolites were re-evaluated according to FOCUS (2006). Modelling endpoints for the parent and its metabolites as well as formation fractions for the metabolites were derived and can be used in environmental fate modelling. Field dissipation studies are triggered for triticonazole.

Comments (RMS AT):

- Evaluation of the Speyer 2.2 loamy sand (10 °C) in Ayliffe & Godward (1993) is missing in this report. Respective evaluation was submitted by Szegedi (2016).

- The **study is not considered reliable** for several reasons. A complete RMS AT synopsis on triticonazole laboratory degradation rates including a full kinetic reassessment of all soil degradation studies is given in Kreschnak (2015) in chapter B.8.1.2.1.1 (aerobic degradation of the active substance).

Reference:	**Kinetic evaluation of laboratory soil degradation of triticonazole (BAS 595 F) and its metabolites RPA 406341 and RPA 404766 in a single soil for derivation of trigger and modelling endpoints according to FOCUS**
Author(s), year:	Szegedi, K., 2016
Report/Doc. Number:	2016/1171410
Guideline(s):	FOCUS (2006): Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration, SANCO/10058/2005, version, 2.0 434 pp.
GLP:	Not applicable (modelling study)
Validity:	Yes
Status:	**New submission**

Material and methods:

The purpose of this evaluation was to analyse the degradation kinetics observed in Speyer 2.2 loamy sand, incubated at 10 °C in Ayliffe & Godward (1993). Kinetic evaluation was performed in order to derive:

- Degradation parameters as triggers for additional work (best-fit endpoints)
- Degradation parameters for environmental fate models (modelling endpoints)

For the test substance triticonazole, the appropriate kinetic model for deriving trigger and modelling endpoints was identified considering the procedures and kinetic models proposed by the FOCUS workgroup on degradation kinetics (FOCUS, 2006). The most appropriate model was selected based on visual and statistical assessment and the corresponding *DegT50* and *DegT90* values are reported as trigger endpoints. Appropriate *DegT50* values for use in environmental fate models were derived depending on the kinetic model.

The first kinetic evaluation was performed considering the parent compound only. The second kinetic evaluation was performed considering the parent compound and its metabolites.

Results and discussion:

The trigger and modelling endpoints for triticonazole derived from the kinetic evaluation considering the parent compound only are summarized in the tables below.

Table B.8.1.2.1.1-4 Endpoints for triticonazole in Speyer 2.2 loamy sand (10 °C)

Endpoint	Kinetic model	χ^2 err. (%)	*DegT50* [d]	*DegT90* [d]
Trigger endpoint	HS	2.58	> 1000	> 1000
Modelling endpoint	DFOP	2.93	> 1000	> 1000

Comments (RMS AT):

- A complete RMS AT synopsis on triticonazole laboratory degradation rates including a full kinetic reassessment of all soil degradation studies is given in Kreschnak (2015) in chapter B.8.1.2.1.1 (aerobic degradation of the active substance).

Reference:	**Kinetic evaluation of the aerobic soil metabolism of BAS 595 F (triticonazole) in a loamy sand soil**
Author(s), year:	Donaldson, F., 2015

Report/Doc. Number:	2015/7001309
Guideline(s):	FOCUS (2006): Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration SANCO/10058/2005, version 2.0, 434 pp.
GLP:	Not applicable (modelling study)
Validity:	None reliable (refer to comment section)
Status:	**New submission**

Material and methods:

One study with one soil was considered in which the parent triticonazole was applied (Ta & Strobush, 2015). Analytical results of triticonazole and its metabolites in soil (in percentage of applied) were obtained from the laboratory soil degradation study and used as input for the kinetic evaluation. Two radiolabels (phenyl, triazole rings) were investigated in the study, and replicate samples were taken for each sampling interval. The data for each radiolabel was combined and analysed as one data set, resulting in four replicates per sampling time. Those metabolites which exceeded 10 % AR at any single sampling time or 5 % AR in two consecutive sampling times were considered in the evaluation. Two metabolites met these criteria: RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) *[RMS AT: results for the metabolites are given in chapter B.8.1.2.1.2, aerobic degradation of metabolites, breakdown and reaction products]*. The simulation modelling was performed using KinGUI (v. 2.2014.224.1704). Degradation rates of triticonazole and its metabolites and, furthermore, the formation fractions of the metabolites were derived. The derived *DegT50* values were normalised to 20 °C (using a Q_{10} of 2.58) and *p*F2.

Results and discussion:

Parent-only kinetics were evaluated with the SFO model as a first step. As this provided an acceptable visual and statistical fit, there was no need to test any biphasic models. The *DegT50* modelling endpoint was derived from the parent-only fitting. A full degradation pathway was also investigated in order to determine metabolite kinetic endpoints (*DegT50*, formation fraction) for RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol). The full degradation pathway fit considered the SFO model for both parent and metabolites. Results for parent are presented in the Table below.

Table B.8.1.2.1.1-5 Triticonazole: Aerobic soil degradation modelling endpoints

Study	Soil	Incubation conditions		Kinetic Model	*DegT50* study cond. (d)	*DegT50* at 20°C, *p*F2 (d)
		Temp. (°C)	Moisture			
Ta & Strobush, 2015	Loamy sand	20	50 % MWHC	SFO	136	116

Conclusion:

The rates of the degradation of triticonazole and its metabolites were evaluated according to FOCUS (2006). Modelling endpoints for the parent and its metabolites as well as formation fractions for the metabolites were derived and can be used in environmental fate modelling.

Comments (RMS AT):

- The **study is not considered reliable** for several reasons. A complete RMS AT synopsis on triticonazole laboratory degradation rates including a full kinetic reassessment of all soil degradation studies is given in Kreschnak (2015) in chapter B.8.1.2.1.1 (aerobic degradation of the active substance).

Reference:	**Summary of kinetic endpoints for Triticonazole and its metabolites from laboratory soil degradation studies**
Author(s), year:	Kreschnak, C., 2015
Report/Doc. Number:	2015/1186987

Guideline(s):	None
GLP:	Not applicable (modelling study)
Validity:	None reliable (refer to comment section)
Status:	**New submission**

The rate of degradation of triticonazole and its metabolites in aerobic laboratory soils was investigated in several studies. The kinetic evaluation of these studies was conducted either directly in the study reports or in separate kinetic reports. In some cases, not all kinetic endpoints were explicitly reported although the necessary data is included in the reports. This statement aims to summarise all kinetic endpoints of triticonazole and its metabolites that were provided in the study reports or in the kinetic reports. The relevant results of this summary (parent only) are presented in the table below.

Table B.8.1.2.1.1-6 Overview of the laboratory aerobic degradation rate studies – active substance triticonazole

Reference	Soil characteristics				Incubation conditions		Trigger Endpoints			Modelling Endpoints		
	Soil origin	Soil type	*p*H ($CaCl_2$)	OC[c] (%)	Moisture	Temp. (°C)	Kinetic Model	*DT50* (days)	*DT90* (days)	Kinetic Model	*DT50* (d) study cond.	*DT50* (d) at 20 °C and pF2
Ayliffe & Austin (1993)	Not reported	Sandy loam	6.42[b]	0.72	75 % of 33 kPa	22	SFO	253	840	SFO	253	176
	Not reported	Clay loam	6.18[b]	5.66		22	SFO	136	452	SFO	136	145
Ayliffe & McMillan-Staff (1994)	Speyer 2.2	Loamy sand	6.8[b]	2.35	75 % of 33 kPa	22	SFO	187	620	SFO	187	206
Ayliffe & Godward (1993)	Not reported	Loamy sand	6.24[b]	18.70	75 % of 33 kPa	22	SFO	249	828	SFO	249	299[d]
	Not reported	Sandy loam	6.30[b]	0.83		10	SFO	347	> 1000	SFO	347	79.8
	Not reported	Clay loam	6.08[b]	3.28		10	SFO	183	607	SFO	183	61.4
	Not reported	Loamy sand	6.24[b]	18.70		10	SFO	599	> 1000	SFO	599	234[d]
Doble et al. (1996)	Not reported	Clay[a]	5.7	1.2	75 % of 33 kPa	25	SFO	492	> 1000	SFO	492	401
Simmonds et al. (1996)	Manningtree (standard)	Sandy loam[a]	6.1	0.8	50 % FC	25	SFO	167	555	SFO	167	166[d]
	Manningtree (reduced rate)				50 % FC	25	SFO	187	620	SFO	187	186[d]
	Manningtree				20 % FC	25	SFO	215	714	SFO	215	344[d]
	Manningtree				50 % FC	10	SFO	413	> 1000	SFO	413	100[d]
Ta & Strobush (2015)	Li10	Loamy sand[a]	6.3	0.81	50 % MWHC	20	DFOP	149	640	SFO	136	116
Grella et al. (2014)	LUFA 2.2	Loamy sand[a]	5.5	2.8	50 % MWHC	20	SFO	317	> 1000	SFO	317	299
	LUFA 2.3	Sandy loam[a]	6.9	1.7		20	FOMC	125	> 1000	SFO	115	100
	LUFA 5M	Sandy loam[a]	7.4	1.7		20	FOMC	149	> 1000	-[e]	-	-
Geometric mean												**161**

(a) Soil type according to USDA, for the other soils the classification is unknown
(b) Buffer solution unknown
(c) If not explicitly mentioned in the study report, OC was calculated: OC (%) = OM (%) / 1.724
(d) The geometric mean value determined from single values for the same soil was used for the calculation of the overall geometric mean value
(e) Modelling endpoints could not be determined since the SFO model did not provide a reliable fit and the slow degradation rate obtained from DFOP model was not significant

Comments (RMS AT):

- In all legacy studies (Ayliffe & Austin, 1993; Ayliffe & McMillan-Staff, 1994; Austin & Godward, 1993; Doble et al., 1996; and Simmonds et al., 1996) as well as in Ta & Strobush (2012) triticonazole was incubated over a period of one year which is indeed much longer than the 120 days recommended by OECD guideline 307. However, OECD guideline 307 also indicates that *where necessary to characterise the decline of the test substance and the formation and decline of major transformation products, studies can be continued for longer periods (e.g. 6 or 12 months).* As degradation of triticonazole and subsequent formation of metabolites in laboratory degradation experiments in indeed rather slow with maximum occurrence of metabolites beyond 120 days, the RMS AT considers the entire incubation period of one year indeed most representative to obtain reliable degradation rates of triticonazole and its metabolites. In principle, this approach was also followed by the applicant. However, the applicant considers the parent decline sufficiently described by the SFO model (see next comment below).

  It may also be noted that on basis of microbial biomass measurements at the beginning and at the end of the one-year incubation period none of the soils is considered to suffer from drastic decline in microbial biomass. In several soils microbial biomass even increased over the incubation period.

- The applicant considers the SFO model sufficient to derive modelling endpoints for triticonazole in all soil degradation studies (with the exception of one soil in Grella et al., 2014), particularly as the χ^2 errors were always below 15 %, as requested by FOCUS degradation kinetics (EC, 2014). In view of the RMS AT, degradation of triticonazole in soil almost consistently follows a biphasic decline pattern which cannot be adequately described by the SFO model (see figures provided below). The biphasic decline pattern is also evident in the only two studies conducted for 120 days (Ta & Strobush, 2015; Grella et al., 2014). For that reason, the RMS AT considers biphasic degradation models (DFOP or HS, no FOMC as 10 % of AR are never reached by study termination) more appropriate for deriving trigger and modelling endpoints as far as these biphasic models allow for reliable fits from a statistical point of view. It is highlighted, that the application of biphasic degradation models for the parent also allows for reliable pathway fits of the two major metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) in most of the soils. This is not necessarily the case if the parent is assumed to follow the SFO model. It is particularly considered important to obtain robust formation fractions of both metabolites as well as robust degradation rates of RPA 404766 (Cis-diol) as for this metabolite no field degradation studies are available (for results on metabolites also refer to B.8.1.2.1.2, aerobic degradation of metabolites, breakdown and reaction products).

- Lab degradation experiments conducted at 10 °C (in Ayliffe & Godward, 1993) or at reduced moisture content (in Simmonds et al., 1996) are not considered appropriate for temperature or moisture normalisation. These experiments are therefore not considered further for modelling endpoints.

- The study Ta & Strobush (2012), investigating degradation of triticonazole in three US soils was originally not included in the applicant dossier but was submitted at late time point in order to support metabolite identification issues. Subsequently, this study was included in the RMS AT re-evaluation of degradation rates of triticonazole and its two metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol).

- One basis of the information provided above, the RMS AT fully re-evaluated the parent soil degradation experiments on basis of pertinent guidance applying the software tool CAKE 3.3 assuming $P_{SFO} \rightarrow M_{SFO}$, $P_{DFOP} \rightarrow M_{SFO}$ or $P_{HS} \rightarrow M_{SFO}$ pathway fits (with M representing RPA 406341, Trans-diol, and RPA 404766, Cis-diol, in parallel). Results for the parent triticonazole are given in the tables below.

- In case of the US clay soil (Doble et al., 1996) no reliable fits could be obtained applying the DFOP or HS model. Fits based on DFOP or HS did also not reveal statistically reliable degradation rates for the metabolites. It is noted that the fits of the metabolites could not be improved by fixing the DFOP k_2 rate of the parent to 1000 days (as suggested by the co-RMS UK). So finally, the SFO model was considered most suitable although the last sampling point of the parent substance is underestimated in this case (see tables below).

- Where necessary, obtained degradation rates have been normalized to standard conditions (20 °C and *p*F2) as given in the table below. It is noted that the normalization procedure applied by the RMS AT deviates from the applicant approach in two cases: i) the default reference MC for the UK loamy sand in Ayliffe & Godward (1993) was set to 12 % whereas it should be 14 %; ii) for the sandy loam in Simmonds et al. (1996) the study MC was set to 9.5 % whereas the study reports quotes 15.5 %.

Table B.8.1.2.1.1-7 Moisture and temperature correction factors for laboratory parent degradation studies conducted at 20 - 25 °C - RMS AT assessment

Study	Soil type	T (°C)	Incubation moisture	Study MC (%)	Ref. MC (*p*F2) (%)	f_T[(c)]	f_{MC}[(d)]	$f_T \times f_{MC}$
Ayliffe & Austin (1993)	Sandy loam	22	75 % 33kPa	8.7	19[(a)]	1.21	0.58	**0.70**
	Clay loam	22	75 % 33kPa	23.6	28[(a)]	1.21	0.89	**1.08**
Ayliffe & McMillan-Staff (1994)	Loamy sand (Speyer 2.2)	22	75 % 33kPa	12.5	14[(a)]	1.21	0.92	**1.11**
Ayliffe & Godward (1993)	Loamy sand (UK)	22	75 % 33kPa	28.9	14[(a)]	1.21	1.00	**1.21**
Doble et al. (1996)	Clay	25	75 % 33kPa	23.8	62.4[(b)]	1.61	0.51	**0.82**
Simmonds et al. (1996)	Sandy loam (standard & red. rate)	25	50 % FC	15.5	19[(a)]	1.61	0.87	**1.40**
Ta & Strobush (2012)	Sand	20	50 % MWHC	9.7	12[(a)]	1.00	0.86	**0.86**
	Loam	20	50 % MWHC	21.3	25[(a)]	1.00	0.89	**0.89**
	Loamy sand	20	50 % MWHC	11.2	14[(a)]	1.00	0.86	**0.86**
Ta & Strobush (2015)	Loamy sand	20	50 % MWHC	11.1	14[(a)]	1.00	0.85	**0.85**
Grella et al. (2014)	Loamy sand	20	50 % MWHC	12.9	14[(a)]	1.00	0.94	**0.94**
	Sandy loam (2.3)	20	50 % MWHC	17.6	19[(a)]	1.00	0.95	**0.95**
	Sandy loam (5M)	20	50 % MWHC	16.8	19[(a)]	1.00	0.92	**0.92**

(a) Default moisture content for this soil type
(b) Measured moisture content
(c) Temperature correction factor = $2.58^{((T_{act}-T_{ref})/10)}$
(d) Moisture correction factor = $(MC_{act}/MC_{ref})^{0.7}$

Table B.8.1.2.1.1-8 Trigger and modelling endpoints for triticonazole in laboratory soil degradation studies conducted at 20 - 25 °C - RMS AT assessment (all pathway fits, fits shaded in grey are considered most reliable)

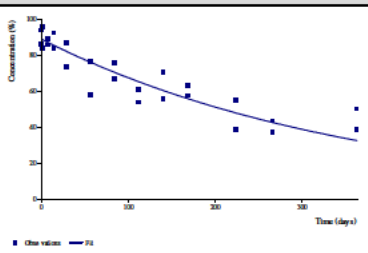
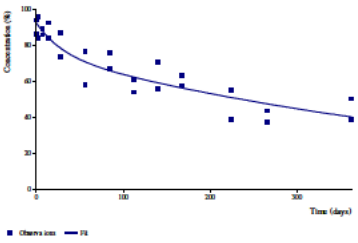
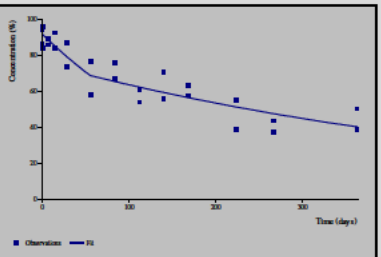
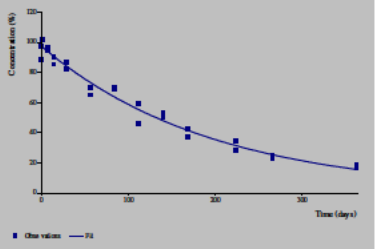
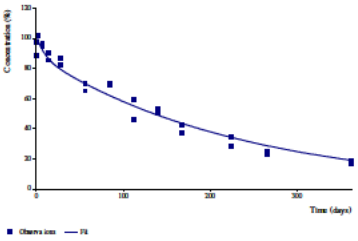
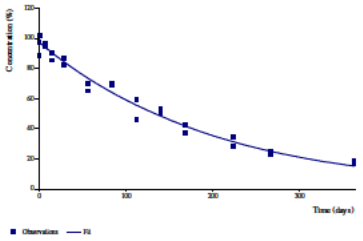
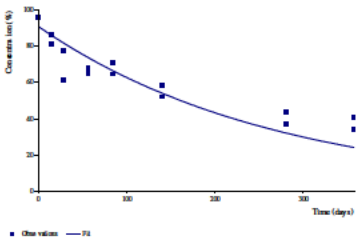
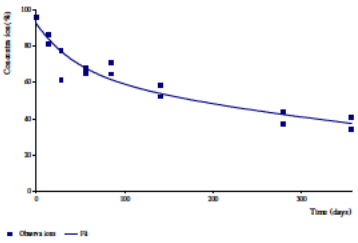
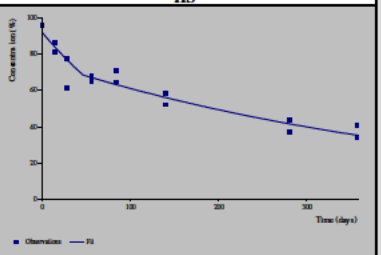
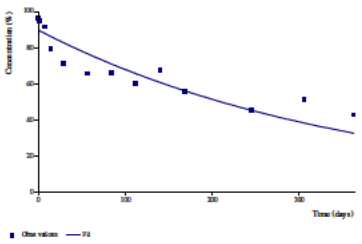
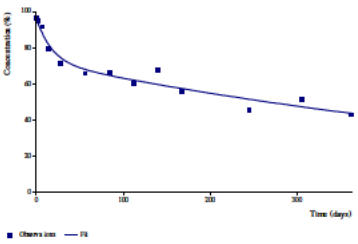
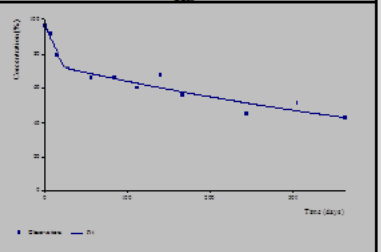
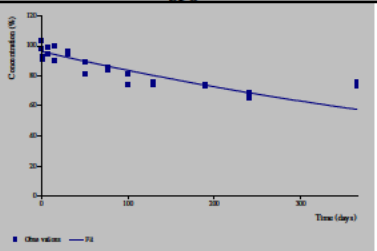
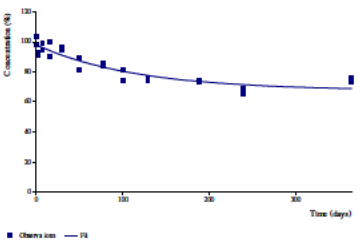
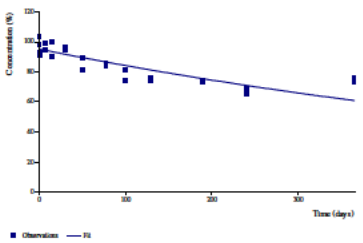
Study	Soil	Kinetic model	Parameter	Value	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	Total system *DegT 50 (d)*	*DegT 90 (d)*	Fast phase *DegT50* (d)	Slow phase *DegT50* (d)	Modelling *DegT50* (d)
Ayliffe & Austin (1993)	Sandy loam	SFO	k	0.003	0.002	0.003	< 0.01	6.0	253	839	na	na	177
		DFOP	k1	0.033	0.000	0.066	0.02						
			k2	0.002	0.001	0.003	< 0.01	5.2	284	> 1000	20.7	404	346[(a)]
			g	0.19	0.03	0.34	na						
		HS	**k1**	0.005	0.002	0.008	< 0.01						
			k2	0.002	0.001	0.002	< 0.01	**5.0**	**289**	**> 1000**	**133**	**400**	**280[(a)]**
			tb	55.4	23.4	87.4	na						
	Clay loam	**SFO**	**k**	**0.005**	**0.005**	**0.005**	**< 0.01**	**4.4**	**137**	**455**	**na**	**na**	**148**
		DFOP	k1	0.110	0.046	0.175	< 0.01						
			k2	0.004	0.004	0.005	< 0.01	5.9	130	510	6.2	163	176[(a)]
			g	0.13	0.07	0.19	na						
		HS	k1	0.005	0.005	0.005	< 0.01						
			k2	0.005	0.004	0.006	< 0.01	4.8	139	448	139	133	144[(a)]
			tb	140	nd	nd	na						
Ayliffe & McMillan-Staff (1994)	Loamy sand (Speyer 2.2)	SFO	k	0.004	0.003	0.0004	< 0.01	9.6	187	620	na	na	208
		DFOP	k1	0.023	0.008	0.037	< 0.01						
			k2	0.002	0.000	0.003	< 0.01	5.4	226	> 1000	30.8	435	483[(a)]
			g	0.29	0.07	0.50	na						
		HS	**k1**	0.006	0.004	0.009	< 0.01						
			k2	0.002	0.001	0.003	< 0.01	**5.0**	**233**	**986**	**109**	**324**	**360[(a)]**
			tb	46.3	27.1	65.4	na						
Ayliffe & Godward (1993)	Loamy sand (UK)	SFO	k	0.003	0.002	0.003	< 0.01	9.1	249	828	na	na	301
		DFOP	k1	0.058	0.022	0.094	< 0.01						
			k2	0.001	0.001	0.002	< 0.01	4.4	292	> 1000	12.0	495	599[(a)]
			g	0.25	0.16	0.33	na						

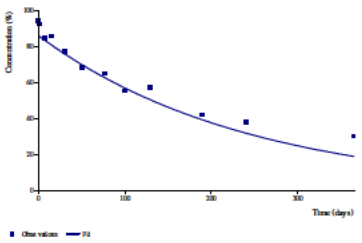
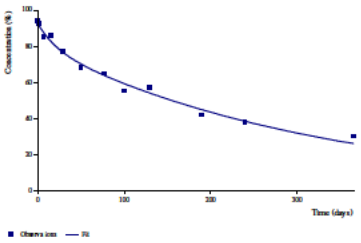
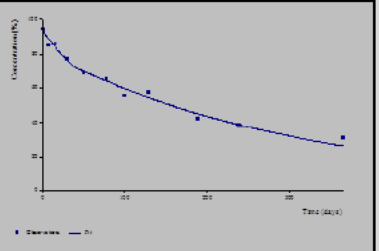
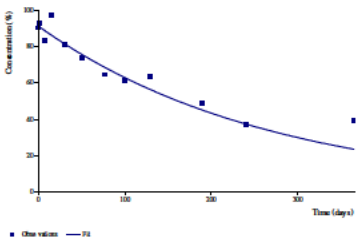
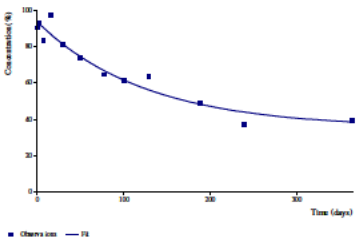
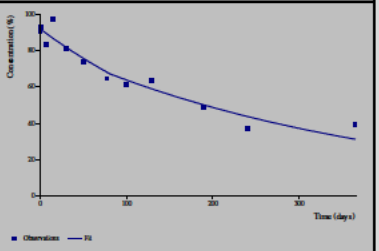
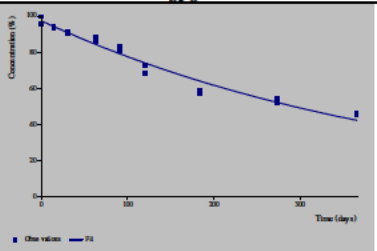
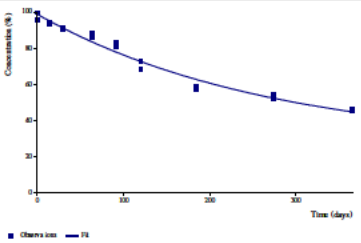
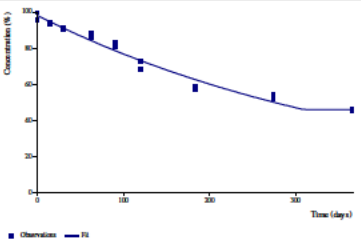
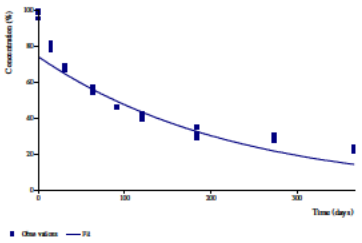
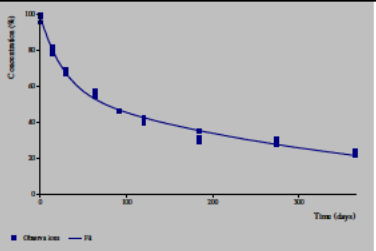
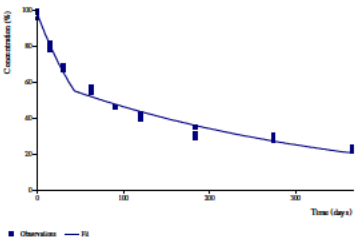
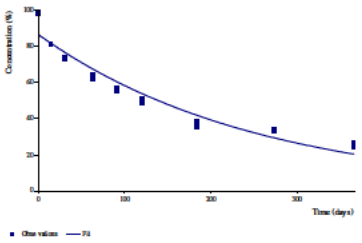
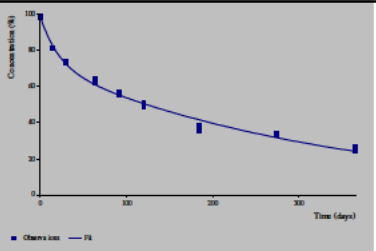
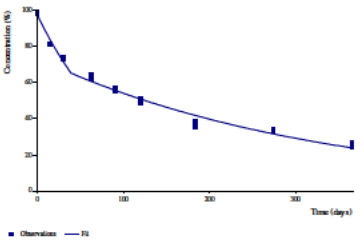
		HS	**k1** **k2** **tb**	**0.012** **0.001** **25.7**	**0.007** **0.001** **16.1**	**0.017** **0.002** **35.2**	**< 0.01** **< 0.01** **na**	**4.2**	**290**	**> 1000**	**59**	**467**	**565[a]**
Doble et al. (1996)	Clay	**SFO**	**k**	**0.001**	**0.001**	**0.002**	**< 0.01**	**5.7**	**495**	**> 1000**	**na**	**na**	**376**
		DFOP	k1 k2 g	0.009 0.000 0.31	-0.001 -0.001 -0.05	0.018 0.001 0.66	0.04 0.50 na	3.4	> 1000	> 1000	80.3	> 1000	na
		HS	k1 k2 tb	0.001 0.001 412	0.001 nd nd	0.001 nd nd	0.001 nd na	5.8	545	> 1000	569	484	397[a]
Simmonds et al. (1996)	Sandy loam (standard)	SFO	k	0.004	0.004	0.004	< 0.01	6.8	169	562	na	na	237
		DFOP	k1 k2 g	0.048 0.003 0.13	0.012 0.003 0.05	0.084 0.004 0.21	0.01 < 0.01 na	3.3	180	706	14.5	226	316[a]
		HS	**k1** **k2** **tb**	**0.006** **0.003** **39.9**	**0.005** **0.003** **22.9**	**0.008** **0.004** **57.0**	**< 0.01** **< 0.01** **na**	**3.3**	**183**	**702**	**111**	**223**	**312[a]**
	Sandy loam (red. rate)	SFO	k	0.004	0.003	0.005	< 0.01	7.5	186	618	na	na	260
		DFOP	k1 k2 g	0.008 0.000 0.62	0.004 -0.002 0.28	0.012 0.002 0.97	< 0.01 0.50 na	6.1	203	> 1000	87.1	> 1000	na
		HS	**k1** **k2** **tb**	**0.004** **0.003** **81.1**	**0.003** **0.002** **49.9**	**0.005** **0.003** **112.4**	**< 0.01** **< 0.01** **na**	**6.5**	**221**	**816**	**179**	**256**	**358[a]**
Ta & Strobush (2012)	Sand	**SFO**	**k**	**0.002**	**0.002**	**0.003**	**< 0.01**	**3.1**	**305**	**> 1000**	**na**	**na**	**262**
		DFOP	k1 k2 g	0.004 0.000 0.74	-0.005 -0.013 -1.72	0.012 0.013 3.19	0.20 0.50 na	3.1	306	> 1000	187	> 1000	na
		HS	k1 k2 tb	0.002 0.000 309	0.002 -0.044 -747	0.003 0.044 1360	< 0.01 0.50 na	3.1	283	> 1000	283	> 1000	na
	Loam	SFO	k	0.004	0.004	0.005	< 0.01	14.5	156	519	na	na	139
		DFOP	**k1** **k2** **g**	0.037 0.003 0.41	0.031 0.002 0.37	0.043 0.003 0.45	**< 0.01** **< 0.01** **na**	**2.4**	**78.8**	**661**	**18.7**	**258**	**230[a]**
		HS	k1 k2 tb	0.013 0.003 43.2	0.012 0.003 38.5	0.015 0.003 47.8	< 0.01 < 0.01 na	3.7	82.8	617	52.1	230	205[a]
	Loamy sand	SFO	k	0.004	0.003	0.005	< 0.01	7.8	176	584	na	na	151
		DFOP	**k1** **k2** **g**	0.048 0.003 0.27	0.032 0.003 0.21	0.063 0.003 0.32	**< 0.01** **< 0.01** **na**	**3.2**	**128**	**664**	**14.5**	**231**	**199[a]**
		HS	k1 k2 tb	0.010 0.003 39.2	0.009 0.003 31.2	0.012 0.004 47.2	< 0.01 < 0.01 na	3.8	134	656	67.6	225	194[a]
Ta & Strobush (2015)	Loamy sand	SFO	k	0.005	0.004	0.006	< 0.01	3.5	138	458	na	na	117
		DFOP	**k1** **k2** **g**	**0.065** **0.003** **0.18**	**0.036** **0.002** **0.09**	**0.093** **0.004** **0.27**	**< 0.01** **< 0.01** **na**	**1.0**	**148**	**633**	**10.7**	**209**	**178[a]**
		HS	k1 k2 tb	0.011 0.005 11.3	0.008 0.004 7.2	0.014 0.005 15.5	0.008 0.004 7.2	2.4	133	478	64.0	148	126[a]
Grella et al. (2014)	Loamy sand	**SFO**	**k**	**0.002**	**0.001**	**0.004**	**0.01**	**7.3**	**317**	**> 1000**	**na**	**na**	**298**
		DFOP	k1 k2 g	5.717 0.001 0.18	-7758 0.000 0.05	7770 0.003 0.32	0.50 0.03 na	5.3	333	> 1000	0.121	471	443[a]
		HS	k1 k2 tb	0.035 0.000 7.3	-0.003 -0.002 -0.1	0.072 0.002 14.6	0.03 0.50 na	7.6	> 1000	> 1000	19.9	> 1000	na
	Sandy Loam (LUFA 2.3)	**SFO**	**k**	**0.006**	**0.005**	**0.007**	**0.01**	**5.9**	**115**	**381**	**na**	**na**	**109**
		DFOP	k1 k2 g	5.746 0.005 0.132	nd 0.004 0.054	nd 0.007 0.209	nd < 0.01 na	4.6	102	399	0.121	128	122[a]
		HS	k1 k2 tb	0.008 < 0.001 74.7	0.006 -0.008 34.7	0.011 0.008 114.6	< 0.01 0.50 na	5.5	> 1000	> 1000	85.8	> 1000	na
	Sandy loam (LUFA 5M)	SFO	k	0.006	0.003	0.008	< 0.01	8.5	123	410	na	na	113
		DFOP	k1 k2 g	0.099 0.003 0.28	-0.083 -0.001 0.02	0.281 0.007 0.53	0.13 0.08 na	6.6	130	697	7.0	244	224[a]
		HS	**k1** **k2**	**0.033** **0.004**	**0.005** **0.002**	**0.062** **0.006**	**0.01** **< 0.01**	**6.3**	**114**	**521**	**20.8**	**175**	**161[a]**

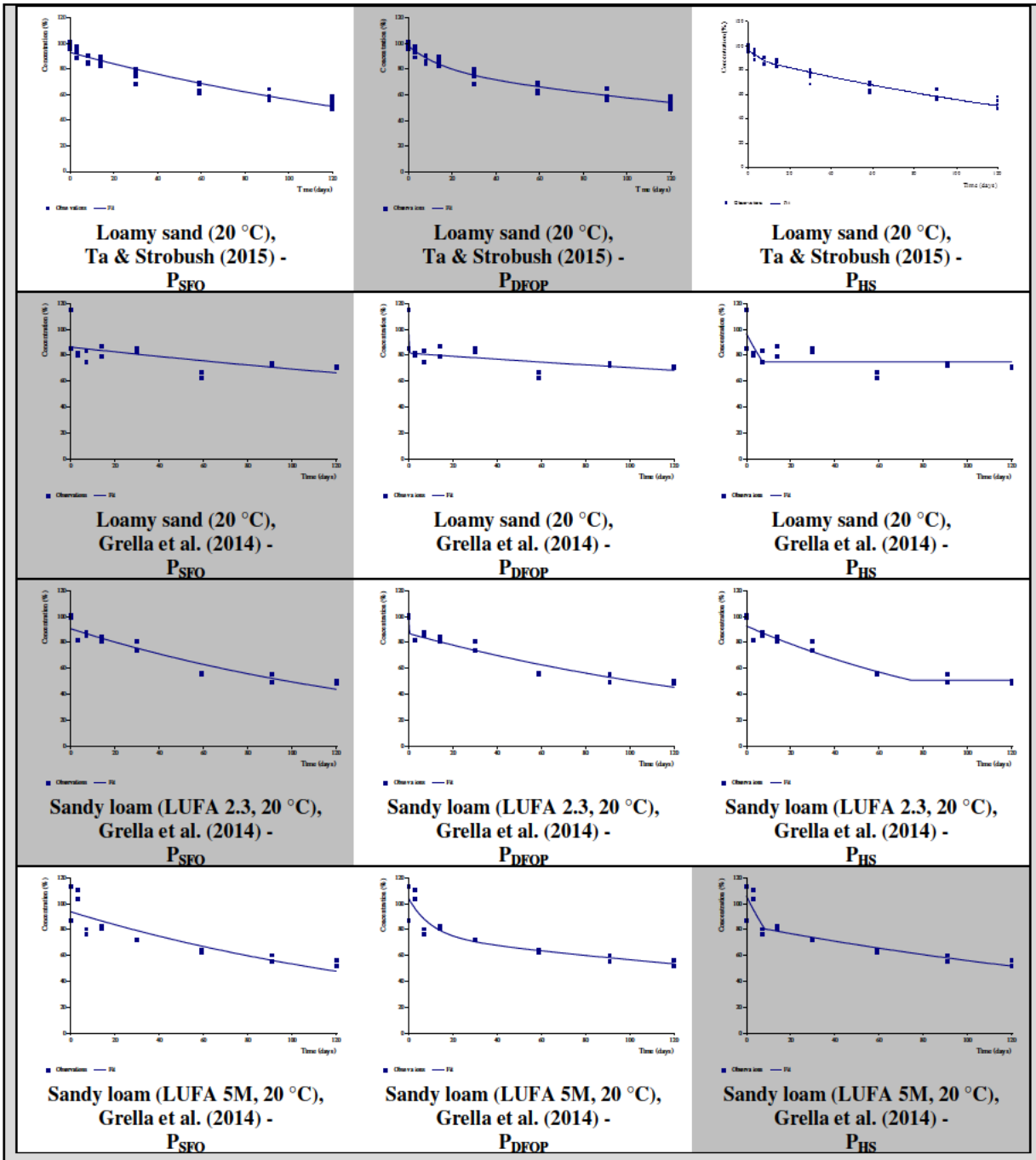
	tb	8.2	0.8	15.6	na

(a) On basis of slow phase (DFOP or HS) *DegT50*

Table B.8.1.2.1.1-9 Fits on trigger and modelling endpoints for triticonazole in laboratory soil degradation studies conducted at 20 - 25 °C - RMS AT assessment (all pathway fits, fits shaded in grey are considered most reliable)

 Sandy loam (22 °C), Ayliffe & Austin (1993) - P_{SFO}	 Sandy loam (22 °C), Ayliffe & Austin (1993) - P_{DFOP}	 Sandy loam (22 °C), Ayliffe & Austin (1993) - P_{HS}
 Clay loam (22 °C), Ayliffe & Austin (1993) - P_{SFO}	 Clay loam (22 °C), Ayliffe & Austin (1993) - P_{DFOP}	 Clay loam (22 °C), Ayliffe & Austin (1993) - P_{HS}
 Loamy sand (Speyer 2.2, 22 °C), Ayliffe & McMillan-Staff (1994) - P_{SFO}	 Loamy sand (Speyer 2.2, 22 °C), Ayliffe & McMillan-Staff (1994) - P_{DFOP}	 Loamy sand (Speyer 2.2, 22 °C), Ayliffe & McMillan-Staff (1994) - P_{HS}
 Loamy sand (UK, 22 °C), Ayliffe & Godward (1993) - P_{SFO}	 Loamy sand (UK, 22 °C), Ayliffe & Godward (1993) - P_{DFOP}	 Loamy sand (UK, 22 °C), Ayliffe & Godward (1993) - P_{HS}
 Clay (25 °C), Doble et al. (1996) -	 Clay (25 °C), Doble et al. (1996) -	 Clay (25 °C), Doble et al. (1996) -

P_{SFO}	P_{DFOP}	P_{HS}
		
Sandy loam (25 °C, standard), Simmonds et al. (1996) - P_{SFO}	Sandy loam (25 °C, standard), Simmonds et al. (1996) - P_{DFOP}	Sandy loam (25 °C, standard), Simmonds et al. (1996) - P_{HS}
		
Sandy loam (25 °C, red. rate), Simmonds et al. (1996) - P_{SFO}	Sandy loam (25 °C, red. rate), Simmonds et al. (1996) - P_{DFOP}	Sandy loam (25 °C, red. rate), Simmonds et al. (1996) - P_{HS}
		
Sand (20 °C), Ta & Strobush (2012) P_{SFO}	Sand (20 °C), Ta & Strobush (2012) P_{DFOP}	Sand (20 °C), Ta & Strobush (2012) P_{SHS}
		
Loam (20 °C), Ta & Strobush (2012) P_{SFO}	Loam (20 °C), Ta & Strobush (2012) P_{DFOP}	Loam (20 °C), Ta & Strobush (2012) P_{SHS}
		
Loamy sand (20 °C), Ta & Strobush (2012) P_{SFO}	Loamy sand (20 °C), Ta & Strobush (2012) P_{DFOP}	Loamy sand (20 °C), Ta & Strobush (2012) P_{SHS}



Loamy sand (20 °C), Ta & Strobush (2015) - P_{SFO}

Loamy sand (20 °C), Ta & Strobush (2015) - P_{DFOP}

Loamy sand (20 °C), Ta & Strobush (2015) - P_{HS}

Loamy sand (20 °C), Grella et al. (2014) - P_{SFO}

Loamy sand (20 °C), Grella et al. (2014) - P_{DFOP}

Loamy sand (20 °C), Grella et al. (2014) - P_{HS}

Sandy loam (LUFA 2.3, 20 °C), Grella et al. (2014) - P_{SFO}

Sandy loam (LUFA 2.3, 20 °C), Grella et al. (2014) - P_{DFOP}

Sandy loam (LUFA 2.3, 20 °C), Grella et al. (2014) - P_{HS}

Sandy loam (LUFA 5M, 20 °C), Grella et al. (2014) - P_{SFO}

Sandy loam (LUFA 5M, 20 °C), Grella et al. (2014) - P_{DFOP}

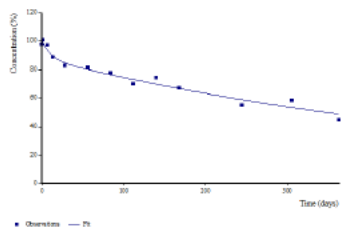
Sandy loam (LUFA 5M, 20 °C), Grella et al. (2014) - P_{HS}

Table B.8.1.2.1.1-10 **Trigger endpoints for triticonazole in laboratory soil degradation studies conducted at 10 °C or reduced moisture - RMS AT assessment (all pathway fits, fits shaded in grey are considered most reliable)**

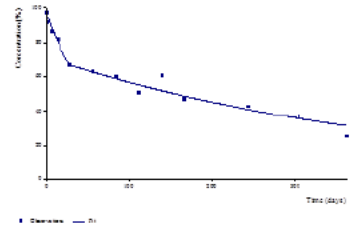
Study	Soil	T (°C)	Kinetic model	Para-meter	Value	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*Total DegT50* (d)	*DegT90* (d)
Ayliffe & Godward (1993)	Sandy loam	10	SFO	k	0.002	0.002	0.002	< 0.01	4.5	347	> 1000
			DFOP	**k1**	**0.090**	**-0.009**	**0.189**	**0.04**			
				k2	**0.002**	**0.001**	**0.002**	**< 0.01**	**3.5**	**341**	**> 1000**
				g	**0.13**	**0.06**	**0.20**	**na**			
			HS	k1	0.002	0.001	0.003	< 0.01			
				k2	0.002	0.000	0.004	0.01	4.7	353	> 1000
				tb	175.9	-604.4	956.1	na			
	Clay loam	10	SFO	k	0.004	0.003	0.005	< 0.01	9.3	187	622
			DFOP	k1	0.083	0.027	0.138	< 0.01			
				k2	0.002	0.002	0.003	< 0.01	5.3	170	866
				g	0.26	0.16	0.36	na			

			HS	**k1** **k2** **tb**	**0.013** **0.002** **26.7**	**0.007** **0.002** **14.6**	**0.019** **0.003** **38.8**	**< 0.01** **< 0.01** **na**	**5.0**	**176**	**892**
	Loamy sand (Speyer 2.2)	10	SFO	k	0.002	0.001	0.002	< 0.01	9.0	407	> 1000
			DFOP	k1 k2 g	0.069 < 0.001 0.22	0.034 < 0.001 0.16	0.103 0.001 0.28	< 0.01 < 0.01 na	3.0	> 1000	> 1000
			HS	**k1** **k2** **tb**	**0.011** **0.000** **22.7**	**0.007** **0.000** **15.6**	**0.015** **0.001** **29.8**	**< 0.01** **< 0.01** **na**	**2.6**	**> 1000**	**> 1000**
	Loamy sand (UK)	10	SFO	k	0.001	0.001	0.002	< 0.01	5.9	607	> 1000
			DFOP	k1 k2 g	0.060 0.001 0.17	-0.007 0.000 0.08	0.127 0.001 0.27	0.04 < 0.01 na	4.2	**865**	**> 1000**
			HS	**k1** **k2** **tb**	**0.007** **0.001** **29.3**	**0.003** **0.000** **13.7**	**0.011** **0.001** **44.9**	**< 0.01** **< 0.01** **na**	**3.9**	**862**	**> 1000**
Simmonds et al. (1996)	Sandy loam (red. temp.)	10	**SFO**	**k**	**0.0012**	**0.0008**	**0.0020**	**< 0.01**	**4.5**	**584**	**> 1000**
			DFOP	Not fitted as SFO is considered appropriate at all (see fit below)							
			HS	Not fitted as SFO is considered appropriate at all (see fit below)							
	Sandy loam (red. moist.)	25	SFO	k	0.003	0.003	0.004	< 0.01	11.1	224	745
			DFOP	**k1** **k2** **g**	**0.053** **0.001** **0.27**	**0.035** **0.001** **0.20**	**0.070** **0.002** **0.35**	**< 0.01** **< 0.01** **na**	**3.7**	**259**	**> 1000**
			HS	k1 k2 tb	0.010 0.002 33.2	0.007 0.001 26.4	0.013 0.002 40.0	< 0.01 < 0.01 na	4.0	261	> 1000

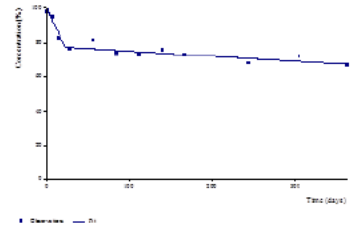
Table B.8.1.2.1.1-11 Fits on trigger endpoints for triticonazole - laboratory studies conducted at 10 °C or reduced moisture - RMS AT assessment (only fits considered most reliable are shown)



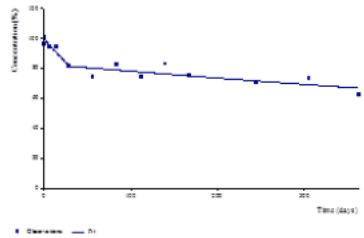
Sandy loam (10 °C), Ayliffe & Godward (1993) - P_{DFOP}



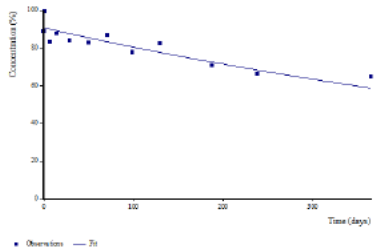
Clay loam (10 °C), Ayliffe & Godward (1993) - P_{HS}



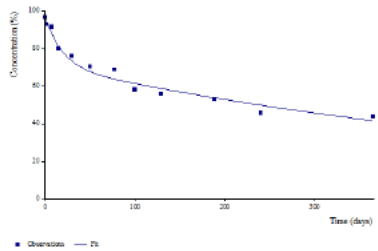
Loamy sand (Speyer 2.2, 10 °C), Ayliffe & Godward (1993) - P_{HS}



Loamy sand (10 °C), Ayliffe & Godward (1993) - P_{HS}



Sandy loam (10 °C), Simmonds et al. (1996) - P_{SFO}



Sandy loam (25 °C, red. moist.), Simmonds et al. (1996) - P_{DFOP}

B.8.1.2.1.2. Aerobic degradation of metabolites, breakdown and reaction products

Studies submitted for first Annex I inclusion:

Parent applied:

- **Ayliffe & Austin (1993)**, investigating phenyl labelled triticonazole in three soils at 22 °C
- **Ayliffe & McMillan-Staff (1994)**, investigating phenyl labelled triticonazole in one soil at 22 °C
- **Ayliffe & Godward (1993)**, investigating phenyl labelled triticonazole in three soils at 10 °C and in one soil at 10 and 22 °C
- **Doble et al. (1996)**, investigating triazole labelled triticonazole in one soil at 25 °C
- **Simmonds et al. (1996)**, investigating phenyl labelled triticonazole in one soil at contrasting incubation conditions

Metabolite applied:

- **McGhee (2000)**, investigating phenyl labelled RPA 406341 (Trans-diol) in three soils at 20 °C
- **Crowe (2002)**, investigating phenyl labelled RPA 404766 (Cis-diol) in three soils at 20 °C
- **Unsworth and Clarke (2000)**, investigating triazole labelled RPA 407922 in three soils at 20 °C

New studies submitted (parent applied):

- **Ta & Strobush (2012)**, investigating phenyl and triazole labelled triticonazole in three US soils at 20 °C
- **Ta & Strobush (2015)**, investigating phenyl and triazole labelled triticonazole in one soil at 20 °C

Parent studies on route and rate (Ayliffe & Austin, 1993; Ayliffe & McMillan-Staff, 1994; Ayliffe & Godward, 1993; Doble et al., 1996; Simmonds et al., 1996; and Ta & Strobush, 2015) have already been discussed in section B.8.1.1.1 (refer to route of degradation in soil).

New kinetic assessment studies submitted:

- **Jarvis & Montesano (2014a)**, investigating modelling endpoints of RPA 406341 (Trans-diol), RPA 404766 (Cis-diol) and RPA 407922 in Ayliffe & Austin (1993), Ayliffe & McMillan-Staff (1994), Ayliffe & Godward (1993), Doble et al. (1996), Simmonds et al. (1996), McGhee (2000), Crowe (2002) and Unsworth & Clarke (2000)
- **Szegedi (2016)**, investigating trigger and modelling endpoints of RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) in one single soil (10 °C) in Ayliffe & Godward (1993)
- **Donaldson (2015)**, investigating modelling endpoints of RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) in Ta & Strobush (2015)
- **Kreschnak (2015)**, summarizing all modelling and trigger endpoints of RPA 406341 (Trans-diol), RPA 404766 (Cis-diol) and RPA 407922
- **Szegedi (2018)**, investigating modelling endpoints for the metabolite fractions 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' observed > 5 % AR at two consecutive sampling points in Ayliffe & Austin (1993)

Notice that kinetic evaluation studies submitted for first Annex I inclusion are considered to be superseded by the new submission.

Reference:	**^{14}C-RPA 406341: Rate of degradation in three soils at 20 °C**
Author(s), year:	McGhee, I., 2000
Report/Doc. Number:	CO10570, GOoD16713, 202643, 16713
Guideline(s):	SETAC (1995), BBA IV, 5.1
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

This study investigated the rate of aerobic degradation of [phenyl-U-^{14}C]-RPA 406341 (Trans-diol) in three soils in the dark at 20 ± 1 °C over a period of 120 days. Soils were treated with a nominal application rate of 200 g/ha. The treatment solution was applied over the soil surface to ensure an even distribution. The specific moisture content of the soil samples was adjusted to 45 % of their maximum water holding capacity.

Single flasks for all soils treated with ^{14}C-RPA 406341 (Trans-diol) were analysed at each sampling date by cold solvent extraction with pure acetonitrile followed by an acetonitrile/water mixture (1/1, v:v). If less than 90 % of AR was extracted using cold solvent extraction then the soil was refluxed with acetonitrile/water (80:20) for 3 or 4 hours.

Extracts for each soil sample were concentrated and analysed by reverse-phase HPLC. Confirmatory TLC was carried out on representative soil extract concentrates. No mass spectroscopy was applied. Reference substances used: None.

Table B.8.1.2.1.2-1 Soil Characteristics

Soil (USDA)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/ 100 g)	Biomass (start) µg C/g soil	Biomass (end) µg C/g soil
Clay loam	25.3	47.1	27.6	4.7	7.0	127	1284	890
Sandy loam	79.3	11.0	9.7	1.8	5.3	10.6	259	213
Loam	33.0	44.0	23.0	1.9	6.2	16.4	333	343

Findings:

The overall mean total radioactivity recoveries were 97.7 %, 96.8 % and 99.5 % for clay loam, sandy loam and clay loam soils, respectively.

Table B.8.1.2.1.2-2 Distribution of radioactivity (% AR)

DAT	Extractable	Bound	Volatiles (CO_2)	Total	RPA 406341 (Trans-diol) (applied)
		Clay loam			
0	100.9	0.2	na	101.1	100.9
1	98.6	0.5	0.0	99.1	98.6
3	97.8	1.1	0.1	99.0	97.8
7	97.5	1.8	0.4	99.7	97.5
14	93.6	3.4	0.7	97.7	93.6
30	93.5	7.6	2.6	103.6	93.5
59	77.1	11.4	2.0	90.4	74.8
120	65.0	21.7	4.3	91.0	61.1
		Sandy loam			
0	99.4	1.8	na	103.1	99.4
1	96.3	3.0	0.0	99.3	96.3
3	95.1	4.2	0.0	99.3	95.1
7	90.5	6.0	0.1	96.6	90.5
14	90.2	7.0	0.6	97.7	90.2
30	92.0	4.7	0.9	97.6	92.0
59	81.7	7.0	2.3	91.0	79.1
120	66.5	20.7	2.9	90.0	62.6
		Loam			
0	95.7	6.2	na	102.0	95.7
1	95.6	5.7	0.0	101.4	95.6
3	90.6	8.7	0.0	99.4	90.6
7	95.7	9.9	0.1	105.7	95.7
14	101.3	2.6	0.5	104.4	101.3
30	88.8	4.8	0.9	94.5	88.8
59	91.4	6.5	1.0	99.0	91.4
120	75.2	12.2	2.6	90.0	72.8

There were no metabolites of RPA 406341 (Trans-diol) observed in extracts from day 0, 1, 3, 7, 14 and 30 soil extracts. A single unknown metabolite was observed on day 59 in the clay loam and sandy loam soil and on day 120 in the loam soil. This metabolite did not exceed 4 % AR.

Conclusion:

RPA 406341 (Trans-diol), one main soil metabolite of the active ingredient triticonazole, can be classified as persistent in soil. Only one metabolite was found which amounted for less than 4 % AR.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some minor deviations:
  - With an application rate of 200 g/ha the study is clearly overdosed (intended use rate of triticonazole is 12.5 g/ha)
  - The organic carbon content of the clay loam (4.7 %) is not in line with the range of 0.5 - 2.5 % recommended
  - No information is given on the field history
  - Only single values were analysed (no replicates)
  - No information is given on the MWHC of the soils. For normalisation of the degradation rate to reference the FOCUS default MWHC is used instead.

  On overall the study is still considered reliable.

- The study was kinetically re-assessed by Jarvis & Montesano (2014a).

Reference:	**^{14}C-RPA 404766: Aerobic soil rate of degradation**
Author(s), year:	Crowe, A., 2002
Report/Doc. Number:	C021045, AES 065/022530
Guideline(s):	SETAC (1995), BBA IV, 5.1
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

This study investigated the rate of aerobic degradation of [phenyl-U-^{14}C]-RPA 404766 (Cis-diol) in three UK soils at 20 ± 2 °C over a period of 120 days. Soils were treated with a nominal application rate of 200 g/ha. The moisture content of the soils was adjusted to between *p*F2 and *p*F2.5. Treated soil samples were incubated in the dark under a controlled stream of moist carbon dioxide-free air. The air leaving the chambers was passed through two traps, each containing 2M aqueous potassium hydroxide, to trap liberated volatile material. On day 24 a third 2M potassium hydroxide trap was added to the chamber containing the silty clay loam soil as the level of radioactivity in the second 2M potassium hydroxide trap was increasing. Single samples for each soil type were removed for analysis after specific time periods.

Extractions were done with acetonitrile and acetonitrile/water (1:1, v/v) and, where less than 90 % AR was extracted at ambient temperature, the soil samples were Soxhlet extracted. Analyses were carried out with HPLC and for selected samples with LC-MS for confirmation. Reference substances used: RPA 406341 (Trans-diol), RPA 407922, triticonazole.

Table B.8.1.2.1.2-3 Soil Characteristics

Soil	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	WHC at *p*F2 (%)	CEC (meq/ 100 g)	Biomass (start) µg C/g soil	Biomass (end) µg C/g soil
Sandy loam	76.9	10.9	12.2	1.2	4.5	17.5	12.0	237	124
Silty clay loam	19.2	49.3	31.5	2.1	7.2	39.5	18.4	1112	847
Clay loam	26.5	50.6	22.9	2.6	6.9	33.0	21.0	995	647

Findings:

Overall recoveries of radioactivity from the soil samples were in the range 85.3 to 98.9 % of applied radioactivity. RPA 404766 (Cis-diol) was metabolised to RPA 406341 (Trans-diol), RPA 407922, triticonazole (the latter < 1 % AR) and six unidentified metabolites. RPA 406341 (Trans-diol) was present at levels up to 20.1 % AR. RPA 407922 was present at levels up to 23.9 % AR. Two of the unidentified metabolites were present at levels greater than 10 % AR each. All other metabolites did not exceed 2.8 % AR each.

Table B.8.1.2.1.2-4 Distribution of radioactivity (% AR)

DAT	Bound resi-dues	CO_2	RPA 404766 (Cis-diol) (applied) R_t ~ 21 min	RPA 406341 (Trans-diol) R_t ~ 23.5 min	RPA 407922 R_t ~ 34.5 min	Unknown R_t ~ 23 min	Unknown R_t ~ 25 min	Unknown R_t ~ 26 min	Total
Sandy loam									
0	0.7	na	98.2	nd	nd	nd	nd	nd	98.9
1	0.7	0.2	90.1	0.5	nd	nd	nd	nd	91.5
3	3.9	0.5	74.2	2.0	nd	2.6	nd	nd	85.3
7	2.3	0.7	78.9	4.4	nd	3.2	nd	nd	92.2
14	3.8	1.1	59.3	3.8	4.5	10.0	4.1	nd	90.2
30	8.1	2.5	50.3	20.1	nd	3.4	nd	2.8	91.5
59	11.3	6.5	24.6	14.1	nd	12.7	11.8	1.5	87.9
120	20.9	19.9	6.9	6.0	13.4	5.8	3.5	0.7	83.8
Silty clay loam									
0	0.9	na	95.2	nd	nd	nd	nd	nd	97.3
1	4.1	0.1	81.3	2.5	nd	2.8	nd	nd	90.8
3	3.1	0.2	69.6	8.1	nd	3.8	nd	0.8	87.3
7	6.0	0.9	63.9	11.1	nd	7.3	nd	2.6	93.8
14	5.0	1.6	32.1	7.3	5.6	19.9	nd	12.6	86.5
30	14.7	2.8	37.8	11.8	nd	8.2	nd	10.5	93.6
59	22.8	6.5	23.0	5.0	20.3	3.9	nd	3.6	90.9
120	30.1	16.0	9.8	2.7	20.4	1.5	nd	nd	84.5
Clay loam									
0	0.7	na	98.0	nd	nd	nd	nd	nd	98.7
1	2.4	0.3	73.1	1.8	nd	1.9	nd	nd	85.8
3	3.5	0.7	74.9	6.8	nd	2.2	nd	0.3	90.2
7	4.4	1.1	66.6	11.6	nd	3.3	nd	2.4	92.5
14	6.3	1.8	48.5	15.8	nd	8.9	nd	7.2	95.0
30	10.8	2.9	45.5	15.2	nd	7.3	nd	11.5	95.9
59	10.5	5.1	42.0	4.5	10.1	1.3	12.0	0.7	90.1
120	17.2	13.8	15.5	6.5	23.9	3.5	4.2	0.4	89.4

nd denotes not detected

Conclusion:

Under laboratory conditions (20 ± 2 °C) soil metabolite RPA 404766 (Cis-diol) metabolised to RPA 406341 (Trans-diol), RPA 407922, triticonazole (< 1 % AR) and six unidentified products.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some minor deviations:
  - With an application rate of 200 g/ha the study is clearly overdoses (intended use rate of triticonazole is 12.5 g/ha)
  - Only single values were analysed (no replicates)

- In a few cases mass total recovery was < 90 % AR

On overall the study is still considered reliable.

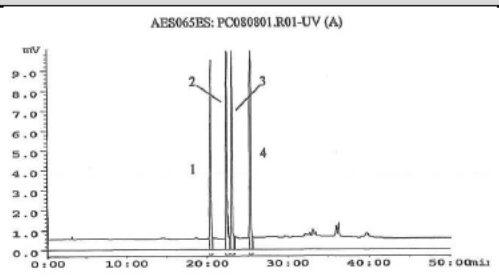
- This study clearly indicates that RPA 404766 (Cis-diol) is indeed much less stable in soil than its isomeric sibling RPA 406341 (Trans-diol) (compared with results obtained in previous study, McGhee, 2000). Obviously, the cis-location of the two hydroxy groups in RPA 404766 (Cis-diol) is less stable than the trans-location in RPA 406341 (Trans-diol). The report even indicates that there is a pronounced transformation from RPA 404766 (Cis-diol) to RPA 406341 (Trans-diol), as RPA 406341 (Trans-diol) was claimed to be found up to 20.1 % AR in this study. Vice versa, RPA 404766 (Cis-diol) was not found in McGhee (2000) dosing RPA 406341 (Trans-diol), thus there is clearly no back-transformation from the trans- to the cis-metabolite.

  The RMS AT challenges the gradient HPLC method used in this study being adequate for metabolites profiling as the elution time from RPA 404766 (Cis-diol) (being the first) to triticonazole (being the last) was only approx. 5 minutes. In consequence, HPLC peaks observed in this study are not well resolved and appear to be smeared (see example chromatograms below). In other studies (e.g. Doble et al., 1996; Simmonds et al., 1996), applying more advanced gradient HPLC methods for metabolite profiling, the time of HPLC elution from RPA 404766 (Cis-diol) to triticonazole covers at least 25 minutes (up to 50 min depending on the HPLC method) with several well resolved peaks within. Nevertheless, the study author claims having identified RPA 406341 (Trans-diol) and RPA 407922 based on mass spectroscopic work and HPLC retention time. In view of the numerous possible degradation products (mono-, di-hydroxylated and oxidised degradates) already observed in parent degradation studies with identical mol masses in several cases, the RMS AT considers identification of RPA 406341 (Trans-diol) and RPA 408922 in this study highly uncertain.

  On overall, the RMS AT is of the opinion that this study does not allow to unambiguously conclude that there is significant transformation from RPA 404766 (Cis-diol) to its isomeric sibling RPA 406341 (Trans-diol) or to RPA 407922, the latter never found in more recent soil degradation studies. For that reason, the RMS AT also does not recommend to kinetically assess residues claimed being RPA 406341 (Trans-diol) in this study.

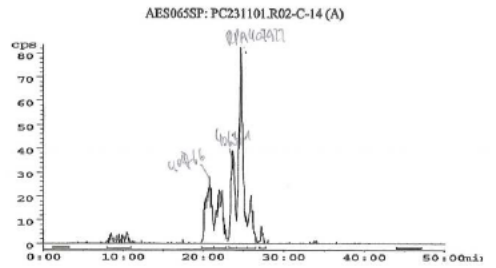
Table B.8.1.2.1.2-5 Example chromatograms of reference compounds and of a soil extract (sandy loam, 120 DAT)

Standard mix (UV) - page 43



Number	Name	RT
1	RPA 404766	20'19
2	RPA 406341	22'19
3	RPA 407922	22'59
4	Triticonazole	25'14

Soil extract (sandy loam, 120 DAT), ^{14}C - page 46



Name	RT	%ROI
Unknown	8'27	3.7
RPA 404766	20'46	18.2
Unknown	21'54	15.5
RPA 406341	23'34	15.9
RPA 407922	24'30	35.6
Unknown	25'51	9.3
Unknown	27'07	1.8

- The study was kinetically re-assessed (RPA 404766 (Cis-diol) only) by Jarvis & Montesano (2014a).

Reference:	**[^{14}C]-RPA 407922: Rate of degradation in three soils at 20 °C**
Author(s), year:	Unsworth, R.H., Clarke, D.E., 2000
Report/Doc. Number:	R012054, GOoD202590
Guideline(s):	SETAC (1995), BBA IV, 5.1
GLP:	Yes
Validity:	Not essential (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

This study investigated the rate of aerobic degradation of [triazole-3(5)-^{14}C]-RPA 407922 in three soils in the dark at 20 ± 1 °C over a period of 100 days. Soils were treated with a nominal application rate of 200 g/ha. The treatment solution was applied over the soil surface to ensure an even distribution. The specific moisture content of the soil samples was adjusted to 45 % of their maximum water holding capacity.

Single flasks for all soils treated with ^{14}C-RPA 407922 were analysed at each sampling date by solvent extraction. Early test point samples were extracted with methanol, methanol/water and Soxhlet acetonitrile/water whereas later time point samples were extracted with acetonitrile and Soxhlet extraction acetonitrile/water. Further, for the day 3 soil residues the amount of unextracted material available to the soil solution was determined by shaking with 0.01 M calcium chloride solution. The dry soil residues for each of the three soil types from the 3 day sampling interval were processed to determine the distribution of unextracted radioactivity between humin, humic and fulvic acid components of the soil.

Analyses were carried out with gradient HPLC, TLC (for confirmation), and structural confirmation of RPA 407922 by LC-MS/MS. Reference substances used: triticonazole.

Table B.8.1.2.1.2-6 Soil Characteristics

Soil (USDA)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/100 g)	MWHC (%)	WHC at 33 kPa (%)	Biomass (start) µg C/g soil	Biomass (end)[(b)] µg C/g soil
Clay loam	18.3	45.8	36.0	4.1	7.4	52.0	105.9	33.7	1030	805 / 674
Clay loam	27.7	45.1	27.1	2.3	7.3	22.3	68.4	24.2	327	201 / 234
Loamy sand	78.5	12.1	9.4	1.3	6.2	6.3	44.3	10.6	178	154 / 178

(a) Silty clay according to ADAS classification
(b) After 100 / 189 days (additional samples)

Findings:

The overall mean total radioactivity recoveries were 97.8, 96.7 and 98.3 % for clay loam (*p*H 7.4), clay loam (*p*H 7.3) and sandy loam soils, respectively.

Extractable radioactivity is expressed as the sum of the different extraction steps (cold extractions plus Soxhlet extraction). The samples extracted at day 56 and day 100 were not analysed chromatographically due to the low levels of RPA 407922 in the 28 day soil extracts (0.4 - 2.3 % AR).

Table B.8.1.2.1.2-7 Distribution of radioactivity (% AR)

DAT	Extractable	Bound	Volatiles (CO_2)	Total	RPA 407922 (applied)	Unknown 1 (rRT ~ 0.1)	Triticonazole (rRT ~ 1.1)
Clay loam (*p*H 7.4)							
0	96.2	5.5	na	101.6	95.8	0.4	nd
1 hr[(a)]	85.3	11.0	0.0	96.4	85.3	nd	nd
3.8 hrs[(a)]	71.8	24.9	0.0	96.7	71.8	nd	nd
12 hrs[(a)]	46.0	49.5	0.0	95.5	43.4	0.7	0.9
1	27.2	70.9	0.1	98.3	18.8	5.2	1.6
3	17.3	85.0	0.3	102.6	3.4	6.6	2.4
7	17.0	77.8	0.7	95.5	2.5	9.0	1.7
14	15.7	81.8	0.9	98.5	1.2	12.4	2.1
28[(a)]	15.7	75.7	0.9	92.3	0.4	12.8	2.6
56	15.5	78.8	2.8	97.1	-[(b)]	-[(b)]	-[(b)]
100	16.8	80.9	3.9	101.5	-[(b)]	-[(b)]	-[(b)]
Clay loam (*p*H 7.3)							
0	99.8	1.4	na	101.2	99.6	0.1	nd
3 hr[(a)]	84.5	11.9	0.0	96.4	84.5	nd	nd
6 hrs[(a)]	72.1	23.2	0.0	95.3	72.1	nd	nd
12 hrs[(a)]	57.0	36.9	0.0	94.0	54.5	nd	0.8
1	50.3	45.7	0.1	96.0	47.7	1.0	1.6
3	28.5	71.0	0.6	100.2	19.0	4.0	3.7
7	19.7	77.4	1.5	98.5	7.9	5.1	4.0
14[(a)]	16.8	78.5	0.1	95.2	3.8	5.7	4.0
28[(a)]	15.6	76.3	1.7	93.6	2.3	9.9	3.5
56	18.1	75.0	4.4	97.5	-[(b)]	-[(b)]	-[(b)]
100	17.4	71.3	7.2	95.9	-[(b)]	-[(b)]	-[(b)]
Loamy sand							
0	98.8	0.5	na	99.3	98.7	0.1	nd
3 hr[(a)]	92.3	8.4	0.0	100.7	92.3	nd	nd
6 hrs[(a)]	88.3	14.3	0.0	102.7	88.3	nd	nd
12 hrs[(a)]	76.1	22.9	0.0	99.0	75.8	0.4	nd
1	53.8	46.9	0.2	100.8	52.5	1.3	nd
3	28.0	67.5	0.4	95.9	15.4	8.4	nd
7	23.3	80.5	0.8	104.6	6.7	10.3	0.3
14[(a)]	25.6	67.5	2.0	95.0	5.3	10.5	2.2
28	18.1	75.5	2.7	96.3	1.8	15.4	1.0
56	18.4	72.6	3.3	94.3	-[(b)]	-[(b)]	-[(b)]
100	17.8	70.4	4.8	93.1	-[(b)]	-[(b)]	-[(b)]

(a) Additional sample treated subsequently to original samples
(b) No HPLC analysis carried out

In all three soil types RPA 407922 rapidly degraded to give one common major unknown metabolite and several minor unknown species (the latter not included in the table above). One of the minor metabolites was identified as triticonazole. Unextractable residues increased with time reaching maximum values after 100 days between 70.4 and 80.9 % AR. The major metabolite increased until the last sampling time for chromatographical analysis (day 28) up to 15.4 % AR. This metabolite was deduced to be more polar than RPA 407922 from its relative retention time. All the other unknown metabolites were found in amounts less than 5 % AR. After 100 days CO_2 production amounted for 3.8 - 7.2 % AR.

Table B.8.1.2.1.2-8 Determination of the distribution of unextracted residues between humin, humic acid and fulvic acid components (% AR)

Soil	Humin	Humic acid	Fulvic acid

Soil	Humin	Humic acid	Fulvic acid
Clay loam (*p*H 7.4)	52.4	15.9	16.7
Clay loam (*p*H 7.3)	38.0	16.5	16.5
Loamy sand	21.8	26.3	19.3

RPA 407922 degrades rapidly in all three soils. The faster degradation in one of the soils could be explained by its higher microbial biomass.

Conclusion:

One of the major soil metabolites of triticonazole, RPA 407922, degrades rapidly in soil. Degradation results in the formation of one major polar metabolite, which was deduced to be more polar than RPA 407922, high amounts of bound residues and several minor metabolites one of it being triticonazole. Except triticonazole the minor metabolites were transient resulting in the formation of CO_2.

Comments (RMS AT):

- The study broadly follows OECD guideline 307 with some minor limitations:
  - With an application rate of 200 g/ha the study is clearly overdoses (intended use rate of triticonazole is 12.5 g/ha)
  - The organic carbon content of the clay loam (4.1 %) is not in line with the range of 0.5 - 2.5 % recommended
  - No information is given on the field history
  - Only single values were analysed (no replicates)

  On overall the study is still considered reliable.

- As already indicated no degradation studies with RPA 407922 are triggered, as RPA 407922 could not be identified in soil degradation studies. **The study is therefore not considered essential**.

- The RMS AT notes that, in contrast to triticonazole and the metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol), degradation of RPA 407922 is strongly driven by distinct formation of non-extractable residues accounting for > 45 % AR already by 1 DAT (with only minor formation of CO_2).

- It is noted that the clay loam (*p*H 7.4) in this applicant summary was erroneously assigned being a silty clay.

- The study was kinetically re-assessed by Jarvis & Montesano (2014a).

Reference:	**Recalculation of Triticonazole laboratory soil degradation kinetics according to FOCUS (2006) guidance**
Author(s), year:	Jarvis, T., Montesano, V., 2014a
Report/Doc. Number:	2016/1171410
Guideline(s):	FOCUS (2006): Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration, SANCO/10058/2005, version 2.0, 434 pp.
GLP:	Not applicable (modelling study)
Validity:	None reliable (refer to comment section)
Status:	**New submission**

DT50 values for the metabolites were obtained from the studies in which the metabolites were applied. Formation fractions for the metabolites were derived from the evaluation of pathway fits using the data from the parent degradation studies. The metabolite *DT50* values obtained from the pathway evaluations were subject to considerable error (χ^2 error values typically >> 15 %) and so were not considered further. However, the formation fractions were considered acceptable for regulatory use. Results are presented in the tables below.

Table B.8.1.2.1.2-9 Metabolites of triticonazole: aerobic soil degradation modelling endpoints

Study	Soil	Incubation conditions Temp. (°C)	Moisture	Kinetic Model	*DT50* study cond. (d)	*DT90* study cond. (d)	*DT50* at 20 °C, *p*F2 (d)
			RPA 406341 (Trans-diol)				
McGhee (2000)	Clay loam	20	45 % MWHC	SFO	165.2	548.8	102.4
	Sandy loam	20	45 % MWHC	SFO	198.9	660.9	143.2
	Loam	20	45 % MWHC	SFO	345.9	> 1000	231.8
			RPA 404766 (Cis-diol)				
Crowe (2002)	Sandy loam	20	*p*F2 - 2.5	SFO	30.9	102.8	30.9
	Silty clay loam	20	*p*F2 - 2.5	DFOP	60.8[b]	137.9	60.8
	Clay loam	20	*p*F2 - 2.5	DFOP	58.7[b]	166.2	58.7
			RPA 407922				
Unsworth & Clarke (2000)	Clay loam (*p*H 7.4)	20	45 % MWHC	SFO	0.44	1.5	0.44
	Clay loam (*p*H 7.3)	20	45 % MWHC	FOMC	2.0[a]	6.6	2.0
	Loamy sand	20	45 % MWHC	SFO	1.1	3.8	1.1

(a) Calculated as follows: *DT90* / 3.32
(b) Calculated using the slow degradation rate: ln(2) / k_2

Table B.8.1.2.1.2-10 Metabolites of Triticonazole: Formation fractions from pathway fits

Study	Soil	Formation fraction from parent RPA 406341 (Trans-diol)	RPA 407922	RPA 404766 (Cis-diol)
Ayliffe & Godward (1993)	Loamy sand	0.688	-[a]	0.312
	Sandy loam	0.404	-[a]	0.253
	Clay loam	0.526	-[a]	0.474
	Loamy sand	0.576	-[a]	0.424
Ayliffe & McMillan-Staff (1994)	Loamy sand	0.512	-[b]	0.488
Ayliffe & Austin (1993)	Sandy loam	0.760	0.040	0.200
	Clay loam	0.343	0.136	0.521
Doble et al. (1996)	Clay	0.581	nd	0.419
Simmonds et al. (1996)	Sandy loam (standard)	0.563	nd	0.437
	Sandy loam (reduced rate)	0.598	nd	0.402
	Sandy loam	0.529	nd	0.471
	Sandy loam	0.655	nd	0.345

(a) Not evaluable (e.g. due to data scattering, insufficient amount of data points).
(b) Formation fraction not reliable.
nd = not determined (metabolite was not detected in these soils).

Comments (RMS AT):

- The **study is not considered reliable** for several reasons. A complete RMS AT synopsis on metabolite laboratory degradation rates including a full kinetic reassessment of all soil degradation studies is given in Kreschnak (2015) in chapter B.8.1.2.1.2 (aerobic degradation of metabolites, breakdown and reaction products).

Reference:	**Kinetic evaluation of laboratory soil degradation of triticonazole (BAS 595 F) and its metabolites RPA 406341 and RPA 404766 in a single soil for derivation of trigger and modelling endpoints according to FOCUS**
Author(s), year:	Szegedi, K., 2016
Report/Doc. Number:	2016/1171410
Guideline(s):	FOCUS (2006): Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration, SANCO/10058/2005, version 2.0, 434 pp.
GLP:	Not applicable (modelling study)
Validity:	Yes
Status:	**New submission**

Material and methods:

The purpose of this evaluation was to analyse the degradation kinetics observed in Speyer 2.2 loamy sand, incubated at 10 °C in Ayliffe & Godward (1993). Kinetic evaluation was performed in order to derive:

- Degradation parameters as triggers for additional work (best-fit endpoints)
- Degradation parameters for environmental fate models (modelling endpoints)

For the test substance triticonazole, the appropriate kinetic model for deriving trigger and modelling endpoints was identified considering the procedures and kinetic models proposed by the FOCUS workgroup on degradation kinetics (FOCUS, 2006). The most appropriate model was selected based on visual and statistical assessment and the corresponding *DegT50* and *DegT90* values are reported as trigger endpoints. Appropriate *DegT50* values for use in environmental fate models were derived depending on the kinetic model.

The first kinetic evaluation was performed considering the parent compound only. The second kinetic evaluation was performed considering the parent compound and its metabolites.

Results and discussion:

Outcome of the kinetic evaluation considering triticonazole and its metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) is presented below. Although the overall fits are acceptable, due to the outcome of the t-test, it cannot be shown that the degradation rates derived for the metabolites are significantly different from 0.

Table B.8.1.2.1.2-11 Estimated parameters and statistics for triticonazole – parameters estimated for the parent compound and its metabolites in Speyer 2.2 loamy sand (10 °C) (parent DFOP, metabolites SFO)

Compound	Estimated Parameter	p (t-test)	χ^2 error [%]	Visual fit	*DegT50* [d]	*DegT90* [d]
Triticonazole	$M_0 = 99.94$ $k_1 = 6.901 \cdot 10^{-2}$ $k_2 = 3.658 \cdot 10^{-4}$ $g = 0.2236$	$< 2 \cdot 10^{-16}$ $8.93 \cdot 10^{-5}$ $7.36 \cdot 10^{-3}$ $2.59 \cdot 10^{-9}$	2.955	Good	> 1000	> 1000
RPA404766 (Cis-diol)	$k = 3.536 \cdot 10^{-5}$ ff = 0.2845	0.4794 0.0458	14.674	Good	> 1000	> 1000
RPA406341 (Trans-diol)	$k = 4.077 \cdot 10^{-4}$ ff = 0.3116	0.294 0.0684	16.036	Good	> 1000	> 1000

Comments (RMS AT):

- A complete RMS AT synopsis on metabolite laboratory degradation rates including a full kinetic reassessment of all soil degradation studies is given in Kreschnak (2015) in chapter B.8.1.2.1.2 (aerobic degradation of metabolites, breakdown and reaction products).

Reference:	**Kinetic evaluation of the aerobic soil metabolism of BAS 595 F (triticonazole) in a loamy sand soil**
Author(s), year:	Donaldson F., 2015
Report/Doc. Number:	2015/7001309
Guideline(s):	FOCUS (2006): Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration, SANCO/10058/2005, version 2.0, 434 pp.
GLP:	Not applicable (modelling study)
Validity:	None reliable (refer to comment section)
Status:	**New submission**

DegT50 values and formation fractions were derived for the metabolites RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) from a study in which the parent triticonazole was applied (Ta & Strobush, 2015). Results are presented below.

Table B.8.1.2.1.2-12 RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol): Aerobic soil degradation modelling endpoints

Compound	Soil	Incubation conditions Temp. (°C)	Moisture	Kinetic Model	*DegT50* at study cond. (d)	*DegT50* at 20 °C, *p*F2 (d)	*ff*
RPA 404766 (Cis-diol)	Loamy sand	20	50 % MWHC	SFO[(a)]	23.6	20.1	0.576
RPA 406341 (Trans-diol)				SFO[(a)]	35.7	30.3	0.386

(a) Pathway fit with parent (= SFO)

Comments (RMS AT):

- The **study is not considered reliable** for several reasons. A complete RMS AT synopsis on metabolite laboratory degradation rates including a full kinetic reassessment of all soil degradation studies is given in Kreschnak (2015) in chapter B.8.1.2.1.2 (aerobic degradation of metabolites, breakdown and reaction products).

Reference:	**Summary of kinetic endpoints for triticonazole and its metabolites from laboratory soil degradation studies**
Author(s), year:	Kreschnak, C., 2015
Report/Doc. Number:	2015/1186987
Guideline(s):	None
GLP:	Not applicable (modelling study)
Validity:	None reliable (refer to comment section)
Status:	**New submission**

The rate of degradation of triticonazole and its metabolites in aerobic laboratory soils was investigated in several studies. The kinetic evaluation of these studies was conducted either directly in the study reports or in separate kinetic reports. In some cases, not all kinetic endpoints were explicitly reported although the necessary data is included in the reports. This statement aims to summarise all kinetic endpoints of triticonazole and its metabolites that were provided in the study reports or in the kinetic reports. The relevant results of this summary are presented in the following tables.

Table B.8.1.2.1.2-13 Overview of the laboratory aerobic degradation rates – major soil metabolite RPA 404766 (Cis-diol)

Reference	Soil characteristics				Incubation conditions		Trigger Endpoints			Modelling Endpoints			
	Soil origin	Soil type	*p*H ($CaCl_2$)	OC[c] (%)	Moisture	Temp. (°C)	Kinetic Model	*DT50* (d)	*DT90* (d)	Kinetic Model	*DT50* (d) study cond.	*DT50* (d) at 20 °C and *p*F2	ff[d]
Ayliffe & Austin (1993)	Not reported	Sandy loam	6.42[b]	0.72	75 % of 33 kPa	22	Degradation rates from pathway fits are not reliable			Degradation rates from pathway fits are not reliable			0.200
	Not reported	Clay loam	6.18[b]	5.66		22							0.521
Ayliffe & Godward (1993)	Not reported	Loamy sand	6.24[b]	18.70	75 % of 33 kPa	22							0.312[e]
	Not reported	Sandy loam	6.30[b]	0.83		10							0.253
	Not reported	Clay loam	6.08[b]	3.28		10							0.474
	Not reported	Loamy sand	6.24[b]	18.70		10							0.424[e]
Ayliffe & McMillan-Staff (1994)	Speyer 2.2	Loamy sand	6.8[b]	2.35	75 % of 33 kPa	22							0.488
Doble et al. (1996)	Not reported	Clay[a]	6.5	1.2	75 % of 33 kPa	25							0.419
Simmonds et al. (1996)	Manningtree (standard)	Sandy loam[a]	6.1	0.8	50 % FC	25							0.437[e]
	Manningtree (reduced rate)				50 % FC	25							0.402[e]
	Manningtree				20 % FC	25							0.471[e]
	Manningtree				50 % FC	10							0.345[e]
Crowe (2002)	Baylham	Sandy loam	4.5	1.2	*p*F2 - 2.5	20	SFO	30.9	102.8	SFO	30.9	30.9	na
	Royston	Silty clay loam	7.2	2.1		20	DFOP	11.0	137.9	DFOP	60.8	60.8	na
	Ongar	Clay loam	6.9	2.6		20	DFOP	30.2	166.2	DFOP	58.7	58.7	na
Ta & Strobush (2015)	Li10	Loamy Sand[a]	6.3	0.81	50 % MWHC	20	DFOP-SFO	-[f]		SFO-SFO	23.6	20.1	0.576
								Geometric mean:				**38.6**	
								Arithmetic mean:					**0.413**

(a) Soil type according to USDA, for the other soils the classification is unknown
(b) Buffer solution unknown
(c) If not explicitly mentioned in the study report, OC was calculated: OC (%) = OM (%) / 1.724
(d) *ff* is the formation fraction from parent triticonazole
(e) The arithmetic mean value determined from single values for the same soil (values in italic) was used for the calculation of the overall arithmetic mean value
(f) The derived trigger *DT50* of 94.6 days is not considered reliable because no degradation of the metabolite was observed and the value differs distinctly from the values obtained from the metabolite study
na denotes not applicable since the metabolite was directly applied to soil

Table B.8.1.2.1.2-14 Overview of the laboratory aerobic degradation rates – major soil metabolite RPA 406341 (Trans-diol)

Reference	Soil characteristics				Incubation conditions		Trigger Endpoints			Modelling Endpoints			
	Soil origin	Soil type	*p*H ($CaCl_2$)	OC[c] (%)	Moisture	Temp. (°C)	Kinetic Model	*DT50* (d)	*DT90* (d)	Kinetic Model	*DT50* (d) study cond.	*DT50* (d) at 20 °C and *p*F2	ff[d]
Ayliffe & Austin (1993)	Not reported	Sandy loam	6.42[b]	0.72	75 % of 33 kPa	22							0.760
	Not reported	Clay loam	6.18[b]	5.66		22							0.343
Ayliffe & McMillan-Staff (1994)	Speyer 2.2	Loamy sand	6.8[b]	2.35	75 % of 33 kPa	22							0.512
Ayliffe & Godward (1993)	Not reported	Loamy sand	6.24[b]	18.70		22							0.688[e]
	Not reported	Sandy loam	6.30[b]	0.83	75 % of 33 kPa	10							0.404
	Not reported	Clay loam	6.08[b]	3.28		10							0.526
	Not reported	Loamy sand	6.24[b]	18.70		10							0.576[e]
Doble et al. (1996)	Not reported	Clay[a]	6.5	1.2	75 % of 33 kPa	25	Degradation rates from pathway fits are not significant			Degradation rates from pathway fits are not significant			0.581
Simmonds et al. (1996)	Manningtree (standard)	Sandy loam[a]	6.1	0.8	50 % FC	25							0.563[e]
	Manningtree (reduced rate)				50 % FC	25							0.598[e]
	Manningtree				20 % FC	25							0.529[e]
	Manningtree				50 % FC	10							0.655[e]
McGhee (2000)	Royston	Clay Loam[a]	7.0	1.2	45 % MWHC	20	SFO	165.2	548.8	SFO	165.2	102.4	na
	Ipswich	Sandy Loam[a]	5.3	2.1		20	SFO	198.9	660.9	SFO	198.9	143.2	na
	Ongar	Loam[a]	6.2	2.6		20	SFO	345.9	> 1000	SFO	345.9	231.7	na
Ta & Strobush (2015)	Li10	Loamy Sand[a]	6.3	0.81	50 % MWHC	20	DFOP-SFO	205	682	SFO -SFO	35.7	30.3	0.386
								Geometric mean:				**100.7**	
								Arithmetic mean:					**0.526**

(a) Soil type according to USDA, for the other soils the classification is unknown
(b) Buffer solution unknown
(c) If not explicitly mentioned in the study report, OC was calculated: OC (%) = OM (%) / 1.724
(d) *ff* is the formation fraction from parent triticonazole
(e) The arithmetic mean value determined from single values for the same soil (values in italic) was used for the calculation of the overall arithmetic mean value
na denotes not applicable since the metabolite was directly applied to soil

Table B.8.1.2.1.2-15 Overview of the laboratory aerobic degradation rates – major soil metabolite RPA 407922

Reference	Soil characteristics				Incubation conditions		Trigger Endpoints			Modelling Endpoints			
	Soil origin	Soil type	*p*H ($CaCl_2$)	OC[c] (%)	Moisture	Temp. (°C)	Kinetic Model	*DT50* (d)	*DT90* (d)	Kinetic Model	*DT50* (d) study cond.	*DT50* (d) at 20 °C and *p*F2	ff[d]
Ayliffe & Austin (1993)	Not reported	Sandy loam	6.42[b]	0.72	75 % of 33 kPa	22	Degradation rates from pathway fits are not significant			Degradation rates from pathway fits are not significant			0.040
	Not reported	Clay loam	6.18[b]	5.66		22							0.136
Ayliffe & McMillan-Staff (1994)	Speyer 2.2	Loamy sand	6.8[b]	2.35	75 % of 33 kPa	22							-[e]
Ayliffe & Godward (1993)	Not reported	Loamy sand	6.24[b]	18.70	75 % of 33 kPa	22							-[e]
	Not reported	Sandy loam	6.30[b]	0.83		10							-[e]
	Not reported	Clay loam	6.08[b]	3.28		10							-[e]
	Not reported	Loamy sand	6.24[b]	18.70		10							-[e]
Doble et al. (1996)	Not reported	Clay[a]	6.5	1.2	75 % of 33 kPa	25							nd
Simmonds et al. (1996)	Manningtree (standard)	Sandy loam[a]	6.1	0.8	50 % FC	25							nd
	Manningtree (reduced rate)				50 % FC	25							nd
	Manningtree				20 % FC	25							nd
	Manningtree				50 % FC	10							nd
Unsworth & Clark (2000)	Not reported	Clay loam[a]	7.4	4.1	45 % MWHC	20	SFO	0.44	1.5	SFO	0.44	0.44	na
	Not reported	Clay loam[a]	7.3	2.3		20	FOMC	0.7	6.6	FOMC	2.0	2.0	na
	Not reported	Loamy sand[a]	6.2	1.3		20	SFO	1.1	3.8	SFO	1.1	1.1	na
								Geometric mean:				**0.99**	
								Maximum:					**0.136**

(a) Soil type according to USDA, for the other soils the classification is unknown
(b) Buffer solution unknown
(c) If not explicitly mentioned in the study report, OC was calculated: OC (%) = OM (%) / 1.724
(d) *ff* is the formation fraction from parent triticonazole
(e) No reliable formation fraction available
na denotes not applicable since the metabolite was directly applied to soil
nd denotes not detected

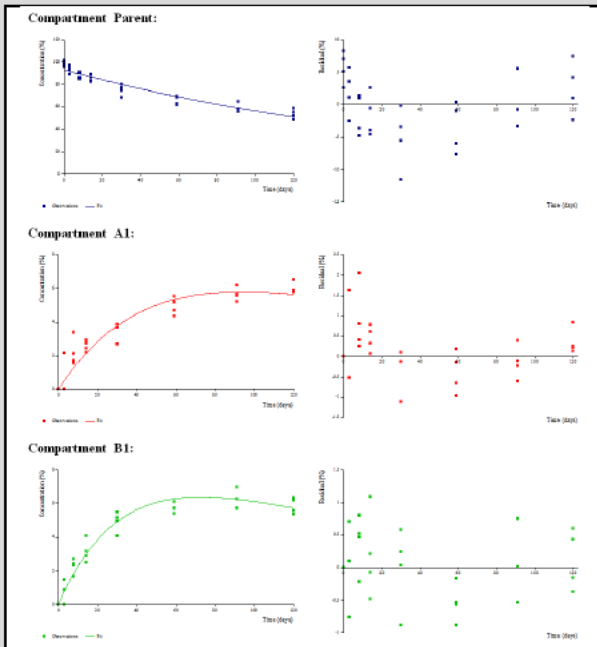
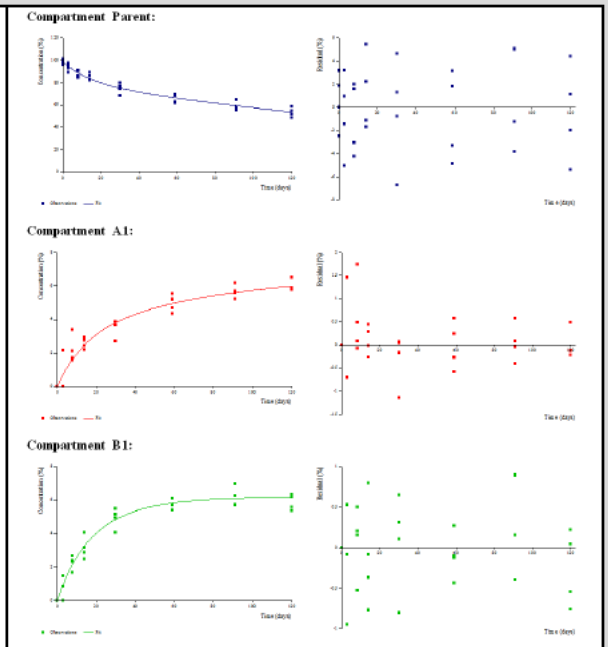
Comments (RMS AT):

- The RMS AT notes that the applicant considers all legacy studies conducted for one year inappropriate to obtain robust degradation rates for the two major soil metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol). However, formation fractions obtained from pathway fits (SFO model for parent and metabolite) were considered suitable as modelling endpoints (see Jarvis & Montesano, 2014a).

  The RMS AT fully re-evaluated the parent soil degradation experiments in line with pertinent guidance applying the software tool CAKE 3.3 assuming $P_{SFO} \rightarrow M_{SFO}$, $P_{DFOP} \rightarrow M_{SFO}$ or $P_{HS} \rightarrow M_{SFO}$ pathway fits (with M representing RPA 406341, Trans-diol and RPA 404766, Cis-diol, in parallel). Notice, that residues of triticonazole did not reach 10 % AR, therefore giving preference to the DFOP and HS model for triticonazole. As already indicated for the parent (refer to Kreschnak (2015) in chapter B.8.1.2.1.1, aerobic degradation of the active substance), the RMS AT considers the entire incubation period up to one year representative and suitable for kinetic evaluation. The RMS AT also notes, that the reliability of the metabolite fits (metabolites following the SFO model) is sensitive to the selection of the parent kinetic model (SFO, DFOP or HS). Although considered appropriate from a statistical point of view (with χ^2 errors < 15 %), the SFO model for the parent does not always lead to reliable fits for the metabolites, whereas the DFOP or HS model for the parent often does so. In view of most reliable degradation rates for both, parent and metabolites, the DFOP or HS model for the parent is given preference if considered appropriate from a statistical point of view. Results on degradation rates obtained for the metabolites (all pathway fits) are given in the tables below.

  An example based on the kinetic evaluation of the loamy sand (20 °C) (Ta & Strobush, 2015) applying either the SFO or DFOP model for the parent may illustrate the situation. Although both fit are considered statistically reliable with χ^2 errors clearly below 15 % for both, the parent as well as the two metabolites, the RMS AT considers the DFOP parent fit superior to the SFO fit as it better describes the residues with less systematic deviation for the parent and metabolites. As already noted, the choice of the parent model has a strong impact on the *DegT50* and formation fraction of the metabolites.

Table B.8.1.2.1.2-16 Illustrative comparison of the kinetic evaluation of the loamy sand (20 °C, Ta & Strobush, 2015) applying either the SFO or DFOP model for the parent - RMS AT assessment

	
Parent SFO	**Parent DFOP**
***DegT50* of the metabolites:**	***DegT50* of the metabolites:**

A1: RPA 406341 (Trans-diol) = **35.7** days, *ff* = 0.39 B1: RPA 404766 (Cis-diol) = **23.7** days, *ff* = 0.57	A1: RPA 406341 (Trans-diol) = **202** days, *ff* = 0.18 B1: RPA 404766 (Cis-diol) = **93.5** days, *ff* = 0.24

- Lab degradation experiments conducted at 10 °C (in Ayliffe and Godward, 1993) or at reduced moisture content (in Simmonds et al., 1996) are not considered appropriate for temperature and moisture normalisation. These experiments are therefore not considered further for modelling endpoints.

- The metabolite doses studies with RPA 406341 (Trans-diol), RPA 404766 (Cis-diol) and RPA 407922 have been re-evaluated by the RMS AT as well. Moisture and temperature correction factors for normalization of obtained degradation rates to reference conditions in the metabolite dosed studies are given in the table below.

- The study Ta & Strobush (2012), investigating degradation of triticonazole in three US soils was originally not included in the applicant dossier but was submitted at late time point in order to support metabolite identification issues. Subsequently, this study was included in the RMS AT re-evaluation of degradation rates of triticonazole and its two metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol).

- As already noted RPA 407922 is not considered to occur at significant amounts in soil degradation studies. Therefore, data on degradation of RPA 407922 obtained in a dedicated soil degradation study (Unsworth & Clarke, 2000) are not considered further (no essential data).

- Degradation rates and formation fraction of the metabolite fractions 'Met 6 (MWT 333)' and 'Met7 (MWT 315)' have been addressed in a separate position paper (Szegedi, 2018).

Table B.8.1.2.1.2-17 Moisture and temperature correction factors for normalization of obtained degradation rates to reference conditions in the metabolite dosed studies - RMS AT assessment

Study	Soil type	T (°C)	Incubation moisture	Study MC (%)	Ref. MC (*p*F2) (%)	f_T[(d)]	f_{MC}[(e)]	$f_{T\times MC}$
McGhee (2000)	Clay Loam	20	45 % MWHC	14[(a)]	28[(b)]	1.00	0.62	**0.62**
	Sandy Loam	20	45 % MWHC	12[(a)]	19[(b)]	1.00	0.72	**0.72**
	Loam	20	45 % MWHC	14[(a)]	25[(b)]	1.00	0.67	**0.67**
Crowe (2002)	Sandy loam	20	*p*F2.5 - 2	13.3 - 17.5	17.5[(c)]	1.00	1.00	**1.00**
	Silty clay loam	20	*p*F2.5 - 2	32.4 - 39.5	39.5[(c)]	1.00	1.00	**1.00**
	Clay loam	20	*p*F2.5 - 2	26.9 - 33.0	33.0[(c)]	1.00	1.00	**1.00**

(a) Based on the default MWHC for this soil type (no information available on measured WHC)
(b) Default moisture content for this soil type (no information available)
(c) Measured moisture content
(d) Temperature correction factor = $2.58^{((T_{act}-T_{ref})/10)}$
(e) Moisture correction factor = $(MC_{act}/MC_{ref})^{0.7}$

Comments (RMS-AT) - continued

Table B.8.1.2.1.2-18 Trigger and modelling endpoints of RPA 406341 (Trans-diol) in laboratory studies conducted at 20 - 25 °C - RMS AT assessment (fits not considered statistically reliable are given in italics)

Study	Soil	Temp. (°C)	Kinetic model	Parameter	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*DegT50* (d)	*DegT90* (d)	*ff* (from parent)	*DegT50* at 20 °C, *p*F2 (d)
Ayliffe & Austin (1993)	Sandy loam	22	P_{HS}→M_{SFO}	k = 0.009	0.002	0.0015	< 0.01	13.2	80.1	266	0.426	56.1
	Clay loam	22	P_{SFO}→M_{SFO}	k = 0.010	0.007	0.013	< 0.01	17.3	68.5	228	0.372	74.0
Ayliffe & McMillan-Staff (1994)	Loamy sand (Speyer 2.2)	22	P_{HS}→M_{SFO}	k = 0.002	0.000	0.004	0.04	7.5	405	> 1000	0.390	450
Ayliffe & Godward (1993)	Loamy sand (UK)	22	P_{HS}→M_{SFO}	k = 0.007	0.002	0.011	< 0.01	21.3	105	349	0.473	127
Doble et al. (1996)	Clay	25	P_{SFO}→M_{SFO}	k = 0.003	0.002	0.006	< 0.01	17.4	170	566	0.583	139
Simmonds et al. (1996)	Sandy loam (standard)	25	P_{HS}→M_{SFO}	k = 0.004	0.002	0.005	< 0.01	7.1	188	623	0.510	263
	Sandy loam (red. rate)	25	P_{HS}→M_{SFO}	k = 0.004	0.003	0.005	< 0.01	5.9	207	686	0.607	290
Ta & Strobush (2012)	Sand	20	P_{SFO}→M_{SFO}	k = 0.001	0.000	0.003	0.02	10.1	462	> 1000	0.207	397
	Loam	20	P_{DFOP}→M_{SFO}	k = 0.003	0.003	0.004	< 0.01	7.8	208	692	0.118	185
	Loamy sand	20	P_{DFOP}→M_{SFO}	k = 0.004	0.003	0.005	< 0.01	6.3	176	584	0.160	151
Ta & Strobush (2015)	Loamy sand	20	P_{DFOP}→M_{SFO}	k = 0.003	-0.001	0.007	0.04	5.8	202	670	0.178	172
McGhee (2000)	Clay loam	20	P_{SFO}	k = 0.004	0.003	0.005	< 0.01	2.0	165	549	na	102
	Sandy loam	20	P_{SFO}	k = 0.004	0.003	0.004	< 0.01	2.3	199	661	na	143
	Loam	20	P_{SFO}	k = 0.002	0.001	0.003	< 0.01	3.5	346	> 1000	na	232

Table B.8.1.2.1.2-19 Kinetic endpoints of RPA 406361 (Trans-diol) in laboratory studies conducted at 10 °C or reduced moisture - RMS AT assessment (fits not considered statistically reliable are given in italics)

Study	Soil	Temp. (°C)	Kinetic model	Parameter	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*DT50* (d)	*DT90* (d)	*ff* (from parent)	*DegT50* at 20 °C, *p*F2 (d)
Ayliffe & Godward (1993)	Sandy loam	10	P_{DFOP}→M_{SFO}	*k < 0.001*	*-0.002*	*0.002*	*0.35*	*14.9*	*> 1000*	*> 1000*	*0.223*	nc
	Clay loam	10	P_{HS}→M_{SFO}	k = 0.002	< 0.001	0.004	0.01	12.5	309	> 1000	0.370	nc
	Loamy sand (Speyer 2.2)	10	P_{HS}→M_{SFO}	*k < 0.001*	*-0.001*	*0.002*	*0.25*	*14.5*	*> 1000*	*> 1000*	*0.321*	nc
	Loamy sand (UK)	10	P_{HS}→M_{SFO}	*k < 0.001*	*-0.003*	*0.003*	*0.47*	*29.5*	*> 1000*	*> 1000*	*0.262*	nc
Simmonds et al. (1996)	Sandy loam (red. temp.)	10	P_{SFO}→M_{SFO}	k = 0.002	0.000	0.004	0.03	18.5	393	> 1000	0.736	nc
	Sandy loam (red. moist.)	25	P_{DFOP}→M_{SFO}	*k = 0.001*	*-0.000*	*0.002*	*0.09*	*6.7*	*951*	*> 1000*	*0.319*	nc

Table B.8.1.2.1.2-20 Trigger and modelling endpoints of RPA 404766 (Cis-diol) in laboratory studies conducted at 20 - 25 °C - RMS AT assessment (fits not considered statistically reliable are given in italics)

Study	Soil	Temp. (°C)	Kinetic model	Parameter	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*DegT50* (d)	*DegT90* (d)	*ff* (from parent)	*DegT50* at 20 °C, *p*F2 (d)
Ayliffe & Austin (1993)	Sandy loam	22	$P_{HS} \rightarrow M_{SFO}$	*k = 0.002*	*-0.002*	*0.005*	*0.19*	*26.1*	*461*	*> 1000*	*0.159*	*nc*
	Clay loam	22	$P_{SFO} \rightarrow M_{SFO}$	k = 0.031	0.024	0.037	< 0.01	19.1	22.7	75.5	0.628	24.5
Ayliffe & McMillan-Staff (1994)	Loamy sand (Speyer 2.2)	22	$P_{HS} \rightarrow M_{SFO}$	k = 0.004	0.001	0.008	< 0.01	9.5	155	516	0.365	172
Ayliffe & Godward (1993)	Loamy sand (UK)	22	$P_{HS} \rightarrow M_{SFO}$	k = 0.016	0.007	0.026	< 0.01	26.2	42.0	141	0.448	50.8
Doble et al. (1996)	Clay	25	$P_{SFO} \rightarrow M_{SFO}$	k = 0.003	0.001	0.006	< 0.01	22.6	213	707	0.418	175
Simmonds et al. (1996)	Sandy loam (standard)	25	$P_{HS} \rightarrow M_{SFO}$	k = 0.007	0.004	0.010	< 0.01	12.4	95.0	315	0.354	133
	Sandy loam (red. rate)	25	$P_{HS} \rightarrow M_{SFO}$	k = 0.007	0.004	0.010	< 0.01	6.2	98.2	326	0.393	137
Ta & Strobush (2012)	Sand	20	$P_{SFO} \rightarrow M_{SFO}$	k = 0.004	0.003	0.005	< 0.01	9.9	170	566	0.305	146
	Loam	20	$P_{DFOP} \rightarrow M_{SFO}$	k = 0.005	0.004	0.006	< 0.01	4.2	139	461	0.181	124
	Loamy sand	20	$P_{DFOP} \rightarrow M_{SFO}$	k = 0.005	0.003	0.006	< 0.01	4.8	148	493	0.214	127
Ta & Strobush (2015)	Loamy sand	20	$P_{DFOP} \rightarrow M_{SFO}$	k = 0.007	0.003	0.012	< 0.01	4.5	93.5	311	0.243	79.5
Crowe (2002)	Sandy loam	20	P_{SFO}	k = 0.022	0.015	0.030	< 0.01	7.2	30.9	103	na	30.9
	Silty clay loam	20	P_{SFO} [(a)]	k = 0.033	0.010	0.057	< 0.01	15.8	20.8	69.0	na	20.8
	Clay loam	20	P_{SFO} [(b)]	k = 0.012	0.006	0.019	< 0.01	9.1	56.1	187	na	56.1

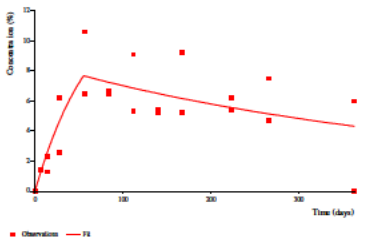
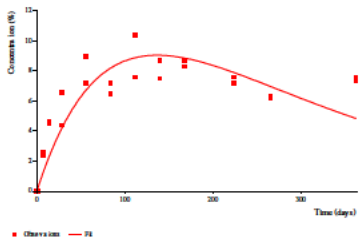
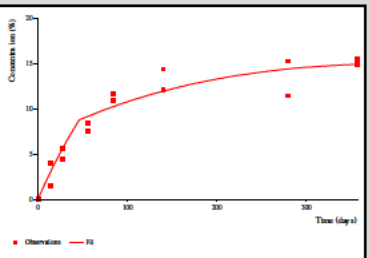
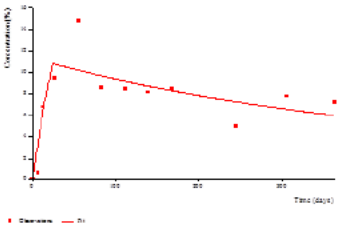
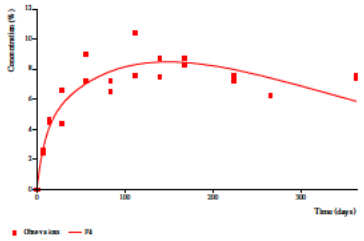
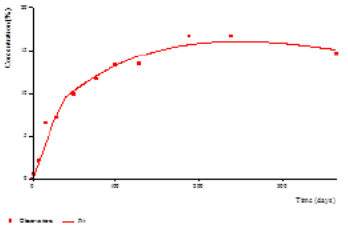
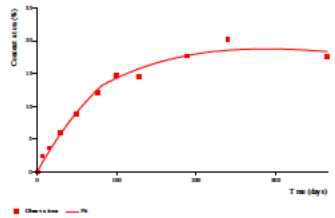
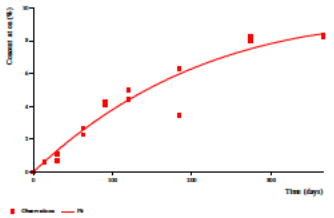
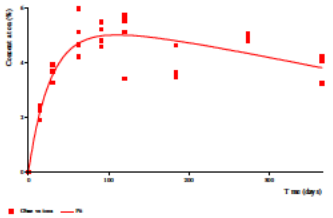
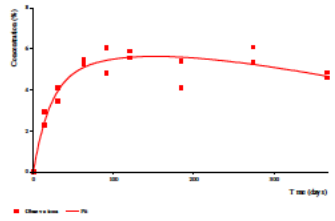
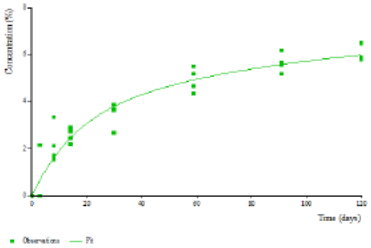
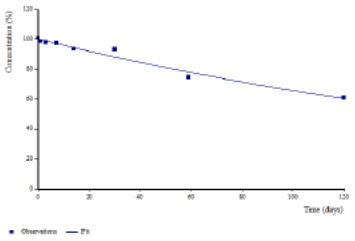
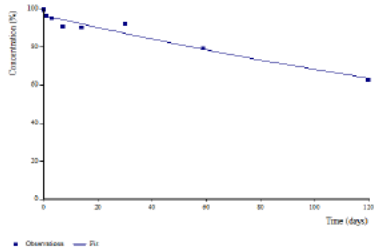
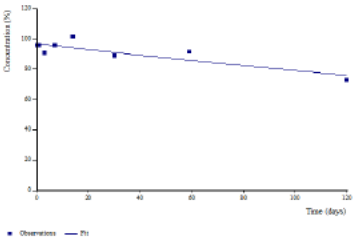
(a) Other kinetic models are not reliable from a statistical point of view
(b) First data point (0 DAT) omitted as an outlier

Table B.8.1.2.1.2-21 Kinetic endpoints of RPA 404766 (Cis-diol) in laboratory studies conducted at 10 °C or reduced moisture - RMS AT assessment (fits not considered statistically reliable are given in italics)

Study	Soil	Temp. (°C)	Kinetic model	Parameter	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*DegT50* (d)	*DegT90* (d)	*ff* (from parent)	*DegT50* at 20 °C, *p*F2 (d)
Ayliffe & Godward (1993)	Sandy loam	10	$P_{DFOP} \rightarrow M_{SFO}$	*k < 0.001*	*-0.002*	*0.003*	*0.45*	*22.3*	*> 1000*	*> 1000*	*0.148*	nc
	Clay loam	10	$P_{HS} \rightarrow M_{SFO}$	k = 0.005	0.002	0.008	< 0.01	21.2	140	464	0.405	nc
	Loamy sand (Speyer 2.2)	*10*	*$P_{HS} \rightarrow M_{SFO}$*	*k < 0.001*	*-0.001*	*0.001*	*0.42*	*12.7*	*> 1000*	*> 1000*	*0.293*	nc
	Loamy sand (UK)	10	*$P_{HS} \rightarrow M_{SFO}$*	*k = 0.005*	*-0.002*	*0.012*	*0.09*	*51.1*	*149*	*496*	*0.282*	nc
Simmonds et al. (1996)	Sandy loam (red. temp.)	10	$P_{SFO} \rightarrow M_{SFO}$	*k = < 0.001*	*-0.003*	*0.004*	*0.43*	*48.0*	*> 1000*	*> 1000*	*0.265*	nc
	Sandy loam (red. moist.)	25	$P_{DFOP} \rightarrow M_{SFO}$	k = 0.002	0.001	0.004	< 0.01	7.0	296	983	0.209	nc

Comments (RMS-AT) - continued

Table B.8.1.2.1.2-22 **Fits on trigger and modelling endpoints for RPA 406341 (Trans-diol) in laboratory studies conducted at 20 - 25 °C - RMS AT assessment (fits not considered statistically reliable are given in italics)**

 Sandy loam (22 °C), Ayliffe & Austin (1993) - P_{HS}→M_{SFO}	 Clay loam (22 °C), Ayliffe & Austin (1993) - P_{SFO}→M_{SFO}	 Loamy sand (Speyer 2.2, 22 °C), Ayliffe & McMillan-Staff (1994)- P_{HS}→M_{SFO}
 Loamy sand (UK, 22 °C), Ayliffe & Godward (1993) - P_{HS}→M_{SFO}	 Clay (25 °C), Doble et al. (1996) - P_{SFO}→M_{SFO}	 Sandy loam (standard, 25 °C), Simmonds et al. (1996) - P_{HS}→M_{SFO}
 Sandy loam (red. rate, 25 °C), Simmonds et al. (1996) - P_{HS}→M_{SFO}	 Sand (20 °C), Ta & Strobush (2012) P_{SFO}→M_{SFO}	 Loam (20 °C), Ta & Strobush (2012) P_{DFOP}→M_{SFO}
 Loamy sand (20 °C), Ta & Strobush (2012) P_{DFOP}→M_{SFO}	 Loamy sand (20 °C), Ta & Strobush (2015) - P_{DFOP}→M_{SFO}	 Clay loam (20 °C), McGhee (2000) - P_{SFO}
 Sandy loam (20 °C), McGhee (2000) -	 Loam (20 °C), McGhee (2000) -	

P_{SFO}	P_{SFO}	

Table B.8.1.2.1.2-23 **Fits on trigger endpoints for RPA 406341 (Trans-diol) in laboratory studies conducted at 10 °C or reduced moisture - RMS AT assessment (fits not considered statistically reliable are given in italics)**

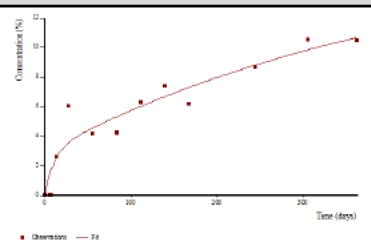
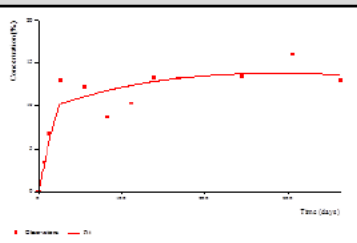
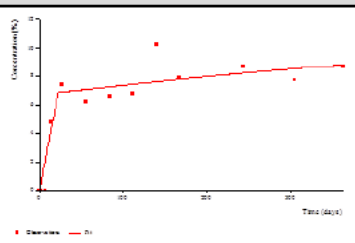
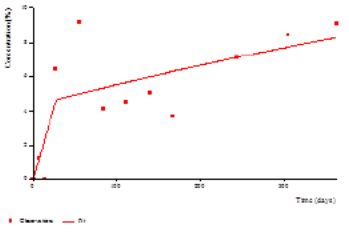
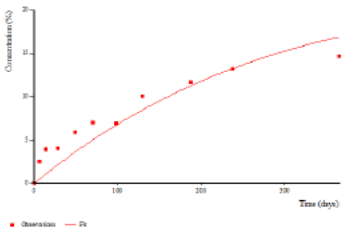
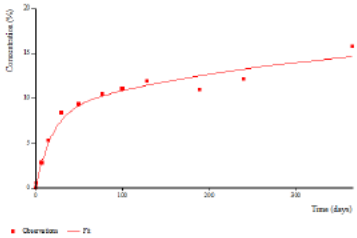
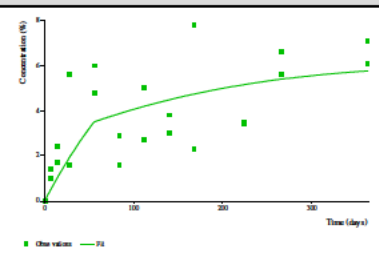
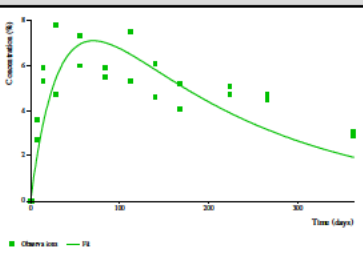
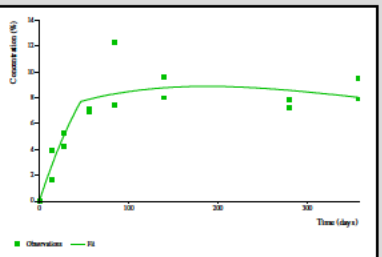
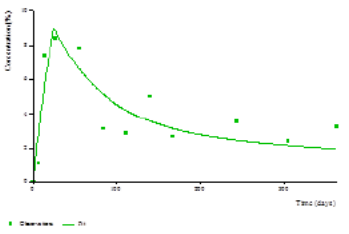
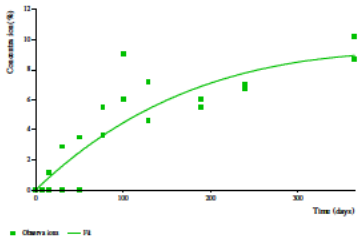
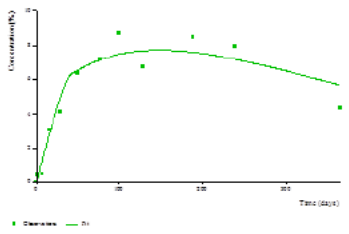
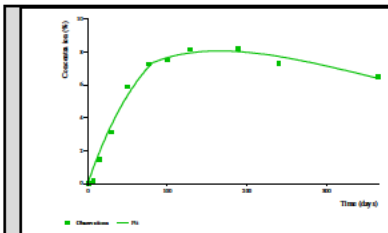
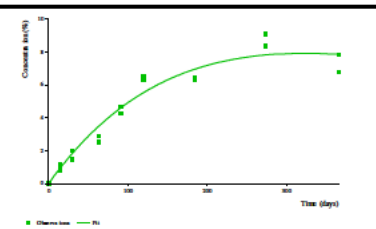
 *Sandy loam (10 °C), Ayliffe & Godward (1993) - P_{DFOP}→M_{SFO}*	 Clay loam (10 °C), Ayliffe & Godward (1993) - P_{HS}→M_{SFO}	 *Loamy sand (2.2, 10 °C), Ayliffe & Godward (1993) - P_{HS}→M_{SFO}*
 *Loamy sand (UK, 10 °C), Ayliffe & Godward (1993) - P_{HS}→M_{SFO}*	 Sandy loam (red. temp., 10 °C), Simmonds (1996) - P_{SFO}→M_{SFO}	 *Sandy loam (red. moist., 25 °C), Simmonds (1996) - P_{DFOP}→M_{SFO}*

Table B.8.1.2.1.2-24 **Fits on trigger and modelling endpoints for RPA 404766 (Cis-diol) in laboratory studies conducted at 20 - 25 °C - RMS AT assessment (fits not considered statistically reliable are given in italics)**

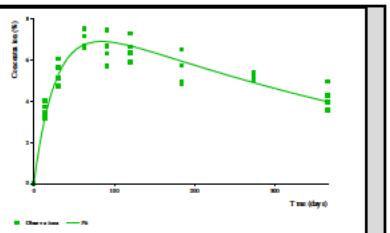
 *Sandy loam (22 °C), Ayliffe & Austin (1993) - P_{HS}→M_{SFO}*	 Clay loam (22 °C), Ayliffe & Austin (1993) - P_{SFO}→M_{SFO}	 Loamy sand (Speyer 2.2, 22 °C), Ayliffe & McMillan-Staff (1994) - P_{HS}→M_{SFO}
 Loamy sand (UK, 22 °C), Ayliffe & Godward (1993), P_{HS}→M_{SFO}	 Clay (25 °C), Doble et al. (1996) - P_{SFO}→M_{SFO}	 Sandy loam (standard, 25 °C), Simmonds et al. (1996) - P_{HS}→M_{SFO}



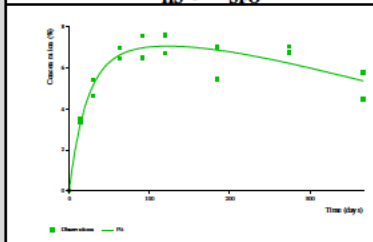
Sandy loam (red. rate, 25 °C), Simmonds et al. (1996) - $P_{HS} \rightarrow M_{SFO}$



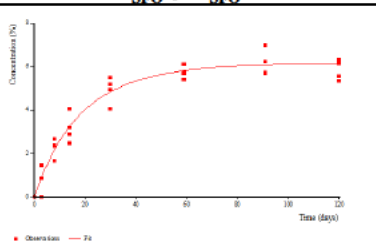
Sand (20 °C), Ta & Strobush (2012) $P_{SFO} \rightarrow M_{SFO}$



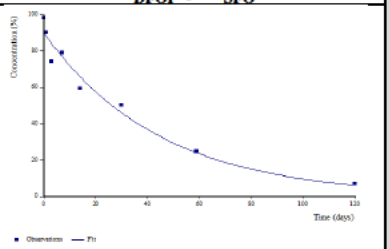
Loam (20 °C), Ta & Strobush (2012) $P_{DFOP} \rightarrow M_{SFO}$



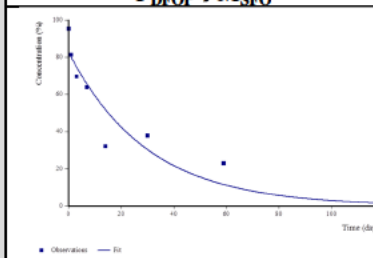
Loamy sand (20 °C), Ta & Strobush (2012) $P_{DFOP} \rightarrow M_{SFO}$



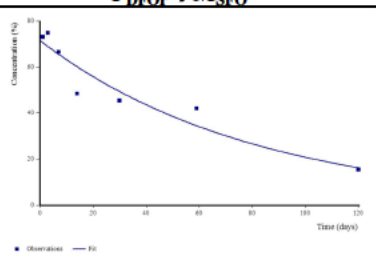
Loamy sand (20 °C), Ta & Strobush (2015) - $P_{DFOP} \rightarrow M_{SFO}$



Sandy loam (20 °C), Crowe (2002) - P_{SFO}

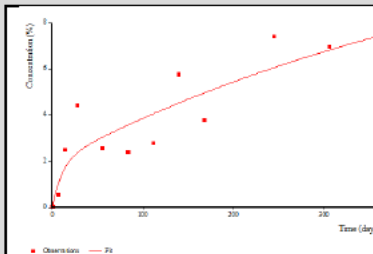


Silty clay loam (20 °C), Crowe (2002) - P_{SFO}

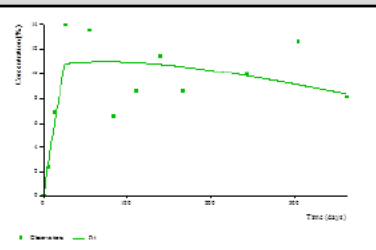


Clay (20 °C), Crowe (2002) - P_{SFO}

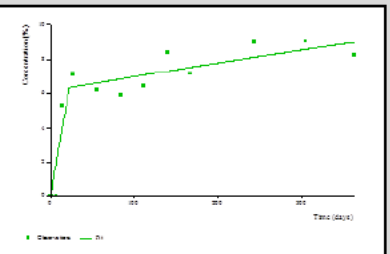
Table B.8.1.2.1.2-25 Fits on trigger endpoints for RPA 404766 (Cis-diol) in laboratory studies conducted at 10 °C or reduced moisture - RMS AT assessment (fits not considered statistically reliable are given in italics)



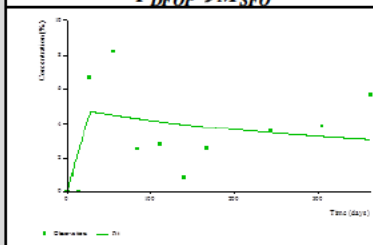
Sandy loam (10 °C), Ayliffe & Godward (1993) - $P_{DFOP} \rightarrow M_{SFO}$



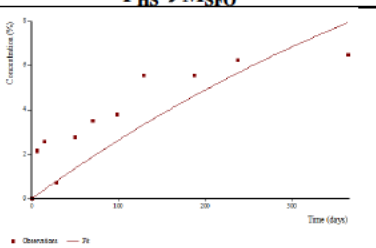
Clay loam (10 °C), Ayliffe & Godward (1993) - $P_{HS} \rightarrow M_{SFO}$



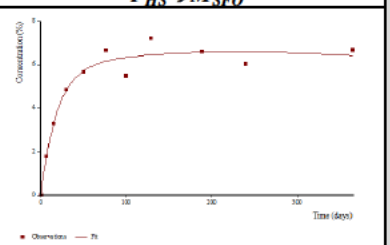
Loamy sand (2.2, 10 °C), Ayliffe & Godward (1993) - $P_{HS} \rightarrow M_{SFO}$



Loamy sand (UK, 10 °C), Ayliffe & Godward (1993) - $P_{HS} \rightarrow M_{SFO}$



Sandy loam (red. temp., 10 °C), Simmonds et al. (1996) - $P_{SFO} \rightarrow M_{SFO}$



Sandy loam (red. moist., 25 °C), Simmonds et al. (1996) - $P_{DFOP} \rightarrow M_{SFO}$

Reference:	**Statement - Exposure assessment for "Met 6" and "Met 7", potential degradation products of BAS 595F triticonazole**
Author(s), year:	Szegedi, K., 2018
Report/Doc. Number:	2018/1091281
Guideline(s):	None
GLP:	Not applicable (statement)
Validity:	Partly (refer to comment section)
Status:	**New submission**

Degradation half-life of 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)':

As a conservative estimate, for both compounds the worst-case default *DegT50* of 1000 days will be assumed. Conservative formation fractions based on residue data in soils from the soil metabolism studies with triticonazole in which maximum occurrence of 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' was observed, respectively: UK clay loam for 'Met 6 (MWT 333)' and UK sandy loam for 'Met 7 (MWT 315)' in Ayliffe & Austin (1993).

Estimating formation of 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)':

For the parent compound triticonazole, the appropriate kinetic model for deriving modelling endpoints was identified by RMS AT considering the procedures and kinetic models proposed by the FOCUS workgroup on degradation kinetics (FOCUS, 2006). *DegT50* values were derived for use in environmental fate models derived for individual soils using selected kinetic the kinetic model.

The kinetic models and half lifes proposed by the RMS for triticonazole for the UK clay loam and for the UK sandy loam, respectively, were used in the current work in combination with the conservative *DegT50* of 1000 d for 'Met 6 (MWT 333)' and for 'Met 7 (MWT 315)'. Degradation rates reported in the (draft) RAR were rounded to three decimals. Values used in the current assessment were calculated based on the reported half-lives. Direct formation of the metabolites from the parent compound was assumed. SFO kinetic was used for the metabolites.

Separate calculations were conducted with KinGUI 2.1 with the IRLS method, with an error tolerance of 10^{-10} and the maximum number of iterations of 500. Only the formation fractions for the metabolites were optimized, all other parameters were fixed.

The first optimisation attempt for the UK clay loam soil resulted in a robust estimation of the formation fraction of 'Met 6 (MWT 333)' from the parent compound. Graphical presentations of the fits, residual plots and KinGUI modelling report summaries are provided in the appendix of the study report.

The first optimisation attempt for 'Met 7 (MWT 315)' did not converge (results are not presented). The run was repeated with optimizing the degradation rate of the metabolite beside its formation fraction. Although this run converged it did not result in a *DegT50* significantly different from 0. Thus, another optimization run was set up in which also degradation rate in the slow phase of the parent compound was also optimized. A further optimization run was set up in which also degradation rate in the slow phase of the parent compound and the formation fraction of the metabolite were optimized. However, degradation rate of the metabolite were not optimized. This approach is justified by the following assumptions: a) the conservative *DegT50* of 1000 days for the metabolite is expected to sufficiently describe its degradation rate in the experiment, b) the optimization of degradation rate of the parent in the slow phase is not expected to significantly change obtained parameters, and c) the change in the degrees of freedom would lead to a more robust estimation. The outcome of the latter fit resulted in a robust estimate for the formation fraction of the metabolite 'Met 7 (MWT 315)' from the parent compound.

And overview of the results of the kinetic evaluation is presented below.

Table B.8.1.2.1.2-26 Estimating formation fraction of 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' derived from residue data collected in UK clay loam and for UK sandy loam in the study Ayliffe & Austin (1993) by RMS AT for triticonazole

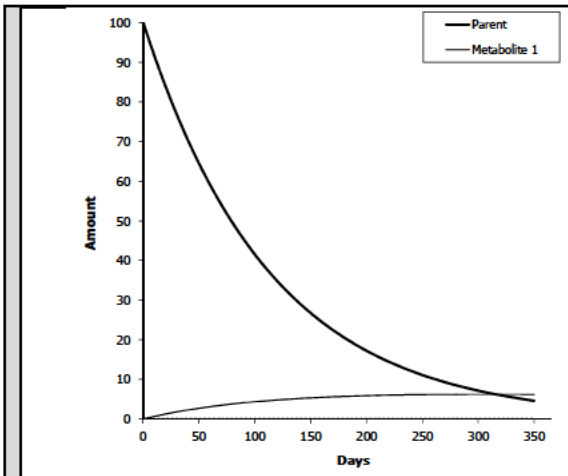
Experiment/ soil name	Kinetic model	χ^2 err. [%]	Visual fit	Formation fraction parent → Met	Remarks
UK clay loam ('Met 6 (MWT 333)')	SFO	5.6	Very good	**0.144**	*DegT50* for 'Met 6 (MWT 333)' = **1000 days** (fixed)
UK sandy loam ('Met 7 (MWT 315)'), formation fraction optimized	Did not converge				
UK sandy loam ('Met 7 (MWT 315)'), formation fraction and *DegT50* for metabolite optimized	HS	5.7	Very good	0.132	*DegT50* for 'Met 7 (MWT 315)' not significantly different from 0
UK sandy loam ('Met 7 (MWT 315)'), formation fraction and *DegT50* for metabolite and DegT50 for parent in slow phase optimized	HS	5.8	Very good	0.125	*DegT50* for 'Met 7 (MWT 315)' not significantly different from 0
UK sandy loam ('Met 7 (MWT 315)'), formation fraction and *DegT50* for parent in slow phase optimized	HS	5.9	Very good	**0.137**	*DegT50* for 'Met 7 (MWT 315)' = **1000 days** (fixed) k_2 for parent = 0.00173 (significantly different from 0)

Bold: values to be used in PEC calculations

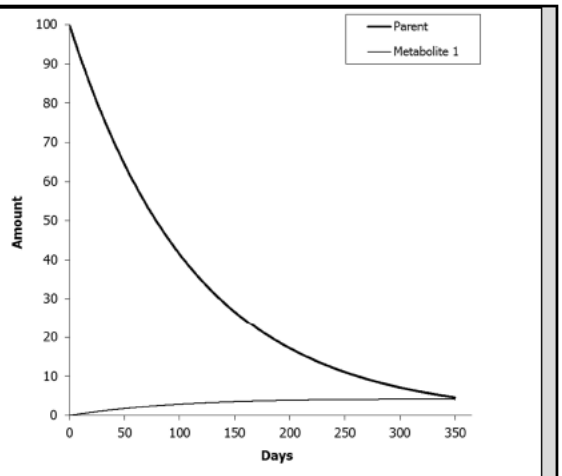
Comments (RMS AT):

- The RMS AT notes that the metabolite fractions 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' have been observed in four legacy soil degradation experiments (conducted at 22 °C) at maximum amounts of 12.8, 4.2, 1.6 and 6.2 % AR ('Met 6 (MWT 333)') and 6.5, 0.9, 3.6 and 5.3 % AR ('Met 7 (MWT 315)') (Ayliffe & Austin, 1993; Ayliffe & McMillan-Staff, 1994; Ayliffe & Godward, 1993). Maximum residues were generally observed at the end of incubation (~ 365 days) or close to the end of incubation. In analogy to averaging substance properties (*DegT50* and formation fraction) of the parent and metabolites in the exposure assessment, the RMS AT considers it defendable to conduct the groundwater assessment for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' also on basis of an average (arithmetic mean) occurrence in soil, which is 6.2 and 4.1 % AR for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)', respectively. Coupling the geometric mean *DegT50* of 78.7 days for the parent (i.e. the modelling endpoint derived from field studies, refer to Chapter B.8.1.2.3, summary on field dissipation/degradation) with a conservative *DegT50* of 1000 days for the two metabolite fractions, a maximum occurrence of 6.2 and 4.1 % for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)', respectively, in the exposure modelling is archived if the formation fraction is set to **0.077** and **0.051** for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)', respectively (see figures below). On overall, the RMS AT considers residues of these two metabolite fractions observed in legacy studies sufficiently covered by this approach.

Table B.8.1.2.1.2-27 Modelled residues of 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' in the exposure assessment on basis of a formation fraction of 0.077 and 0.051 for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)', respectively - RMS AT assessment



Modelled residues of 'Met 6 (MWT 333)' (= Metabolite 1) on basis of a parent *DegT50* of 78.7 days, a metabolite *DegT50* of 1000 days and a formation fraction fixed to 0.077 (maximum occurrence = 6.2 %).



Modelled residues of 'Met 7 (MWT 315)' (= Metabolite 1) on basis of a parent *DegT50* of 78.7 days, a metabolite *DegT50* of 1000 days and a formation fraction fixed to 0.051 (maximum occurrence = 4.1 %).

B.8.1.2.1.3. Anaerobic degradation of the active substance

Triticonazole was shown to be stable under conditions of anaerobic soil conditions (one soil).

B.8.1.2.1.4. Anaerobic degradation of metabolites, breakdown and reaction products

In general anaerobic degradation rate studies with metabolites of triticonazole are not considered necessary as degradation rates obtained under aerobic conditions are used for environmental exposure modelling.

B.8.1.2.1.5. Summary on laboratory degradation rates in soil (compiled by the RMS AT)

The rate of degradation in soil of triticonazole and metabolites has been assessed in laboratory studies and is summarised in the tables below. Notice that the kinetic assessment provided by the RMS AT is based on the entire period of incubation (so one year in most cases). Metabolite RPA 407922 is not considered to occur at significant amounts in soil degradation studies. Therefore degradation data obtained for RPA 407922 in a dedicated soil degradation study are not considered further. Conservative degradation rates and formation fractions for the two metabolite fractions 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' have been proposed in a separate position paper (Szegedi, 2018).

Table B.8.1.2.1.5-1 Summary on aerobic degradation rates of triticonazole in laboratory soil degradation studies conducted at 20 - 25 °C - trigger & modelling endpoints

Soil origin	Soil type (USDA)	Label	*p*H ($CaCl_2$)	T (°C)	Water content	*DegT50* (d)	*DegT90* (d)	*DegT50* (d) 20 °C, *p*F2	χ^2 err. (%)	Kinetic model	Ref.[a]
UK	Sandy loam[b]	Ph	6.4[c]	22	75 % 33 kPa	289	> 1000	280[d]	5.0	HS	1
UK	Clay loam[b]	Ph	6.2[c]	22	75 % 33 kPa	137	455	148	4.4	SFO	
Speyer 2.2	Loamy sand[b]	Ph	6.8[c]	22	75 % 33 kPa	233	986	360[d]	5.0	HS	2
UK	Loamy sand[b]	Ph	6.3[c]	22	75 % 33 kPa	290	> 1000	565[d]	4.2	HS	3
US	Clay	T	5.7	25	75 % 33 kPa	495	> 1000	376	5.7	SFO	4
Manningtree	Sandy loam	Ph	6.1	25	50 % FC	183[e] 221[f]	702 816	312[d] 358[d]	3.3 6.5	HS HS	5
California	Sand	T	8.1[h]	20	50 % MHWC	305	> 1000	262	3.1	SFO	
New Jersey	Loam	Ph & T	6.8[h]	20	50 % MHWC	78.8	661	230[d]	2.4	DFOP	6
Wisconsin	Sandy loam	T	6.0[h]	20	50 % MHWC	128	664	199[d]	3.2	DFOP	
Li 10	Loamy sand	Ph & T	6.3	20	50 % MWHC	148	633	178[d]	1.0	DFOP	7
LUFA 2.2	Loamy sand	-	5.5	20	50 % MWHC	317	> 1000	298	7.3	SFO	
LUFA 2.3	Sandy loam	-	6.9	20	50 % MWHC	115	381	109	5.9	SFO	8
LUFA 5M	Sandy loam	-	7.4	20	50 % MWHC	114	521	161[d]	6.3	HS	
					Maximum (n = 13)	**495**	**> 1000**	-	-	SFO	
					Geometric mean (n = 13)[g]	-	-	**246**	-	SFO	
					pH-dependency: y/n	**n**	-	**-**	-	-	

(a) Reference:
1: Ayliffe & Austin (1993)
2: Ayliffe & McMillan-Staff (1994)
3: Ayliffe & Godward (1993)
4: Doble et al. (1996)
5: Simmonds et al. (1996)
6: Ta & Strobush (2012)
7: Ta & Strobush (2015)
8: Grella et al. (2014)
(b) Soil texture classification not specified
(c) Matrix not specified
(d) On basis of slow phase *DegT50* (DFOP or HS)
(e) Standard conditions
(f) Reduced application rate
(g) Two experiments in Simmonds et al. (1996) averaged (geometric mean) before averaging different soils
(h) In water

Table B.8.1.2.1.5-2 Summary on aerobic degradation rates of triticonazole in laboratory soil degradation studies conducted at 10 °C or reduced soil moisture

Soil origin	Soil type (USDA)	Label	*p*H ($CaCl_2$)	T (°C)	Water content	*DegT50* (d)	*DegT90* (d)	*DegT50* (d) 20 °C, *p*F2	χ^2 err. (%)	Kinetic model	Reference
UK	Sandy loam[a]	Ph	6.3[b]	10	75 % 33 kPa	341	> 1000	nc	3.5	DFOP	Ayliffe & Godward (1993)
UK	Clay loam[a]	Ph	6.1[b]	10	75 % 33 kPa	176	892	nc	5.0	HS	
Speyer 2.2	Loamy sand[a]	Ph	6.3 [b]	10	75 % 33 kPa	> 1000	> 1000	nc	2.6	HS	
UK	Loamy sand[a]	Ph	6.2[b]	10	75 % 33 kPa	862	> 1000	nc	3 9	HS	
Manning-tree	Sandy loam	Ph	6.1	10	50 % FC	584	> 1000	nc	4.5	SFO	Simmonds et al. (1996)
				25	20 % FC	259	> 1000	nc	13.1	DFOP	

(a) Soil texture classification not specified
(b) Matrix not specified

Table B.8.1.2.1.5-3 Summary on aerobic degradation rates of RPA 406341 (Trans-diol) in laboratory soil degradation studies conducted at 20 - 25 °C - trigger & modelling endpoints

Soil origin	Soil type (USDA)	Label	*p*H ($CaCl_2$)	T (°C)	Water content	*DegT 50* (d)	*DegT 90* (d)	*ff*[i]	*DegT50* (d) 20 °C, *p*F2	χ^2 err. (%)	Kinetic model	Ref.[a]
UK	Sandy loam[b]	Ph	6.4[c]	22	75 % 33 kPa	80.1	266	0.426	56.1	13.2	P_{HS}→M_{SFO}	1
UK	Clay loam[b]	Ph	6.2[c]	22	75 % 33 kPa	68.5	228	0.372	74.0	17.3	P_{SFO}→M_{SFO}	
Speyer 2.2	Loamy sand[b]	Ph	6.8[c]	22	75 % 33 kPa	405	> 1000	0.390	450	7.5	P_{HS}→M_{SFO}	2
UK	Loamy sand[b]	Ph	6.3[c]	22	75 % 33 kPa	105	349	0.473	127	21.3	P_{HS}→M_{SFO}	3
US	Clay	T	5.7	25	75 % 33 kPa	170	566	0.583	139	17.4	P_{SFO}→M_{SFO}	4
Manningtree	Sandy loam	Ph	6.1	25	50 % FC	188[d]	623	0.510	263	7.1	P_{HS}→M_{SFO}	5
						207[e]	686	0.607	290	5.9	P_{HS}→M_{SFO}	
California	Sand	T	8.1[h]	20	50 % MHWC	462	> 1000	0.207	397	10.1	P_{SFO}→M_{SFO}	
New Jersey	Loam	Ph & T	6.8[h]	20	50 % MHWC	208	692	0.118	185	7.8	P_{DFOP}→M_{SFO}	6
Wisconsin	Sandy loam	T	6.0[h]	20	50 % MHWC	176	584	0.160	151	6.3	P_{DFOP}→M_{SFO}	
Li 10	Loamy sand	Ph & T	6.3	20	50 % MWHC	202	670	0.178	172	5.8	P_{DFOP}→M_{SFO}	7
Royston	Clay Loam	Ph	7.0	20	45 % MWHC	165	549	na	102	2.0	SFO	
Ipswich	Sandy Loam	Ph	5.3	20	45 % MWHC	199	661	na	143	2.3	SFO	8
Ongar	Loam	Ph	6.2	20	45 % MWHC	346	> 1000	na	232	3.5	SFO	
					Maximum (n = 13)	**462**	**> 1000**	-	-	-	SFO	
					Geometric mean (n = 13)[f]	-	-	**-**	**163**	-	SFO	
					Arithmetic mean (n = 13)[g]	-	-	**0.347**	**-**	-		
					***p*H-dependency: y/n**	**n**	-	**-**	**-**	-		

(a) Reference:
1: Ayliffe & Austin (1993)
2: Ayliffe & McMillan-Staff (1994)
3: Ayliffe & Godward (1993)
4: Doble et al. (1996)
5: Simmonds et al. (1996)
6: Ta & Strobush (2012)
7: Ta & Strobush (2015)
8: McGhee (2000)
(b) Soil texture classification not specified
(c) Matrix not specified
(d) Standard conditions
(e) Reduced application rate
(f) Two experiments in Simmonds et al. (1996) averaged (geometric mean) before averaging different soils
(g) Two experiments in Simmonds et al. (1996) averaged (arithmetic mean) before averaging different soils
(h) In water
(i) From parent

Table B.8.1.2.1.5-4 Summary on aerobic degradation rates of RPA 406341 (Trans-diol) in laboratory soil degradation studies conducted at 10 °C or reduced soil moisture

Soil origin	Soil type (USDA)	Label	*p*H ($CaCl_2$)	T (°C)	Water content	*DegT 50* (d)	*DegT 90* (d)	*ff*[d]	*DegT 50* (d) 20 °C, *p*F2	χ^2 err. (%)	Kinetic model	Ref.[a]
UK	Clay loam[b]	Ph	6.1[c]	10	75 % 33 kPa	309	> 1000	0.370	nc	12.5	P_{HS}→M_{SFO}	1
Manningtree	Sandy loam	Ph	6.1	10	50 % FC	393	> 1000	0.736	nc	18.5	P_{SFO}→M_{SFO}	2

(a) Reference:
1: Ayliffe & Godward (1993)
2: Simmonds et al. (1996)
(b) Soil texture classification not specified
(c) Matrix not specified
(d) From parent

Table B.8.1.2.1.5-5 Summary on aerobic degradation rates of RPA 404766 (Cis-diol) in laboratory soil degradation studies conducted at 20 - 25 °C - trigger & modelling endpoints

Soil origin	Soil type (USDA)	Label	*p*H (Ca Cl_2)	T (°C)	Water content	*DegT 50* (d)	*DegT 90* (d)	*ff*[(i)]	*DegT 50* (d) 20 °C, *p*F2	χ^2 err. (%)	Kinetic model	Ref.[(a)]
UK	Clay loam[(b)]	Ph	6.2[(c)]	22	75 % 33 kPa	22.7	75.5	0.628	24.5	19.1	P_{SFO}→M_{SFO}	1
Speyer 2.2	Loamy sand[(b)]	Ph	6.8[(c)]	22	75 % 33 kPa	155	516	0.365	172	9.5	P_{HS}→M_{SFO}	2
UK	Loamy sand[(b)]	Ph	6.3[(c)]	22	75 % 33 kPa	42.0	141	0.448	50.8	26.2	P_{HS}→M_{SFO}	3
US	Clay	T	5.7	25	75 % 33 kPa	213	707	0.418	175	22.6	P_{SFO}→M_{SFO}	4
Manningtree	Sandy loam	Ph	6.1	25	50 % FC	95.0[(d)] 98.2[(e)]	315 326	0.354 0.393	133 137	12.4 6.2	P_{HS}→M_{SFO} P_{HS}→M_{SFO}	5
California	Sand	T	8.1[(h)]	20	50 % MHWC	170	566	0.305	146	9 9	P_{SFO}→M_{SFO}	6
New Jersey	Loam	Ph & T	6.8[(h)]	20	50 % MHWC	139	461	0.181	124	4.2	P_{DFOP}→M_{SFO}	
Wisconsin	Sandy loam	T	6.0[(h)]	20	50 % MHWC	148	493	0.214	127	4.8	P_{DFOP}→M_{SFO}	
Li 10	Loamy sand	Ph & T	6.3	20	50 % MWHC	93.5	311	0.243	79.5	4.5	P_{DFOP}→M_{SFO}	7
Baylham	Sandy loam	Ph	4.5	20	*p*F2.5 - 2	30.9	103	na	30.9	7.2	SFO	
Royston	Silty clay loam	Ph	7.2	20	*p*F2.5 - 2	20.8	69.0	na	20.8	15.8	SFO	8
Ongar	Clay loam	Ph	6.9	20	*p*F2.5 - 2	56.1	187	na	56.1	9.1	SFO	
					Maximum (n = 12)	**213**	**707**	-	-	-	SFO	
					Geometric mean (n = 12)[(f)]	-	-	**-**	**75.3**	-	SFO	
					Arithmetic mean (n = 12)[(g)]	-	-	**0.353**	**-**	-		
					***p*H-dependency: y/n**	**n**	**-**	**-**	**-**	**-**		

(a) Reference:
1: Ayliffe & Austin (1993)
2: Ayliffe & McMillan-Staff (1994)
3: Ayliffe & Godward (1993)
4: Doble et al. (1996)
5: Simmonds et al. (1996)
6: Ta & Strobush (2012)
7: Ta & Strobush (2015)
8: Crowe (2002)
(b) Soil texture classification not specified
(c) Matrix not specified
(d) Standard conditions
(e) Reduced application rate
(f) Two experiments in Simmonds et al. (1996) averaged (geometric mean)
(g) Two experiments in Simmonds et al. (1996) averaged (arithmetic mean)
(h) In water
(i) From parent

Table B.8.1.2.1.5-6 Summary on aerobic degradation rates of RPA 404766 (Cis-diol) in laboratory studies conducted at 10 °C or reduced soil moisture

Soil origin	Soil type (USDA)	Label	*p*H (Ca Cl_2)	T (°C)	Water content	*DegT 50* (d)	*DegT 90* (d)	*ff*[(d)]	*DegT 50* (d) 20 °C, *p*F2	χ^2 err. (%)	Kinetic model	Ref.[(a)]
UK	Clay loam[(b)]	Ph	6.1[(c)]	10	75 % 33 kPa	140	464	0.405	nc	21.2	P_{HS}→M_{SFO}	1
Manningtree	Sandy loam	Ph	6.1	25	20 % FC	296	983	0.209	nc	7.0	P_{DFOP}→M_{SFO}	2

(a) Reference:
1: Ayliffe & Godward (1993)
2: Simmonds et al. (1996)
(b) Soil texture classification not specified
(c) Matrix not specified
(d) From parent

The RMS AT investigated degradation rates of triticonazole and its metabolites in relation to soil *p*H. No such relationship could be established (see figure below).

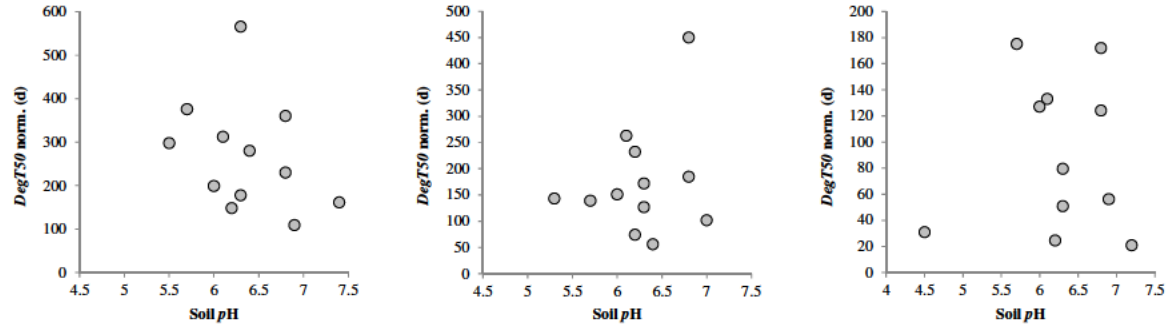


Figure B.8.1.2.1.5-1: Normalized *DegT50* of triticonazole, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) in relation to soil *p*H (measured in various matrices)

The RMS AT notes that the metabolite fractions **'Met 6 (MWT 333)'** and **'Met 7 (MWT 315)'** have been observed in four legacy soil degradation experiments (conducted at 22 °C) at maximum amounts of 12.8, 4.2, 1.6 and 6.2 % AR ('Met 6 (MWT 333)') and 6.5, 0.9, 3.6 and 5.3 % AR ('Met 7 (MWT 315)') (Ayliffe & Austin, 1993; Ayliffe & McMillan-Staff, 1994; Ayliffe & Godward, 1993). Maximum residues were generally observed at the end of incubation (~ 365 days) or close to the end of incubation. In analogy to averaging substance properties (*DegT50* and formation fraction) of the parent and metabolites in the exposure assessment, the RMS AT considers it defendable to conduct the groundwater assessment for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' also on basis of an average (arithmetic mean) occurrence in soil, which is 6.2 and 4.1 % AR for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)', respectively. Coupling the geometric mean *DegT50* of 78.7 days for the parent (i.e. the modelling endpoint derived from field studies, refer to Chapter B.8.1.2.3, summary on field dissipation/degradation) with a conservative *DegT50* of 1000 days for the two metabolite fractions, a maximum occurrence in the exposure modelling of 6.2 and 4.1 % for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)', respectively, is archived if the formation fraction is set to **0.077** and **0.051** for 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)', respectively. On overall, the RMS AT considers residues of these two metabolite fractions observed in legacy studies sufficiently covered by this approach.

Under **anaerobic conditions** triticonazole is considered to be stable.

In comparison to dark conditions, the rate of degradation of triticonazole under conditions of **photolysis on soil surface** is relatively fast (*DissT50* of 65.3 days under environmental conditions, 50 °N). However, as triticonazole is intended to be used as a seed treatment the impact of soil photolysis is negligible.

B.8.1.2.2. Field studies

B.8.1.2.2.1. Soil dissipation studies

Although field dissipation studies were conducted with formulated triticonazole, these studies are reported in this Volume 3CA as they are relevant for deriving modelling endpoints for the active substance and metabolite RPA 406341 (Trans-diol).

Studies submitted for first Annex I inclusion:

- **Wicks & Guyot (1993)**, investigating formulated triticonazole in three European field trials planted with winter wheat (seed treatment)
- **Doble & Parsons (1994)**, investigating formulated triticonazole in one European outdoor lysimeter planted with winter wheat (seed treatment)
- **Wicks (1996)**, investigating formulated triticonazole in four European field trials planted with winter wheat (spray application and seed treatment)
- **Duncan et al. (2003)**, investigating formulated triticonazole in four European field trials planted with winter wheat (spray application)

New studies submitted:

- **Richter (2009)**, investigating RPA 406341 (Trans-diol) in four European field trials on bare soil

New kinetic assessment studies submitted:

- **Huber (2007)**, investigating non-normalized residues of triticonazole in Wicks (1996) and Duncan et al. (2003)
- **Schwarz & Jarvis (2014a)**, investigating time-step normalized residues of triticonazole in Wicks (1996) and Duncan et al. (2003)
- **Huber (2008)**, investigating non-normalized and normalized residues of RPA 406341 (Trans-diol) in Richer (2009)
- **Schwarz & Jarvis (2014b)**, investigating normalized residues of RPA 406341 (Trans-diol) in Richter (2009)

Reference:	**RPA 400727: Field soil study in France**
Author(s), year:	Wicks, R. J., Guyot, C. N., 1993
Report/Doc. Number:	R012975, 200193 / P92/085 / GOoD3866
Guideline(s):	US-EPA guidelines
GLP:	No
Validity:	None reliable (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The dissipation of triticonazole in soil was studied under wheat growing conditions at Muizon (near Reims), Coinces (near Orléans) and Frans (near Lyon) in France over a period of 10 months. The test sites were planted with winter wheat at seed application rates of 147 - 280 kg/ha using seed which had been dressed with triticonazole at a rate of 1.9 g ai/kg seed. The test material was EXP 80378, Lot No. OP910614, containing 211 g/l triticonazole and 87.2 g/l anthraquinone for seed dressing. Three times soil samples were taken in increments of 30 cm down to 0.9 m. Samples were extracted with acetone and analysed by GC (with ECD). The limit of quantification was 5 µg/kg.

Table B.8.1.2.2.1-1 Soil Characteristics (0 - 30 cm stratum)

Field trial	Soil texture[(a)]	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H (water)
Muizon	Loam	43	32	25	1.7	7.8
Coinces	Silty clay loam	10	61	29	2.3	6.6
Frans	Silty clay loam	19	52	29	1.8	5.6

(a) Unknown classification scheme

Findings:

Amounts of triticonazole remaining in soil are given in the table below. Below 30 cm no residues were found above the LOD.

Table B.8.1.2.2.1-2 Determination of triticonazole residues

Site	DAT	Concentration (mg/kg)	Total amount remaining (g/ha) min - max
Muizon	**0**		280
	195	83	160 - 370
	281	50	90 - 230
Coinces	**0**		420
	189	175	320 - 790
	273	120	220 - 540
Frans	**0**		530
	190	80	190 - 360
	279	43	100 - 190

The reduction in residues between the two sampling intervals suggests that the half-life of triticonazole was approximately 4 - 6 months.

Conclusion:

This report can be used as an indicative study only.

Comments (RMS AT):

- The study has some severe deficiencies like only 2 sampling points after the day of application, time between sampling and freezing is not given and a kinetic evaluation is not possible.
- The study was not conducted according to GLP.
- The study is considered **non-reliable**.

Reference:	**Triticonazole (^{14}C-Phenyl): Soil persistence study using lysimeter tubes**
Author(s), year:	Doble, M., Parsons, R. G., 1993
Report/Doc. Number:	R012980, 200248
Guideline(s):	Non-guideline study
GLP:	Yes
Validity:	Supplemental information only (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

An outdoor soil persistence study was carried out with [phenyl-U-^{14}C]-triticonazole formulated (FS) and applied to winter wheat as a seed dressing. PVC tubes (15 cm diameter × 50 cm) were driven into sandy loam soil at RPAL Aldhams Farm Manningtree, Essex, UK. Ten treated seeds were planted in each tube (equivalent to a dose rate of 412 g/ha). Fertilisers and agrochemicals were applied according to normal agricultural practice. At each of 7 sampling points, between 3 and 15 months after sowing, one or two tubes were removed from the soil and cut open. The wheat plants were cut at ground level in the lysimeter tubes. The soil inside was divided into 2.5 cm layers down to a depth of 25 cm and thereafter into 5 cm layers. The amount of radioactivity in each layer as well as in plant samples was determined by soil combustion followed by liquid scintillation counting. The soil layers 0 to 7.5 cm for all time-points, and down to 12.5 cm for the 15 month sample, were extracted and analyses carried out by isocratic HPLC, TLC or LC/MS. Soxhlet extraction with acetonitrile/water was carried out.

Table B. 8.1.2.2.1-3: Soil Characteristics

Soil[(a)]	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H[(b)]	CEC (meq/100 g)	WHC at 0.33 bar (%)
UK sandy loam	73	13.5	13.5	1.43	6.3	5.99	12.0

(a) Texture classification not specified
(b) Matrix non specified

Findings:

At 3 months no radioactivity was detected below 10 cm. At 4 months a small quantity (< 2 % AR) was present in layers below 10 cm. The proportion of radioactivity found below 10 cm increased during the experiment such that at 15 month 17.5 % AR was found below 10 cm, but only 1.3 % AR was found in the 35 to 40 cm soil layer. Several metabolites were separated but not reliably identified. They appeared only in very small amounts (max. single value: 2.2 % AR, 0 - 2.5 cm after 5 months). The number of metabolites detected increased over the course of the study.

Table B.8.1.2.2.1-4 Amount of triticonazole and total radioactivity recovered from lysimeter tubes (% AR)

Months after application	Triticonazole recovered from lysimeter tube	Total recovered from lysimeter tube	Total recovered in crop cover
3	67.2	71.2	na
4	56.0	65.0	1.1
5	49.9	62.2	na
6	56.2	86.7	2.5
7	46.9	73.3	3.6
8	43.1	70.9	na
15	26.6	59.3	na

Table B.8.1.2.2.1-5 Total radioactivity and triticonazole (in bold) recovered from soil tubes, with time and depth (% of AR)

Soil depth	Months after application						
	3	**4**	**5**	**6**	**7**	**8**	**15**
0 - 2.5 cm	**56.3** 59.0	**51.3** 57.5	**37.6** 41.1	**42.4** 60.7	**25.7** 35.2	**18.3** 26.2	**4.1** 8.6
2.5 - 5 cm	**7.4** 8.5	**4.2** 5.2	**10.5** 16.7	**12.6** 20.6	**14.5** 23.0	**12.5** 18.8	**7.8** 15.1
5 - 7.5 cm	**3.3** 3.4	**0.2** 0.8	**1.3** 3.2	**0.4** 1.8	**3.9** 8.9	**5.2** 11.0	**5.3** 10.8
7.5 - 10 cm	0.2	0.2	0.7	0.5	3.2	4.8	**3.3** 7.2
10 - 12.5 cm	0.0	0.0	0.3	0.6	1.2	3.5	**1.7** 4.7
12.5 - 15 cm	0.0	0.0	0.2	0.2	0.9	2.5	3.1
15 - 17.5 cm	0.0	0.2	0.0	0.4	0.3	1.2	2.4
17.5 - 20 cm	0.0	0.0	0.0	0.4	0.3	1.0	2.2
20 - 22.5 cm	0.0	0.2	0.0	0.3	0.0	0.6	1.2
22.5 - 25 cm	0.0	0.3	0.0	0.4	0.2	0.5	0.9

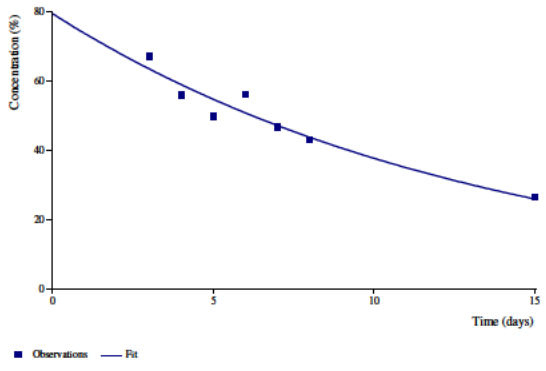
25 - 30 cm	0.0	0.4	0.0	0.9	0.2	0.5	1.2
30 - 35 cm	0.0	0.0	0.0	0.0	0.0	0.2	0.6
35 - 40 cm	0.0	0.3	0.0	0.0	0.0	0.0	1.3
Total radioactivity	71.2	65.0	62.2	86.7	73.3	70.9	59.3

Conclusion:

Total radioactivity recovered from the tubes showed a small decline over the course of the study. At three months after application 71 % was recovered, at 15 months 59 %. HPLC results showed that the proportion of parent compound declined over the course of the study and that the proportion of parent also declined with depth.

Comments (RMS AT):

- As this study does not investigate the degradation in field soil but in outdoor lysimeters, the results can only be used as **supplemental information**.
- The RMS AT notes, that the soil used in this outdoor lysimeter study (i.e. the Manningtree soil) is identical to the UK sandy loam soil used in Ayliffe & Austin (1993). It is worthwhile to notice that under conditions of the outdoor lysimeter conducted for 15 month none of the metabolites exceeded 5 % AR, whereas in the lab RPA 406431 (Trans-diol), RPA 404766 (Cis-diol) and the metabolite fraction 'Met 7 (MWT 315)' were observed above 5 % AR. Based on mass spectroscopic work mol masses (MWT) of 315, 331, 333, 347 and 349 were tentatively attributed to unknown metabolites in this study. This is well in line with findings in Ayliffe & Austin (1993) as well as with more recent laboratory soil degradation experiments.
- Dissipation half-life of triticonazole in this outdoor lysimeter study was calculated by the RMS AT to be 9.32 months, equivalent to approx. 280 days (SFO, χ^2 error = 5.3 %). This result is similar to the degradation rate obtained for the same soil in the lab. Notice that in the figure below the time is given in days whereas it should be in months (one 'day' in the figure equals one month).



Reference:	**Triticonazole: Terrestrial Field Soil Dissipation Study in Europe**
Author(s), year:	Wicks, R. J., 1996
Report/Doc. Number:	R012996, 201284
Guideline(s):	US-EPA
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

A two year field soil dissipation study was conducted to study the environmental behaviour of triticonazole and its main metabolite RPA 406341 (Trans-diol) under wheat growing conditions at four locations in Europe: Italy (Bologna), Germany (Goch), UK (Manningtree) and France (Mereville). In autumn triticonazole was sprayed on the plots at a nominal rate of 240 g ai/ha, incorporated to approximately 5 cm and then winter wheat was planted. An additional plot was used in the UK where winter wheat seed dressed with triticonazole was planted at the same rate. Soil samples from different depths to a maximum of 0.9 m below the surface were then collected at regular intervals and analysed for triticonazole and its metabolite RPA 406341 (Trans-diol). The formulation used for both treatments was a suspension concentrate EXP80441A (lot no. OP920602).

Rainfall was supplemented with irrigation which was generally stopped during the winter months, in accordance with the local practice. Different chemicals were applied to the plots during the course of the study, flurtamone and diflufenican were applied to each sprayed plot on the same day triticonazole was applied.

The weather data for the duration of the study were obtained from nearby weather stations.

Soil samples were taken prior to treatment, within four hours of application, and approximately 0.5, 1, 2 and every 2 months after application until the results of two consecutive samplings were below the limit of quantifiable residues (LOQ 0.005 mg/kg). Triticonazole and RPA 406341 (Trans-diol) were quantified by GC (with TSD). Extractions of soil were either done with acetone for triticonazole or with acetonitrile for the metabolite.

Table B.8.1.2.2.1-6 Soil Characteristics (0 - 10 cm, average of 4 subplots)

Field trial	Texture (USDA)	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H (water)	FC (%)	CEC (meq/100 g)	Biomass[(a)] (µg C/g soil)
Bologna (IT)	Loam	31	43	27	1.62	8.4	22.3	12.9	234
Goch (DE)	Sandy loam	62	24	15	2.04	6.6	13.2	6.2	265
Manningtree (UK)	Sandy loam	61	30	9	1.49	5.3	12.2	5.3	108 (spray) / 118 (seed)
Mereville (FR)	Silty clay loam	4	67	29	2.35	7.8	24.6	17.8	336

(a) Ca. 16 months post application

The climatic conditions during the duration of the study were obtained from nearby weather stations. Summary results on temperature and precipitation are presented in the table below.

Table B.8.1.2.2.1-7 Summary of climatic conditions at the trial sites used to investigate the field dissipation of triticonazole

Location	Bologna, Italy		Goch, Germany		Manningtree, UK		Mereville, France	
Climatic conditions	T_{mean} air [°C]	Rainfall[(a)] [mm]	T_{mean} air [°C]	Rainfall[(a)] [mm]	T_{mean} air [°C]	Rainfall[(a)] [mm]	T_{mean} air [°C]	Rainfall[(a)] [mm]
October 1992	12.5	160	7.8	62	-	-	9.2	65
November 1992	8.1	25	7.9	101	7.2	74	9.1	81
December 1992	3.8	106	3.4	57	3.8	42	4.6	49
January 1993	2.1	2	4.8	69	6.1	62	6.6	64
February 1993	3.0	1	1.6	25	4.1	9	2.4	20
March 1993	7.2	83	6.2	5	5.7	15	7.3	6
April 1993	12.4	80	11.3	53	9.5	57	10.8[(b)]	74
May 1993	18.3	40	14.9	83	12.1	30	14.0	119
June 1993	22.0	55	16.3	39	15.2	41	17.4[(c)]	60
July 1993	22.7	73	16.8	122	15.9	44	17.2[(d)]	23
August 1993	24.3	72	15.6	35	15.6	30	17.9	11
September 1993	18.5	70	13.2	164	13.5	115	18.0	93
October 1993	13.8	73	9.1	80	9.7	96	9.2	89
November 1993	6.2	74	2.2	50	5.0	61	2.6	17
December 1993	3.9	66	5.0	151	5.4	80	6.2	74
January 1994	4.6	56	5.0	111	4.8	63	5.4	61
February 1994	3.5	27	1.4	24	3.3	38	4.5	73
March 1994	11.3	20	7.5	114	7.6	42	9.2	44
April 1994	11.7	124	8.7	68	8.3	56	9.0	43

Location	Bologna, Italy		Goch, Germany		Manningtree, UK		Mereville, France	
Climatic conditions	**T_{mean} air [°C]**	**Rainfall[(a)] [mm]**	**T_{mean} air [°C]**	**Rainfall[(a)] [mm]**	**T_{mean} air [°C]**	**Rainfall[(a)] [mm]**	**T_{mean} air [°C]**	**Rainfall[(a)] [mm]**
May 1994	17.6	29	12.9	63	11.0	57	13.8	67
June 1994	20.8	129	16.3	39	14.8	50	17.1	47
July 1994	25.0	47	16.8	122	19.4	35	22.0	65
August 1994	25.7	19	15.8	35	17.4	69	19.3	61
September 1994	19.3	203	14.0	74	12.5	58	14.0	71
October 1994	12.3	54	9.4	81	9.5	81	11.1	39
November 1994	-	-	10.2	52	8.9	16	-	-

(a) Without irrigation
(b) Average of the available data (day 1 and day 21 are missing)
(c) Average of the available data (day 23 and day 24 are missing)
(d) Average of the available data (day 15 is missing)

Findings:

No triticonazole could be detected after 21 months at Bologna, and at the other sites the residue levels were close to the limit of quantification after 24 months. The metabolite RPA 406341 (Trans-diol) achieved a maximum of 11 % of applied parent (on a parent equivalent basis) at 6 to 10 months after application and could not be detected after 18 months.

Dissipation characteristics were similar at all sites except for Bologna. The relatively reduced dissipation during the four months after application at Bologna may have been due to a combination of low winter temperatures and two extremely dry months. The dissipation rate increased during the spring and summer probably due to warmer and wetter conditions.

Triticonazole remained in the surface to 20 cm layer in soil samples from the four plots except for a few samples when residues were found in the 20 to 30 cm layer. These deeper residues were at or below the limit of quantification. No residues were found below 30 cm. Except for a few detections of RPA 406341 (Trans-diol) between 10 and 20 cm deep the metabolite was confined to the upper 10 cm of soil.

Table B.8.1.2.2.1-8 Determination of residues: Triticonazole and RPA 406341 (Trans-diol), Bologna; field dissipation (as g/ha triticonazole equivalents, mean of four replicates)

DAT	Triticonazole	RPA 406341 (Trans-diol)
0	173.6	0.0
15	132.9	0.0
31	158.4	0.0
57	132.9	0.0
122	169.5	0.0
183	131.8	0.0
246	70.2	nd
301	6.5	nd
365	10.9	0.0
434	10.0	nd
486	19.5	nd
548	0.0	nd
629	3.0	nd
730	0.0	nd

nd denotes not determined

Table B.8.1.2.2.1-9 Determination of residues: Triticonazole and RPA 406341 (Trans-diol), Goch; field dissipation (as g/ha triticonazole equivalents, mean of four replicates)

DAT	Triticonazole	RPA 406341 (Trans-diol)
0	238.1	0.0
14	156.4	0.0
28	116.4	0.0
56	119.6	0.0
119	180.5	2.4
184	72.7	0.0

DAT	Triticonazole	RPA 406341 (Trans-diol)
252	67.3	nd
313	47.1	nd
384	40.5	0.0
448	40.0	nd
504	33.6	nd
547	16.7	nd
644	19.2	nd
744	7.3	nd

nd denotes not determined

Table B.8.1.2.2.1-10 Determination of residues: Triticonazole and RPA 406341 (Trans-diol), Manningtree; field dissipation (as g/ha triticonazole equivalents, mean of four replicates)

	Spray application		Seed treatment	
DAT	**Triticonazole**	**RPA 406341 (Trans-diol)**	**Triticonazole**	**RPA 406341 (Trans-diol)**
0	253.2	0.0	119.8	0.0
15	218.7	0.0	-	-
29	180.9	0.0	235.5	0.0
60	95.7	0.0	152.2	1.4
119	103.2	4.6	195.2	6.8
182	90.9	7.0	185.2	7.3
241	65.0	23.6	66.7	12.1
303	50.0	24.9	61.3	11.5
372	21.7	8.1	43.1	7.7
436	36.9	0.0	49.3	3.8
484	36.9	0.0	35.3	4.1
549	40.2	0.0	8.4	0.0
647	11.8	nd	6.2	n.d.
723	15.1	nd	7.5	n.d.

nd denotes not determined

Table B.8.1.2.2.1-11 Determination of residues: Triticonazole and RPA 406341 (Trans-diol), Mereville; field dissipation (as g/ha triticonazole equivalents, mean of four replicates)

DAT	Triticonazole	RPA 406341 (Trans-diol)
0	197.5	0.0
15	216.2	0.0
34	205.4	0.0
61	124.9	0.0
121	109.3	0.0
183	96.8	22.5
246	81.3	0.0
314	34.9	0.0
373	48.0	0.0
460	47.3	nd
484	76.1	nd
548	48.5	nd
646	37.3	nd
735	16.3	nd

nd denotes not determined

Conclusion:

Total triticonazole residues were below or close to the limit of quantification at all five of the test plots in Europe by the end of the field study. Triticonazole was found to have low mobility under wheat growing conditions at the four sites in Europe. About 95 % of triticonazole residues were found in the upper 10 cm of soil and no residues could be detected below 30 cm.

Comparison of the dissipation between the two treatments (spray and seed dressing) indicates that the method of application has little effect on the dissipation of triticonazole.

Comments (RMS AT):

- The study broadly follows the pertinent guidance for terrestrial field dissipation with some deviations:
  - Historical use is reported for 2 instead for 3 years
  - No untreated control plots were included
  - Duration of shipment is not stated
  - Further shipment at ambient temperature for later sampling intervals (except for DAT 0 and 14)
  - Procedures applied are not always described in detail

  On overall the study is still considered reliable.

- With a nominal application rate of 240 g/ha the field study is clearly overdosed considering an intended application rate of 12.5 g/ha only.

- The RMS AT notes that the study was not conducted on bare soil; instead winter cereals were sown immediately after application or at application (seed treatment in one field trial). In this respect the study does not fulfil the requirements for deriving modelling endpoints (e.g. after time-step normalisation) according to EFSA (2014)[1]. However, as the field study indeed closely mirrors the intended use of triticonazole as a seed treatment, the RMS AT considers degradation rates obtained in this field study appropriate for the intended use in winter cereals. Uses in other crops are not considered to be covered by these field trials. In order to avoid double counting of potential plant uptake, plant uptake has to be switched off in the numerical exposure models.

- The study was kinetically re-assessed by Huber (2007) (non-normalized residues) and Schwarz & Jarvis (2014a) (time-step normalized residues).

Reference:	**Triticonazole: Field soil dissipation study in Europe**
Author(s), year:	Duncan, P., Doran, A., Old, J., 2003
Report/Doc. Number:	C032147, Inveresk 680045
Guideline(s):	Directive 95/36/EC
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The environmental behaviour of triticonazole was studied in the field under winter wheat (year 1) and grass (year 2, except for trial 3 (Balaguer, Spain), where wheat was used in year 2 as well) growing conditions at four locations in Western Europe: Brentwood, UK; St. Trivier sur Moignans, Southern France; Balaguer, Northwest Spain and Goch, Northern Germany. In autumn 2000 the plots were seeded with winter wheat following a single application of triticonazole and incorporation into the soil at a nominal rate of 240 g ai/ha. Soil samples from various soil strata to a maximum of 0.9 m (soil profiles were divided into depths of 0 - 30 cm, 30 - 60 cm and 60 - 90 cm increments) below the surface were collected at regular intervals and analysed for triticonazole and its metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol).

Prior to application, a calibration of the sprayers to be used at each site demonstrated good spray uniformity. Triticonazole was applied in a single application on 26th of October (Brentwood, UK), 1st of December (St.

[1] EFSA (2014) EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662

Trivier sur Moignans, FR), 22th of November (Balaguer, ES) and 25th of October (Goch, DE) to bare soil, at a nominal rate of 240 g ai/ha, and incorporated pre-planting to a depth of ca 5 - 10 cm by rotovation equipment just prior to drilling of winter wheat. Filter papers were placed on the soil surface, five within each sub-plot, randomly sited, just before application and these were removed for analysis after the application was complete. Soil samples were taken soon after application (see below). Rainfall was supplemented with irrigation to maintain the crop and achieve a total precipitation above the average precipitation on a monthly basis. Irrigation was generally stopped during the winter months, in accordance with the local practice. Weather data were collected for the duration of the study from nearby weather stations.

Summary results on temperature and precipitation are presented in the table below.

Table B.8.1.2.2.1-12 Summary of climatic conditions at the trial sites used to investigate the field dissipation of triticonazole

Location	Brentwood (UK)		St. Trivier sur Moignans (FR)		Balaguer (ES)		Goch (DE)	
Climatic conditions	T_{mean} air [°C]	Rainfall[(a)] [mm]	T_{mean} air [°C]	Rainfall[(a)] [mm]	T_{mean} air [°C]	Rainfall[(a)] [mm]	T_{mean} air [°C]	Rainfall[(a)] [mm]
January 2000	4.9	13.8	-	-	-	-	-	-
February 2000	6.3	62.6	-	-	-	-	-	-
March 2000	7.5	14.4	-	-	-	-	-	-
April 2000	8.6	95.1	-	-	-	-	-	-
May 2000	13.0	99.6	-	-	-	-	-	-
June 2000	16.0	19.3	-	-	-	-	-	-
July 2000	15.7	41.4	-	-	-	-	-	-
August 2000	17.5	14.2	-	-	-	-	-	-
September 2000	15.7	76.9	-	-	-	-	15.3	95.8
October 2000	10.8	151.6	-	-	-	-	10.9	110.0
November 2000	7.1	106.6	9.4	141.6	8.6	57.5	7.5	74.6
December 2000	6.1	70.2	7.7	56.3	7.6	41.8	4.7	53.6
January 2001	3.4	57.7	6.1	65.9	7.1	30.8	2.4	87.0
February 2001	4.8	103.5	6.2	37.4	6.7	4.3	4.3	44.4
March 2001	6.0	90.4	11.1	171.9	12.9	26.9	4.9	94.6
April 2001	8.2	63.6	10.2	102.9	12.8	79.2	8.8	77.5
May 2001	12.7	42.1	17.3	70.3	17.8	39.0	14.4	54.6
June 2001	14.5	56.6	18.8	66.9	23.0	7.6	14.7	75.1
July 2001	18.0	63.0	21.7	91.1	23.5	55.9	18.4	69.0
August 2001	18.1	53.3	21.7	93.5	25.6	5.4	18.5	101.6
September 2001	13.6	105.7	14.9	62.8	18.9	28.3	12.7	176.6
October 2001	14.1	106.2	16.0	133.1	17.8	9.0	13.9	65.8
November 2001	6.9	47.0	5.0	43.9	7.2	28.9	5.9	68.0
December 2001	3.3	15.5	1.1	23.0	-0.2	8.2	2.3	40.4
January 2002	5.5	50.8	3.2	27.4	5.7	7.8	3.7	75.4
February 2002	7.6	67.5	8.8	46.3	8.2	4.8	6.8	126.2
March 2002	7.5	34.5	9.8	40.8	11.8	8.6	6.7	40.2
April 2002	9.3	42.0	11.4	23.0	13.6	38.2	9.1	40.6
May 2002	12.3	67.4	13.5	142.2	16.7	26.7	13.5	60.0
June 2002	15.1	44.9	20.4	84.2	22.7	14.9	16.9	73.2
July 2002	16.8	49.8	19.6	110.8	23.9	4.4	17.7	95.0
August 2002	17.8	38.0	19.3	49.9	22.8	38.8	18.7	74.0
September 2002	14.1	29.9	15.7	76.4	21.4	76.4	14.4	31.6
October 2002	10.3	63.4	12.0	100.3	15.3	44.6	9.4	86.8
November 2002	8.7	125.6	9.3	252.3	11.2[(b)]	26.1[(b)]	-	-
December 2002	6.2	101.8	-	-	-	-	-	-

(a) Without irrigation
(b) Average of the available data (day 21-31 are missing)

Soil samples were collected prior to treatment, within four hours after application (time 0), and at approximately 0.5, 1, 2, 4, 6, 8, 10, 12 months and then every 3 months following application. Sampling continued until total residues were less than 10 % of the applied dose and no further useful information could be gained on dissipation or movement of residues. Shortly after application cores consisting of a single 20 cm stratum were taken with a 7.6 cm diameter stainless steel tube. Five cores from each sub-plot (twenty in total) were combined and thoroughly mixed. A sub-sample was then transferred to a labelled container. Samples to a depth of 30 cm were

collected with a device composed of three stainless steel tubes with plastic flanges that allowed the collection of 0 - 10 cm, 10 - 20 cm and 20 - 30 cm strata with a minimal risk of cross-contamination. Deeper increments, if required, were collected with a bucket auger or motorised corer (Humax). All samples were transferred to a freezer as soon as possible after collection. The samples were transported to the analytical laboratory by refrigerated vehicles. Upon reception at the analytical laboratory the samples were transferred to a freezer (~ -20 °C).

The determination of triticonazole, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) was carried out by solid-liquid extraction from soil using sonication and shaking with 0.1 M ammonium hydroxide and acetone, followed by sample clean-up by solid phase extraction using a C_{18} phase. For later time-points a concentration step (by evaporation) was introduced. The three analytes were detected and quantified by HPLC/MS/MS. A similar method was used for analysis of the filter papers. Depth increments were analysed at each interval until a residue-free or a very low level residue stratum was reached. The water content of the soil was determined by drying samples overnight at about 110 °C. The analytical method for each analyte was validated by the analysis of soil portions that had been fortified with the analyte in the laboratory. The levels of fortification were at the limit of quantification (LOQ = 0.002 mg/kg) and 10 × LOQ. Recoveries at each time-point were determined by use of batches of samples at the same two levels.

Determination of biomass was conducted on soil cores taken to depth of 10 cm from throughout each plot. The results of the analyses of the top-soil (0 - 30 cm) and the biomass determinations at each of the sites are presented below.

Table B.8.1.2.2.1-13 Soil Characteristics (0 - 30 cm)

Field trial	Texture (BBA)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/ 100 g)	Biomass at start/finish (µg C/g soil)
Brentwood (UK)	Sandy silt loam	26	58	16	1.9	7.3	9.4	107 / 131
St. Trivier sur Moignans (FR)	Sandy silt loam	22	62	16	1.1	7.1	10.8	157 / 118
Balaguer (ES)	Clay loam	26	55	20	1.2	7.4	11.9	479 / 366
Goch (DE)	Sandy silt loam	27	61	12	0.9	6.7	12.8	142 / 90

Findings:

The results from the method validation experiments are presented in the table below. The mean recoveries at LOQ were 91, 87.2 and 76.1 % for triticonazole, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol), respectively. The corresponding values at 10 × LOQ were 82.5, 88.6 and 79.6 %.

Table B.8.1.2.2.1-14 Recoveries of triticonazole, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) from fortified field soil samples

Matrix	Analyte	Nominal conc. (mg/kg)	Number of replicates	Mean recovery (%)	Precision
Clay loam	Triticonazole	0.002	5	82.4	4.2
		0.020	5	86.6	2.4
	RPA 406341 (Trans-diol)	0.002	5	83.7	4.7
		0.020	5	89.3	3.6
	RPA 404766 (Cis-diol)	0.002	5	82.9	4.3
		0.020	5	87.3	7.2
Sandy silt loam	Triticonazole	0.002	5	81.8	2.8
		0.020	5	89.8	1.8
	RPA 406341 (Trans-diol)	0.002	5	86.7	6.7
		0.020	5	92.1	3.3
	RPA 404766 (Cis-diol)	0.002	5	75.8	4.2
		0.020	5	88.3	7.9

The application rates, calculated from the calibrated sprayer output and the recorded pass time were 240 g/ha to 257 g/ha. Results from filter paper analysis indicated application rates of 153 to 196 g/ha.

The results from the residue analyses for each site for triticonazole and the two metabolites are presented in in the tables below. On occasions it was noted that there was insufficient batch recovery data to meet the protocol

acceptance criteria. Data from these batches are reported for the sake of completeness and are presented in italics in the tables. The tables show the concentrations of the analytes found in the top 10 cm of soil and the total amounts detected as if they had all been in the top 10 cm.

Table B.8.1.2.2.1-15 Levels of triticonazole, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) in soil with time at Brentwood (UK), mean results of four sub-plots

Time-point (months)	Triticonazole (mg/kg, dry weight)		RPA 404766 (Cis-diol) (mg/kg, dry weight)		RPA 406341 (Trans-diol) (mg/kg, dry weight)	
	0 - 10 cm	Total	0 - 10 cm	Total	0 - 10 cm	Total
0.5	0.136	0.138	nd	nd	< 0.002	< 0.002
1	0.129	0.130	nd	nd	< 0.002	< 0.002
2	0.210	0.211	0.005	0.005	0.007	0.007
4	0.091	0.097	0.003	0.004	0.004	0.004
6	0.050	0.055	0.002	0.003	0.003	0.004
8	*0.072*[(a)]	*0.078*[(a)]	0.004	0.004	0.007	0.008
10	0.053	0.057	0.003	0.004	0.006	0.007
12	0.048	0.051	0.003	0.004	0.005	0.006
15	0.045	0.049	0.004	0.005	0.007	0.008
18	0.027	0.031	0.003	0.004	*0.005*[(a)]	*0.005*[(a)]
21	0.035	0.037	*< 0.002*[(a)]	*< 0.002*[(a)]	*0.002*[(a)]	*0.002*[(a)]
24	0.020	0.021	*< 0.002*[(a)]	*< 0.002*[(a)]	*0.002*[(a)]	*0.003*[(a)]

nd denotes not detected
LOQ = 0.002 mg/kg
(a) No valid data due to insufficient batch recovery

Table B.8.1.2.2.1-16 Levels of triticonazole, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) in soil with time at St. Trivier sur Moignans (FR), mean results of four sub-plots

Time-point (months)	Triticonazole (mg/kg, dry weight)		RPA 404766 (Cis-diol) (mg/kg, dry weight)		RPA 406341 (Trans-diol) (mg/kg, dry weight)	
	0 - 10 cm	Total	0 - 10 cm	Total	0 - 10 cm	Total
0.5	0.091	0.092	0.003	0.003	0.003	0.003
1	0.133	0.134	0.006	0.006	0.006	0.006
2	0.087	0.090	0.006	0.006	0.006	0.006
4	0.074	0.080	0.010	0.011	0.013	0.013
6	ns	ns	ns	ns	ns	ns
8	*0.012*[(a)]	*0.013*[(a)]	0.002	0.002	0.003	0.003
10	0.007	0.008	< 0.002	< 0.002	0.003	0.003
12	0.005	0.005	< 0.002	< 0.002	< 0.002	< 0.002
15	0.004	0.005	*< 0.002*[(a)]	*< 0.002*[(a)]	0.002	0.002
18	0.006	0.007	< 0.002	< 0.002	*0.002*[(a)]	*0.003*[(a)]
21	< 0.002	< 0.002	*nd*[(a)]	*nd*[(a)]	nd	nd
24	< 0.002	< 0.002	*nd*[(a)]	*nd*[(a)]	*nd*[(a)]	*nd*[(a)]

nd denotes not detected
ns denotes no sample
LOQ = 0.002 mg/kg
(a) No valid data due to insufficient batch recovery

Table B.8.1.2.2.1-17 Levels of triticonazole, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) in soil with time at Balaguer (ES), mean results of four sub-plots

Time-point (months)	Triticonazole (mg/kg, dry weight)		RPA 404766 (Cis-diol) (mg/kg, dry weight)		RPA 406341 (Trans-diol) (mg/kg, dry weight)	
	0 - 10 cm	Total	0 - 10 cm	Total	0 - 10 cm	Total
0.5	0.130	0.134	< 0.002	< 0.002	< 0.002	< 0.002
1	0.181	0.185	0.004	0.004	0.002	0.002
2	0.081	0.084	< 0.002	< 0.002	0.002	0.002
4	0.059	0.065	*0.004*[(a)]	*0.004*[(a)]	0.006	0.006
6	*0.062*[(a)]	*0.063*[(a)]	*0.005*[(a)]	*0.005*[(a)]	*0.010*[(a)]	*0.010*[(a)]
8	0.089	0.090	0.002	0.002	0.023	0.023
10	0.013	0.015	< 0.002	< 0.002	0.002	0.002
12	0.015	0.015	*< 0.002*[(a)]	*< 0.002*[(a)]	*< 0.002*[(a)]	*< 0.002*[(a)]
15	0.009	0.011	< 0.002	< 0.002	< 0.002	< 0.002

18	0.006	0.006	*< 0.002*[(a)]	*< 0.002*[(a)]	< 0.002	< 0.002
21	0.003	0.004	nd	nd	nd	nd
24	0.004	0.005	< 0.002	< 0.002	< 0.002	< 0.002

nd denotes not detected
LOQ = 0.002 mg/kg
(a) No valid data due to insufficient batch recovery

Table B.8.1.2.2.1-18 Levels of triticonazole, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) in soil with time at Goch (DE), mean results of four sub-plots

Time-point (months)	Triticonazole (mg/kg, dry weight)		RPA 404766 (Cis-diol) (mg/kg, dry weight)		RPA 406341 (Trans-diol) (mg/kg, dry weight)	
	0 - 10 cm	Total	0 - 10 cm	Total	0 - 10 cm	Total
0.5	0.188	0.194	0.004	0.004	0.004	0.004
1	0.141	0.141	0.005	0.005	0.005	0.005
2	0.098	0.098	0.004	0.004	0.005	0.005
4	0.069	0.070	0.007	0.008	0.008	0.008
6	*0.096*[(a)]	*0.097*[(a)]	*0.011*[(a)]	*0.012*[(a)]	*0.024*[(a)]	*0.024*[(a)]
8	0.067	0.069	0.005	0.005	0.013	0.013
10	0.032	0.032	0.003	0.003	0.006	0.006
12	0.042	0.042	0.005	0.005	0.010	0.010
15	0.016	0.016	*0.002*[(a)]	*0.003*[(a)]	0.005	0.005
18	0.029	0.030	0.004	0.005	*0.009*[(a)]	*0.010*[(b)]
21	0.011	0.012	< 0.002	< 0.002	0.003	0.003
24	0.012	0.013	0.002	0.002	0.004	0.004

LOQ = 0.002 mg/kg
(a) No valid data due to insufficient batch recovery

Maximum triticonazole residue levels were detected at the second, third or fourth time-point after application.

The concentrations of the two metabolites, RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol), always remained low. The maximum concentration of RPA 404766 (Cis-diol) detected was 0.010 mg/kg. The concentrations of RPA 406341 (Trans-diol) were generally higher than those of RPA 404766 (Cis-diol) (in line with laboratory experiments) and this compound reached a maximum concentration of 0.023 mg/kg. At the end of the study the concentrations of both metabolites had declined to at or below the LOQ for RPA 404766 (Cis-diol) and at or below 2 × LOQ for RPA 406341 (Trans-diol). It was not possible to derive reliable kinetic data from the results but it was clear that neither metabolite was formed in significant quantities and that the amounts which were formed were dissipated so that there was no likelihood of accumulation.

A summary of the analytical results of deeper soil layers is presented in the table below.

Table B.8.1.2.2.1-19 Levels of triticonazole in different soil layers after application of nominal 240 g ai/ha at four European sites (mg/kg range of 4 subplots)

Months after appl. / soil layer (cm)	0 - 10	10 - 20	20 - 30	30 - 60	60 - 90
	Brentwood (UK)				
0.6 hrs	0 - 20 cm: 0.024 - 0.079		na	na	na
0.5	0.107 - 0.158	nd - 0.003	nd - 0.004	na	na
1	0.083 - 0.166	nd - 0.003	nd	na	na
2	0.169 - 0.257	nd	nd - 0.004	na	na
4	0.053 - 0.153	0.003 - 0.006	< 0.002 - 0.006	na	na
6	0.037 - 0.068	0.003 - 0.004	< 0.002	na	na
8	*0.045 - 0.100*[(b)]	*0.003 - 0.005*[(b)]	*< 0.002*[(b)]	*nd - 0.004*[(b)]	na
10	0.046 - 0.064	< 0.002 - 0.002	< 0.002	nd - 0.002	na
12	0.022 - 0.072	< 0.002 - 0.003	< 0.002	nd - < 0.002	na
15	0.026 - 0.062	< 0.002 - 0.006	< 0.002	nd - < 0.002	nd
18	0.021 - 0.031	< 0.002 - 0.004	< 0.002 - 0.002	< 0.002	nd - < 0.002[(a)]
21	0.021 - 0.043	< 0.002 - 0.003	nd - < 0.002	nd - < 0.002	nd
24	0.016 - 0.023	< 0.002	nd	nd	nd
	St. Trivier sur Moignans (FR)				
Months after appl. / soil layer (cm)	**0 - 10**	**10 - 20**	**20 - 30**	**30 - 60**	**60 - 90**

0.6 hrs	0 - 20 cm: 0.036 - 0.096		na	na	na
0.5	0.038 - 0.124	nd - 0.006	nd	na	na
1	0.075 - 0.246	nd - 0.005	nd	na	na
2	0.021 - 0.121	nd - 0.006	nd	na	na
4	0.065 - 0.085	< 0.002 - 0.008	< 0.002- 0.002	na	na
6	na	na	na	na	na
8	*0.009 - 0.014*[(b)]	*< 0.002*[(b)]	*nd - < 0.002*[(b)]	*nd*[(b)]	na
10	0.004 - 0.009	< 0.002	nd - < 0.002	nd	na
12	0.003 - 0.009	na	na	nd	na
15	0.002 - 0.005	< 0.002	< 0.002 - < 0.002	nd	nd
18	0.004 - 0.008	< 0.002	nd - < 0.002	nd	nd
21	< 0.002	nd	nd	nd	nd
24	nd - < 0.002	nd - < 0.002	nd	nd	nd
		Balaguer (ES)			
Months after appl. / soil layer (cm)	**0 - 10**	**10 - 20**	**20 - 30**	**30 - 60**	**60 - 90**
0.6 hrs	0 - 20 cm: 0.054 - 0.146		na	na	na
0.5	0.047 - 0.216	nd - 0.017	nd	na	na
1	0.117 - 0.244	nd - 0.008	nd	na	na
2	0.058 - 0.126	nd - 0.009	nd	na	na
4	0.045 - 0.086	0.002 - 0.008	< 0.002	na	na
6	*0.021 - 0.099*[(b)]	*nd - 0.028*[(b)]	*nd - 0.002*[(b)]	na	na
8	0.040 - 0.122	nd - < 0.002	nd - < 0.002	nd	na
10	0.006 - 0.033	nd - 0.004	nd	nd	na
12	0.008 - 0.026	nd - < 0.002	nd	nd	na
15	0.006 - 0.014	< 0.002 - 0.003	nd	nd	nd
18	0.002 - 0.009	nd - < 0.002	nd	nd	nd
21	< 0.002 - 0.004	nd - < 0.002	nd	nd	nd
24	0.002 - 0.008	< 0.002	nd	nd	nd
		Goch (DE)			
Months after appl. / soil layer (cm)	**0-10**	**10-20**	**20-30**	**30-60**	**60-90**
0.6 hrs	0 - 20 cm: 0.089 - 0.217		na	na	na
0.5	0.134 - 0.245	0.002 - 0.007	nd	na	na
1	0.097 - 0.179	nd	nd	na	na
2	0.085 - 0.120	nd	nd	na	na
4	0.041 - 0.105	< 0.002	nd - < 0.002	na	na
6	*0.044 - 0.132*[(b)]	*nd - < 0.002*[(b)]	*nd - < 0.002*[(b)]	na	na
8	0.045 - 0.085	< 0.002	nd - < 0.002	nd - < 0.002[(a)]	na
10	0.015 - 0.044	nd - < 0.002	nd	nd	na
12	0.019 - 0.086	nd - < 0.002	nd	nd	na
15	0.009 - 0.030	nd - < 0.002	nd	nd	nd - < 0.002[(a)]
18	0.018 - 0.049	< 0.002	nd - < 0.002	nd - < 0.002[(a)]	nd - < 0.002
21	0.007 - 0.017	nd - < 0.002	nd	nd	nd
24	0.010 - 0.015	nd - < 0.002	nd	nd	nd

na denotes not analysed
nd denotes not detected
(a) Detected only in one of the four subplots
(b) No valid data due to insufficient batch recovery
LOQ: 0.002 mg/kg

In fact the levels of triticonazole detected in the 0 - 20 cm layer were low and those in the 20 - 30 cm layer were very low and sporadic. With the exception of one of the sixteen sub-plots at two sampling time-points the analyses gave lower than LOQ or not detectable for the 30 - 60 cm stratum samples for all sub-plots at all the time-points and lower than LOQ or not detectable for all 60 - 90 cm stratum samples.

In deeper soil layers (below 10 cm) the two soil metabolites were found only in trace amounts (< 0.002 mg/kg) with one exception for metabolite RPA 404766 (Cis-diol): 0.003 mg/kg 6 month after application at the Spain site (10 - 20 cm soil layer), and one exception for metabolite RPA 406341 (Trans-diol): 0.003 mg/kg 15 months after application at the UK site (10 - 20 cm soil layer). Below 30 cm metabolites were not detected (one exception: RPA 404766 (Cis-diol) < 0.002 mg/kg 18 months after application at the UK site, 30 - 60 cm soil depth).

Table B.8.1.2.2.1-20 Levels of soil metabolites after application of nominal 240 g ai/ha (mg/kg range of 4 subplots) (soil layer 0 - 10 cm)

Months after appl.	Brentwood (UK) RPA 404766 (Cis-diol)	Brentwood (UK) RPA 406341 (Trans-diol)	St. Trivier sur Moignans (FR) RPA 404766 (Cis-diol)	St. Trivier sur Moignans (FR) RPA 406341 (Trans-diol)
0.6 hrs	0 - 20 cm: nd	0 - 20 cm: nd	0 - 20 cm: nd	0 - 20 cm: nd
0.5	nd	nd - 0.003	nd - 0.005	nd - 0.004
1	nd	nd - 0.003	0.004 - 0.012	0.004 - 0.11
2	0.004 - 0.006	0.005 - 0.008	nd - 0.009	nd - 0.009
4	0.002 - 0.004	0.003 - 0.005	0.007 - 0.014	0.009 - 0.017
6	0.002 - 0.004	0.003 - 0.004	na	na
8	0.003 - 0.005	0.002 - 0.011	< 0.002 - 0.003	0.002 - 0.003
10	0.003 - 0.004	0.004 - 0.007	nd - < 0.002	< 0.002 - 0.004
12	< 0.002 - 0.006	0.002 - 0.008	< 0.002	< 0.002 - 0.002
15	0.003 - 0.004	0.005 - 0.008	*< 0.002*[(b)]	*< 0.002 - 0.003*
18	0.02 - 0.004	*0.003 - 0.005*[(b)]	< 0.002	*< 0.002 - 0.003*[(b)]
21	*< 0.002 - 0.002*[(b)]	*< 0.002 - 0.003*[(b)]	*nd*[(b)]	nd
24	*< 0.002*[(b)]	*< 0.002 - 0.003*[(b)]	*nd*[(b)]	*nd*[(b)]

Months after appl.	Balaguer (ES) RPA 404766 (Cis-diol)	Balaguer (ES) RPA 406341 (Trans-diol)	Goch (DE) RPA 404766 (Cis-diol)	Goch (DE) RPA 406341 (Trans-diol)
0.6 hrs	0 - 20 cm: nd	0 - 20 cm: nd	0 - 20 cm: nd	0 - 20 cm: nd
0.5	nd - 0.003	nd - 0.003[(a)]	0.003 - 0.007	0.003 - 0.005
1	nd - 0.006	nd - 0.005	nd - 0.009	0.003 - 0.006
2	nd - 0.004	nd - 0.005	0.004 - 0.005	0.004 - 0.005
4	*0.002 - 0.006*[(b)]	0.003 - 0.009	0.004 - 0.012	0.005 - 0.012
6	*0.003 - 0.007*[(b)]	0.005 - 0.014[(b)]	*0.007 - 0.014*[(b)]	*0.017 - 0.034*[(b)]
8	< 0.002 - 0.002	0.016 - 0.032	0.003 - 0.005	0.009 - 0.018
10	nd	< 0.002 - 0.003	< 0.002 - 0.006	0.003 - 0.010
12	*nd - < 0.002*[(b)]	*nd - 0.002*[(b)]	0.003 - 0.007	0.006 - 0.015
15	< 0.002	< 0.002	*< 0.002 - 0.003*[(b)]	0.004 - 0.006
18	*nd - < 0.002*[(b)]	< 0.002	0.003 - 0.006	*0.006 - 0.013*[(b)]
21	nd	nd	< 0.002	< 0.002 - 0.004
24	*nd - < 0.002*[(a)]	nd - < 0.002[(a)]	< 0.002 - 0.002	0.002 - 0.005

na denotes not analysed
nd denotes not detected
(a) Detected only in one of the four subplots
(b) No valid data, due to insufficient batch recovery data
LOQ: 0.002 mg/kg

Conclusion:

Although this study was not initiated as a leaching study some conclusions can be drawn with regard to the leaching potential of triticonazole and its main soil metabolites. In this study triticonazole was found in soil layers below 20 cm only sporadically above the LOQ (0.002 mg/kg) at the UK site. At the other two sites the LOQ was not exceeded. Below 30 cm soil layer triticonazole was not detected at the site in Spain and France, at two occasions (< 0.002 mg/kg) at the German site, and from 8 months after application onwards in amounts of < 0.002 - 0.004 mg/kg at the UK site. This indicates that small amounts of triticonazole migrate through the soil profile rather slowly.

Degradation of triticonazole to its main soil metabolites is obvious. The two soil metabolites (RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol)) were found mainly in the upper soil layer (0 - 10 cm). In deeper soil layers they were found above the LOQ (0.002 mg/kg) only at one sampling point each.

When considering the much lower intended application rate of triticonazole of 12.5 g ai/ha compared to the application in this study (more than 10-fold) it seems to be very unlikely that triticonazole or its metabolites will be detected in deeper soil layers or will leach into groundwater in significant amounts when applied according to the intended use.

Comments (RMS AT):

- The study broadly follows the pertinent guidance for terrestrial field dissipation with some deviations:
    - Historical use is reported for only 2 instead of 3 years
    - At the UK and FR field site other azoles (epoxiconazole, cyproconazole, fluquinconazole, tebucoanzole, propiconazole, difenoconazole) were used in previous years before application of triticonazole
    - No untreated control plots were included
    - The duration of shipment is not stated
    - Procedures applied are not always described in detail
    - Analytical results are of medium quality (scattering data, occasionally insufficient batch recovery)

  On overall the study is still considered reliable.

- With a nominal application rate of 240 g/ha the field study is fairly overdosed considering an intended application rate of 12.5 g/ha only.

- The RMS AT notes that the study was not conducted on bare soil; instead winter cereals were sown immediately after application. In this respect the study does not fulfil the requirements for deriving modelling endpoints after (time-step) normalisation according to EFSA (2014)[2]. However, as the field study indeed closely mirrors the intended use of triticonazole as a seed treatment, the RMS AT considers degradation rates obtained in this field study appropriate for the intended use in winter cereals. Uses in other crops are not considered to be covered by these field trials. In order to avoid double counting of potential plant uptake, plant uptake has to be switched off in the numerical exposure models.

- The study was kinetically re-assessed by Huber (2007) (non-normalized residues) and Schwarz & Jarvis (2014a) (time-step normalized residues).

Reference:	**Field soil dissipation study of RPA 406341 (metabolite of BAS 595 F - Triticonazole) in the formulation EXP 5059144 F on bare soil at four different locations in Europe, 2007-2008**
Author(s), year:	Richter, T., 2009
Report/Doc. Number:	2009/1049703
Guideline(s):	EEC 95/36, EEC 91/414, SETAC Procedures for assessing the environmental fate and behaviour and ecotoxicity of pesticides (March 1995), BBA VI 4-1 (December 1986), ECPA Guidance Document on Field Soil Dissipation Studies Aug. 1997, EPA 171-4(e), IVA-Leitlinie Rückstandsversuche Teil II Lagerstabilität von Rückstandsproben (Frankfurt/Main 1990), SANCO/825/00 rev. 7 (17 March 2004), SANCO/3029/99 rev. 4 (11 July 2000)
GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Field sites, sampling, and analysis

The dissipation of metabolite RPA 406341 (Trans-diol) was studied under bare soil conditions for up to 12 months in Germany, Belgium, South of France and Spain. Basic soil properties for the top layer of the four sites are listed in the table below.

Table B.8.1.2.2.1-21 Basic soil properties of sites

[2] EFSA (2014) EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662

Soil properties	L070921 (Germany)	L070922 (Belgium)	L070923 (France)	L070924 (Spain)
Location	Goch-Nierswalde	Rummen	Meauzac	Alberic/Valencia
Top soil depth [cm]	0 - 30	0 - 30	0 - 20	0 - 30
Soil Type (USDA)	Silt loam	Silt loam	Loam	Clay
Sand [%]	26.6	44.2	48.9	5.8
Silt [%]	70	51.3	40.3	70.3
Clay [%]	3.5	4.4	10.8	23.9
Organic carbon [%]	1.71	1.39	1.19	1.50
Organic matter [%][(a)]	2.95	2.40	2.05	2.59
pH ($CaCl_2$) [-]	4.7	5.1	5.4	7.6

(a) OM = OC × 1.724

The selected fields represented typical regions of agricultural practice and had been under cultivation for many years. The sites were flat without any significant slope. Before commencement of the first sampling, the soil at each trial site was prepared as for sowing and was rolled if considered necessary, but then was left fallow. Field maintenance measurement, crop and pesticide history information were not subjected to GLP.

The trial area at each site was divided into two plots, one untreated control plot (size: 30 - 72 m^2) and one treated plot (size: 168 - 180 m^2) which consisted of four equal sized subplots A, B, C and D that were assigned for replicates. The untreated control plot was subdivided into 2 subsubplots of the equal size. Each of the four treated subplots was subdivided into eight subsubplots of equal size and 2 buffer stripes. The width of the treated subplots was 2.5 or 3 m and adapted to the size of the spraying boom used. The buffer stripes at the beginning and at the end of each treated subplot were treated with the test item but were not sampled. The distance between the treated subplots was at least 2 m, the distance between treated and untreated plot at least 10 m.

In late summer of 2007 (29^{th} of August to 11^{th} of September), RPA 406341 (Trans-diol) was applied using broadcast sprayer on the bare plots at a nominal rate of 100 g/ha. To avoid any potential effect of photolysis the plots were irrigated with a rate of about 10 mm after application to wash in the substance.

No tillage or fertilization was performed during the course of the study from first to last sampling and no crop were grown throughout any of the trials. The plots were kept free of vegetation via the application of glyphosate or acetochlor.

Climatic conditions were based on records of appropriate weather stations located on-site or at a distance of maximal 12 km from site. Monthly summary results on temperature and precipitation are presented in the study report.

Replicate soil specimens (20 per treated plot and 20 per control plot) were taken at intervals up to about 340 days and down to a soil depth of up to 50 cm. At day 0, immediately after application, the treated plots were sampled down to 10 cm only.

Soil samples were analysed for RPA 406341 (Tans-diol) according to the validated method No. 0051, which is presented in chapter CA 4.1.2 of this dossier, i.e. by solid-liquid extraction using sonication and shaking with ammonium hydroxide and acetone, followed by sample clean-up by solid phase using C_{18} phase. The analyte was detected and quantified by HPLC/MS/MS.

Application verification and recovery rates

Procedural recovery experiments were conducted with untreated field soil as well as with untreated LUFA 2.2 soil (during analysis of storage samples) which was used for the Petri dish samples that served as application monitors. Untreated and fortified samples of field soil were analyzed along with the applied Petri dishes as well as with samples from the field. Fortification levels were at 0.01, 2.0 and 5.0 mg/kg. The fortification experiments yielded average recoveries for RPA 406341 (Trans-diol) at 0.01 mg/kg level of 88 ± 10 % (n = 25), at 2.0 mg/kg level of 84 ± 7 % (n = 10) and at 5.0 mg/kg level of 85 ± 7 % (n = 14). These data prove that the analytical method applied is able to accurately determine RPA 406341 (Trans-diol) residues in soil down to a concentration of 0.01 mg/kg. Residues in blank samples were not detectable.

Residue levels of RPA 406341 (Trans-diol) achieved on extraction and analysis of the application monitors (Petri dishes filled with soil LUFA 2.2) were corrected for mean procedural recoveries of the respective analytical set of samples and then converted into residue rates (in g/ha) taking into account the area of the Petri

dishes (91.6 cm^2). The obtained rates ranged from 70 to 94 g/ha (see Table 3 for individual figures) representing 70 - 94 % of the target application rate.

Sample storage and Storage stability
All soil specimens (inclusive of Petri dish samples, main samples and double samples) were placed into freezer storage at about -18 °C within a maximum of 6.5 hours of being taken. The specimens remained frozen at about -18 °C until shipment to BASF SE, Limburgerhof, Germany. For exceptions, the temperature was higher (max. -8 ° C), this was only for a short period and the samples remained in any case frozen.

In order to verify that residues in soil specimens did not deteriorate during the time of storage in the freezers, the storage stability of RPA 406341 (Trans-diol) was checked in frozen soil. The soil arrived in the laboratory in Brazil on September 1th, 2007. From this time the soil was stored at the cold chamber at -20 ° C or cooler. The shipment was conducted at frozen conditions and the samples were homogenised before analysis. For all experiments, LUFA 2.2 soil, batch 07/736/01, was used. Untreated soil aliquots of 5 g were weighed into plastic containers. Five sets of samples were prepared at one time point consisting of 5 specimens each. Each set of samples was intended for an analytical queue covering one nominal sampling time point between 14 and 365 days. Two specimens of each set were spiked at a level of 100 ng/kg and were intended for storage. The other 3 specimens of each set were not initially treated but two of them were intended to be freshly fortified on the day of analysis of the sample set. The fifth specimen remained untreated and served as control sample. An additional set of samples consisting of one untreated and two freshly fortified specimens was prepared and worked up immediately. This set served as the day 0 sample. All samples besides the day 0 samples were stored in the dark at about -20 °C for the intended storage period. These conditions were in agreement with those used for the storage of field residue samples.

The storage stability samples were worked up and analysed for RPA 406341 (Trans-diol) according to the same method used for the analysis of field residue samples.

Results:

Residue data
For all sampling dates and at all sites residue of RPA 406341 (Trans-diol) was only found in the top 10 cm of the soil profile. No movement below this first soil layer occurred.

Table B.8.1.2.2.1-22 Residue data of RPA 406341 (Trans-diol) (mg/kg) for 0 - 10 cm soil depth

Goch-Nierswalde (Germany)		Rummen (Belgium)		Meauzac (France)		Alberic/Valencia (Spain)	
DAT	**mg/kg**	**DAT**	**mg/kg**	**DAT**	**mg/kg**	**DAT**	**mg/kg**
0	0.082	**0**	0.065	**0**	0.044	**0**	0.087
3	0.059	**4**	0.072	**3**	0.041	**2**	0.047
9	0.067	**11**	0.033	**10**	0.028	**12**	0.051
28	0.050	**32**	0.047	**31**	0.025	**30**	0.020
65	0.026	**67**	0.032	**64**	0.020	**62**	0.018
97	0.022	**103**	0.022	**100**	0.025	**96**	0.017
176	0.020	**175**	0.019	**184**	0.017	**182**	0.010
346	< 0.01	**344**	< 0.01	**336**	< 0.01	**351**	< 0.01

nd denotes not detected
LOQ = 0.01 mg/kg

Storage stability
The results show no significant decline of RPA 406341 (Trans-diol) concentrations up to 365 days. From these data it can be concluded that residues of RPA 406341 (Trans-diol) are stable in soil for at least 365 days when stored frozen at about -20 °C. This period covers the maximum storage time from sampling to the first analysis of samples collected during the course of the field soil dissipation study except three samples from the 20 - 30 cm layer. They were analysed later in order to demonstrate two residue free soil layers below the 0 - 10 cm horizon which provide residues.

Conclusion:

The study delivers appropriate data to derive endpoints for subsequent model calculations.

Comments (RMS AT):

- The study follows pertinent guidance and is considered reliable.
- The test substance was applied at late August/early September. This application date is not necessarily representative for the intended use in winter cereals. However, as the peak occurrence of the metabolite RPA 406431 (Trans-diol) under real field situation is roughly around late summer / early autumn in case of application in spring cereals and somewhere in spring in case of application in winter cereals dissipation rates obtained in this study are considered sufficiently robust for trigger endpoints as well as PEC soil calculation.

Reference:	**Determination of trigger endpoints for triticonazole (BAS 595 F) from field dissipation studies**
Author(s), year:	Huber, S., 2007
Report/Doc. Number:	2007/1058036
Guideline(s):	FOCUS Kinetics (2006)
GLP:	Not applicable (modelling study)
Validity:	Partly (refer to comment section)
Status:	**New submission**

Material and methods:

Two field soil dissipation studies (Wicks, 1996, and Duncan et al., 2003) with altogether eight trials across Europe (Germany, UK, France, Italy, Spain) were considered. The parent triticonazole was applied in all trials. Residues of triticonazole in the soil layers were accumulated on a 10-cm basis and used as input for the kinetic evaluation. The simulation modelling was performed with the software package ModelMaker 3.0.4 (Family Genetix Ltd). Trigger endpoints of triticonazole were derived following the recommended procedures outlined by FOCUS (2006).

Results and discussion:

For all but two sites the dissipation behaviour could be best described by bi-phasic kinetics. For the Italian site (Bologna), a modified hockey-stick model was fitted to the data to account for the initial lag-phase (the first degradation rate constant k_1 was fixed to zero). Results are valid for use as persistence endpoints and are presented in the table below:

Table B.8.1.2.2.1-23 Triticonazole: Trigger endpoints in field soils

Study	System	Kinetic model	*DT50* (d)	*DT90* (d)
Wicks (1996)	Bologna (IT)	Modified HS[(a)]	230	360
	Goch (DE)	DFOP	85	632
	Manningtree (UK), spray treatment	DFOP	55	641
	Mereville (FR)	FOMC	133	1237
Duncan et al. (2003)	Brentwood (UK)	DFOP	250	831
	Saint Trivier sur Moignans (FR)	SFO	109	360
	Balaguer (ES)	DFOP	54	398
	Goch (DE)	DFOP	38	500

(a) First degradation rate k_1 fixed to zero to account for the initial lag-phase.

Conclusion:

Field soil dissipation of triticonazole was re-evaluated according to FOCUS (2006). Trigger endpoints for the parent were derived.

Comments (RMS AT):

- Residue data of triticonazole in the field trials are fairly scattered (see figures below) leading to rather high χ^2 errors. Nevertheless, the RMS AT considers them sufficiently robust for kinetic evaluation.

- The RMS AT notes that residue data of triticonazole observed in Wicks (1996) and Duncan et al. (2003) were inconsistently handled in this study (investigating non-normalized residues) and in the next study, Schwarz & Jarvis (2014a), investigating time-step normalized data. This is particularly true with respect to setting of detections < LOQ below detections above LOQ and handling of 'estimated' values < LOQ in Wicks (1996). In order to allow for a consistent fitting approach for both, non-normalized as well as time-step normalized residues, the RMS AT reprocessed triticonazole residues in the following consistent way:

  - Residues < LOQ below residues > LOQ were set to 1/2 LOQ
  - Residues < LOQ below residues < LOQ or non-detects were set to zero
  - 'Estimated' residues < LOQ in Wicks (1996) below residues > LOQ where set to the estimated value
  - 'Estimated' residues < LOQ in Wicks (1996) below residues < LOQ or non-detects were set to zero
  - Residues from samples with insufficient batch recovery (in Duncan et al., 2003, only) where omitted from the fitting procedure

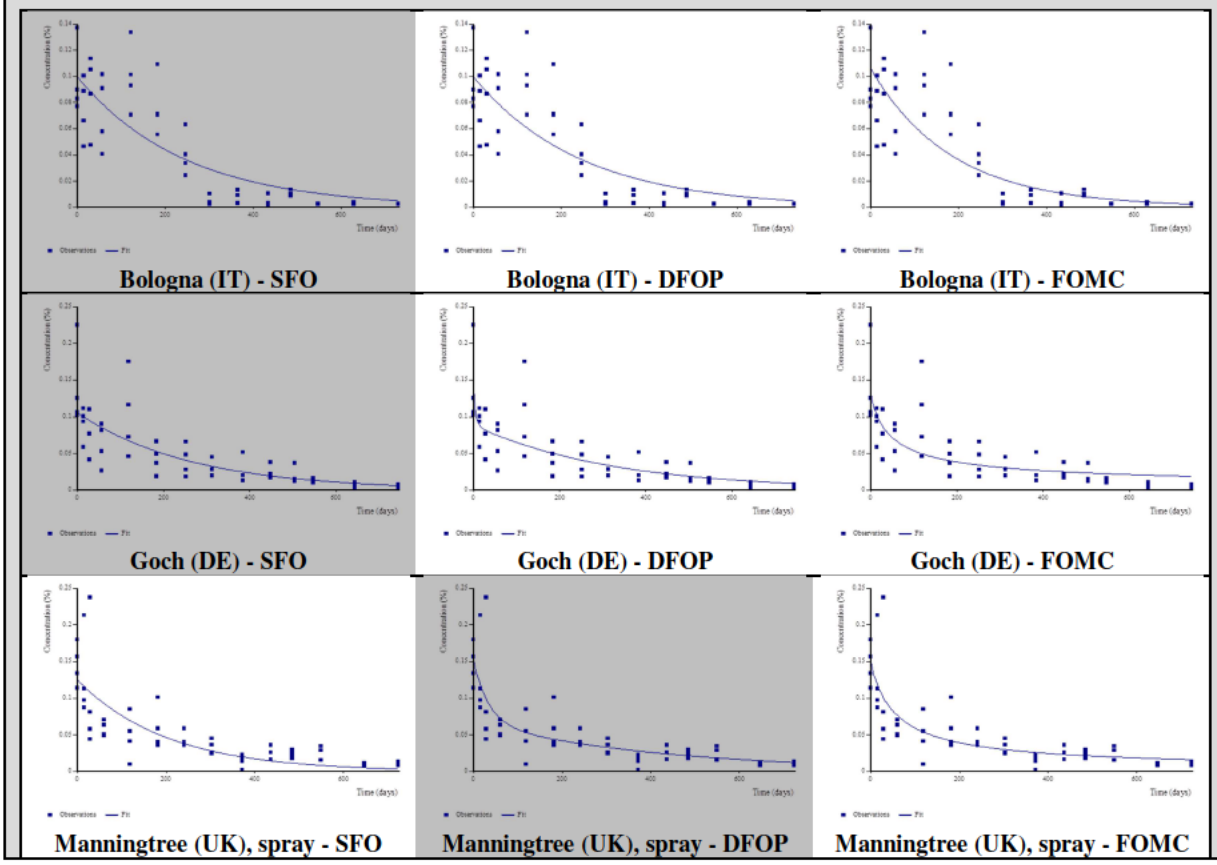
- Following re-processing as stated above the RMS AT re-assessed dissipation rates of triticonazole in both field trials in line with pertinent guidance applying the software tool CAKE 3.3. Results are given below.

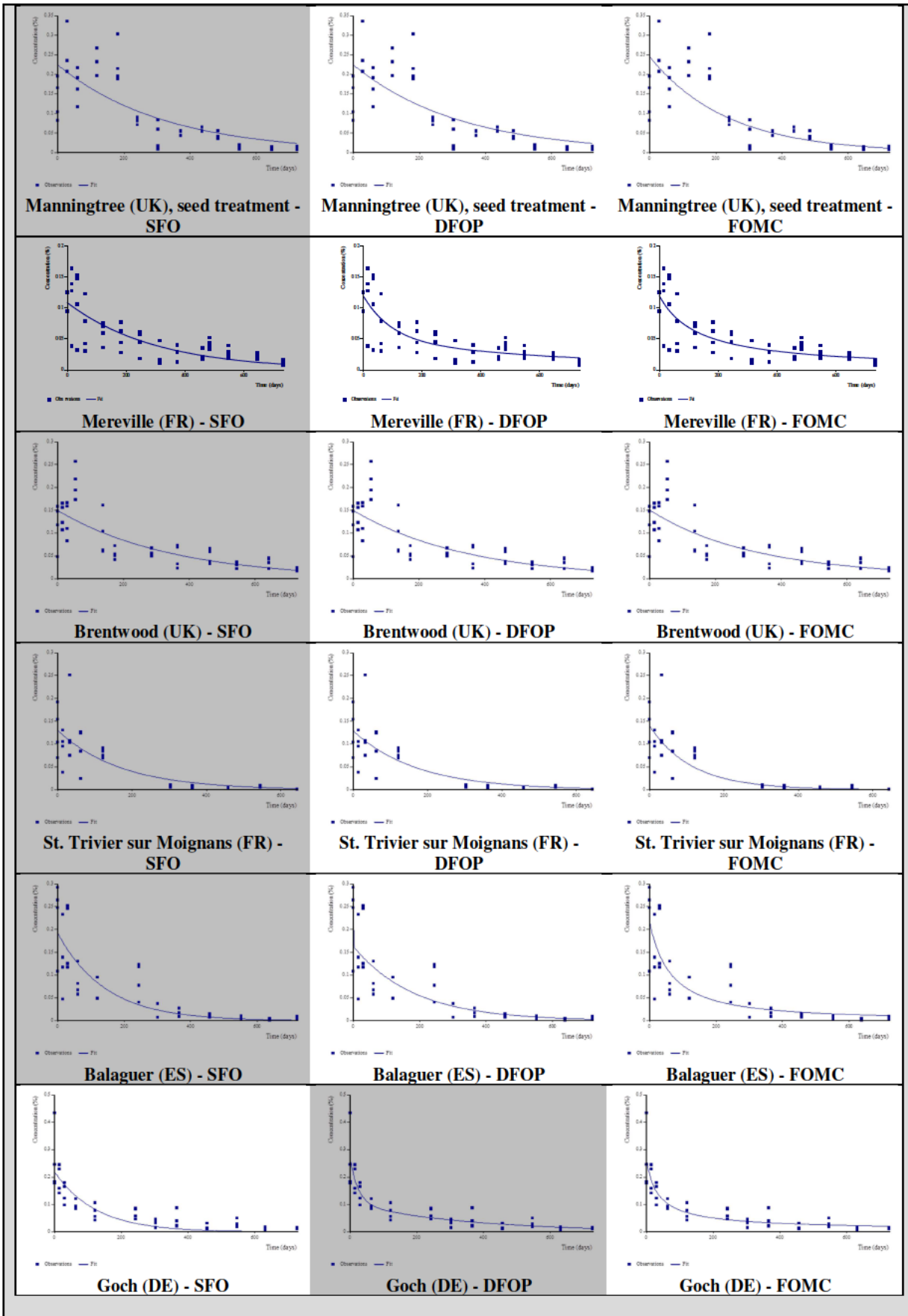
Table B.8.1.2.2.1-24 Field dissipation rates of triticonazole (non-normalized residues) - RMS AT assessment (fits shaded in grey are considered most reliable as trigger endpoints)

Study	Site	Kinetic model	Para-meter	Value	Confidence interval (95%) Lower	Upper	p > t	χ^2 err. (%)	*DissT50* (d)	*DissT90* (d)
Wicks (1996)	Bologna (IT)	**SFO**	**k_1**	**0.004**	**0.003**	**0.005**	**< 0.01**	**32.5**	**169**	**563**
		DFOP	k_1	0.238	nd	nd	nd	34.8	169	563
			k_2	0.004	0.003	0.005	< 0.01			
			g	0.001	nd	nd	na			
		FOMC	α	38	30	47	na	33.9	129	436
			β	6990	6120	7860	na			
	Goch (DE)	**SFO**	**k_1**	**0.004**	**0.002**	**0.005**	**< 0.01**	**28.5**	**183**	**609**
		DFOP	k_1	0.182	-0.465	0.830	0.29	22.8	76.8	598
			k_2	0.003	0.002	0.004	< 0.01			
			g	0.37	0.15	0.58	na			
		FOMC	α	0.58	0.16	1.01	na	29.9	64.3	1430
			β	28.29	-25.27	81.85	na			
	Manningtree (UK), spray	SFO	k_1	0.005	0.003	0.007	< 0.01	23.1	140	465
		DFOP	**k_1**	**0.029**	**-0.006**	**0.064**	**0.05**	**13.5**	**55.0**	**633**
			k_2	**0.002**	**0.000**	**0.005**	**0.03**			
			g	**0.56**	**0.23**	**0.90**	**na**			
		FOMC	α	0.78	0.21	1.35	na	14.4	62.7	798
			β	43.56	-27.87	115.00	na			
	Manningtree (UK), seed treatment	**SFO**	**k_1**	**0.003**	**0.002**	**0.004**	**< 0.01**	**38.2**	**223**	**741**
		DFOP	k_1	0.003	-0.288	0.294	0.49	41.2	223	741
			k_2	0.003	-90.790	90.790	0.50			
			g	1.00	-6893.00	6900.00	na			
		FOMC	α	170	133	206	na	39.6	162	541
			β	39500	38600	40400	na			
	Mereville (FR)	**SFO**	**k_1**	**0.003**	**0.002**	**0.004**	**< 0.01**	**17.6**	**204**	**678**
		DFOP	k_1	0.010	-0.007	0.028	0.12	14.2	126	1130
			k_2	0.001	-0.002	0.005	0.26			
			g	0.61	-0.14	1.36	na			
		FOMC	α	1.0	-0.1	2.1	na	14.1	132	1200
			β	129.8	-135.8	395.5	na			

Duncan et al. (2003)	Brentwood (UK)	**SFO**	**k_1**	**0.003**	**0.002**	**0.004**	**< 0.01**	**27.8**	**242**	**803**
		DFOP	k_1	0.003	-0.016	0.021	0.38	30.2	241	805
			k_2	< 0.001	-3.791	3.791	0.50			
			g	1.00	-7.29	9.28	na			
		FOMC	α	8	-82	99	na	28.8	234	857
			β	2750	-28970	34500	na			
	St. Trivier sur Moignans (FR)	**SFO**	**k_1**	**0.006**	**0.003**	**0.009**	**< 0.01**	**21.1**	**118**	**392**
		DFOP	k_1	4.801	-2862.000	2870.000	0.5	23.5	116	393
			k_2	0.006	0.002	0.009	< 0.01			
			g	0.02	-0.34	0.39	na			
		FOMC	α	28	-13	68	na	22.6	78.9	270
			β	3090	-3717	9900	na			
	Balaguer (ES)	**SFO**	**k_1**	**0.007**	**0.004**	**0.010**	**< 0.01**	**31.4**	**99.1**	**329**
		DFOP	k_1	1.198	0.778	1.617	< 0.01	29.2	65.9	362
			k_2	0.005	0.003	0.008	< 0.01			
			g	0.28	0.09	0.48	na			
		FOMC	α	1.3	-0.2	2.8	na	30.0	58.3	398
			β	84.7	-81.2	250.6	na			
	Goch (DE)	SFO	k_1	0.008	0.005	0.011	< 0.01	25.0	85.9	285
		DFOP	**k_1**	**0.040**	**0.003**	**0.076**	**0.02**	**8.2**	**36.1**	**477**
			k_2	**0.003**	**0.001**	**0.005**	**0.01**			
			g	**0.60**	**0.34**	**0.87**	**na**			
		FOMC	α	0.8	0.4	1.2	na	9.8	39.0	512
			β	26.4	-5.1	57.9	na			

Table B.8.1.2.2.1-25 Fits on field dissipation rates of triticonazole (non-normalized residues) - RMS AT assessment (fits shaded in grey are considered most reliable as trigger endpoints)





Manningtree (UK), seed treatment - SFO

Manningtree (UK), seed treatment - DFOP

Manningtree (UK), seed treatment - FOMC

Mereville (FR) - SFO

Mereville (FR) - DFOP

Mereville (FR) - FOMC

Brentwood (UK) - SFO

Brentwood (UK) - DFOP

Brentwood (UK) - FOMC

St. Trivier sur Moignans (FR) - SFO

St. Trivier sur Moignans (FR) - DFOP

St. Trivier sur Moignans (FR) - FOMC

Balaguer (ES) - SFO

Balaguer (ES) - DFOP

Balaguer (ES) - FOMC

Goch (DE) - SFO

Goch (DE) - DFOP

Goch (DE) - FOMC

Reference:	**Determination of normalised rates of decline for triticonazole from two field dissipation studies**
Author(s), year:	Schwarz, N., Jarvis, T., 2014a
Report/Doc. Number:	2014/1083344
Guideline(s):	FOCUS Kinetics (2006)
GLP:	Not applicable (modelling study)
Validity:	Partly (refer to comment section)
Status:	**New submission**

Material and methods:

Two field soil dissipation studies carried out at eight sites in different regions of Europe (Italy, Germany, UK, France, Spain) were considered (Wicks, 1996, and Duncan et al., 2003). The parent triticonazole was applied onto bare soil at a nominal application rate of 240 g ai/ha and then incorporated into the soil on the same day and winter wheat was then planted. The application of triticonazole was conducted as spray application at all sites. At one site (Manningtree, UK) the application was additionally carried out as seed treatment. Residue data of triticonazole in different depths (in percentage of applied) were obtained from the studies and used as input for the kinetic evaluation. Replicates from four subplots per trial site were considered.

Due to the incorporation of triticonazole into soil, the EFSA (2010) recommendation of incorporation to about 10 cm to prevent surface processes taking place was considered to be fulfilled and all data points were considered for the kinetic evaluation.

The field data were normalised to 20 °C and *p*F2 using the time-step normalisation approach. The PERSIST model was used to calculate normalised day lengths based on temperature and moisture data which requires that daily average soil moisture and temperature data are either directly available or can be calculated from other data, e.g. daily maximum/minimum air temperatures. Weather data from all sites were provided in the reports and were sufficient for normalisation.

The simulation modelling was performed using KinGUI Version 2. Degradation rates of triticonazole were derived. FOCUS (2006, 2011) approaches were used to determine the appropriate kinetic fit in each soil.

Results and discussion:

In general, the replicate results from the subplots showed high variability and hence in all cases the χ^2 error values were considerably high.

The SFO model did not always provide acceptable fits. Biphasic degradation kinetics (FOMC or DFOP) were considered more appropriate at Manningtree (UK, spray treatment), Balaguer (ES), Goch (DE) and Mereville (FR), both by statistical and visual measure. There was no significant difference in the *DegT50* values for spray application and seed treatment at the Manningtree site, hence indicating that the differing methods of application did not affect the degradation rate. The derived modelling endpoints are shown in the table below.

Table B.8.1.2.2.1-26 Triticonazole - soil degradation modelling endpoints from field studies

Study	Site	Application method	Kinetic Model	χ^2 error (%)	*DegT50* at 20 °C, *p*F2 (d)	*DegT90* at 20 °C, *p*F2 (d)
Wicks, 1996	Bologna (IT)	Spray	SFO	22.8	75.5	251
	Goch (DE)	Spray	DFOP	21.6	81.4[(a)]	211
	Manningtree (UK)	Spray	FOMC	15.7	92.2[(b)]	306
	Manningtree (UK)	Seed treatment	SFO	36.5	88.8	295
	Mereville (FR)	Spray	DFOP	14.1	252[(a)]	467
Duncan et al, 2003	Brentwood (UK)	Spray	SFO	32.9	100	333
	Saint Trivier sur Moignans (FR)	Spray	SFO	19.3	49.5	165
	Balaguer (ES)	Spray	FOMC	33.4	57.2[(b)]	190
	Goch (DE)	Spray	FOMC	12.6	52.4[(b)]	174

(a) Calculated using the slow degradation rate: $\ln(2)/k_2$
(b) Calculated as follows: *DT90*/3.32

Conclusion:

Field soil dissipation of triticonazole was re-evaluated according to FOCUS (2006, 2001) and EFSA (2010). Modelling endpoints for the parent were derived.

Comments (RMS AT):

- Residue data of triticonazole in the field trials are fairly scattered (see figures below) leading to rather high χ^2 errors. Nevertheless, the RMS AT considers them sufficiently robust for kinetic evaluation.

- The RMS AT is not in the positon to fully re-do the time-step normalization provided by the study authors applying the PERSIST model. However, the information provided in the study report is fairly detailed and considered sufficient to conclude on the appropriateness of the time-step normalization procedure performed by the study authors.

- As already noted in Huber (2007) (study before) residue data of triticonazole observed in Wicks (1996) and Duncan et al. (2003) were inconsistently handled in Huber (2007), investigating non-normalized residues, and in this study, investigating time-step normalized data, This is particularly the case with respect to setting of detections < LOQ below detections above LOQ and handling of 'estimated' values < LOQ in Wicks (1996). In order to re-assess the kinetic evaluation of the time-step normalized residues of triticonazole the RMS AT reprocessed triticonazole residues in a consistent way as given in Huber (2007).

- The RMS AT notes that residues at study end (2 years study duration) where on average clearly below 10 % of the initial dose (with the exception of the Brentwood field trial, ~ 17 %, and the Mereville field trial, ~ 10 %) thus giving preference to the FOMC model in case of biphasic degradation patterns according to pertinent guidance in most cases. However, as the FOMC model did not deliver fully reliable fits (with 95th confidence interval of α and β including zero in most cases), biphasic models other than FOMC where tested by the RMS AT and partly accepted as the most reliable degradation model. However, as final residues were clearly below 10 % of the initial dose in all of these cases, the RMS AT recommends deriving a pseudo modelling *DegT50* from the overall DFOP or HS *DegT90* divided by 3.32 in line with the usual FOMC approach instead of applying an overly conservative slow-phase DFOP or HS *DegT50*.

- The RMS AT redid the kinetic evaluation following pertinent guidance applying CAKE 3.3 on basis of revised residue data (as indicated above). Results on RMS AT fits are given below.

- It may be noted that all field trials have been planted with winter cereals shortly after application of triticonazole (in one case, Manningtree, treated seeds from winter cereals have been applied). In principal, this is not in line with the EFSA guidance on *DegT50* (EFSA, 2014)[3] recommending the soil to be kept free from any vegetation in order to exclude any possible uptake by plants. However, as the intended use is seed treatment in winter cereals the RMS AT considers the *DegT50* values obtained in these field trials at least sufficiently robust for the intended use. Notice that in the exposure model plant uptake has to be set to zero in order to avoid double counting of plant uptake. Any use of *DegT50* values obtained in these field trials in crops other than winter cereals or at deviating crop stages in winter cereals is subject to some uncertainties.

- Actual and time-step normalized days are not given in the applicant study summary. These data are provided in the table below.

Table B.8.1.2.2.1-27 Actual and time-step normalised days after application of triticonazole in Wicks (1996)

Bologna (IT)	Goch (DE)	Manningtree (UK)	Mereville (FR)

[3] EFSA (2014) EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662

Sample day	Normalised day	Sample day	Normalised day	Sample day	Normalised day	Sample day	Normalised day
0	0.0	**0**	0.0	**0**	0.0	**0**	0.0
15	7.5	**14**	4.0	**15**	4.40	**15**	5.4
31	12.8	**28**	8.2	**29**	8.4	**34**	11.9
57	20.8	**56**	15.8	**60**	16.7	**61**	20.8
122	32.5	**119**	27.1	**119**	33.8	**121**	36.2
183	52.7	**184**	44.0	**182**	57.4	**183**	53.8
246	110.8	**252**	87.2	**241**	97.5	**246**	91.9
301	182.4	**313**	129.4	**303**	142.5	**314**	142.5
365	234.4	**384**	160.6	**372**	174.1	**373**	177.6
434	255.1	**448**	174.4	**436**	189.5	**460**	200.8
486	266.8	**504**	186.1	**484**	200.7	**484**	207.8
548	289.7	**547**	198.4	**549**	224.0	**548**	246.7
629	363.3	**644**	256.0	**647**	295.9	**646**	301.3
730	463.7	**744**	317.9	**723**	332.6	**735**	375.2

Table B.8.1.2.2.1-28 Actual and time-step normalised days after application of triticonazole in Duncan et al. (2003)

Brentwood (UK)		Saint Trivier sur Moignans (FR)		Balaguer (ES)		Goch (DE)	
Sample day	Normalised day	Sample day	Normalised day	Sample day	Normalised day	Sample day	Normalised day
0	0.0	**0**	0.0	**0**	0.0	**0**	0.0
15	5.5	**14**	7.2	**15**	5.8	**14**	5.9
29	8.7	**33**	12.3	**30**	9.6	**30**	10.6
54	18.3	**62**	19.5	**61**	18.3	**63**	19.5
138	31.4	**122**	36.4	**120**	38.1	**121**	27.4
174	41.4	**181**	71.1	**181**	70.3	**181**	41.9
221	63.6	**249**	137.1	**245**	139.1	**243**	79.2
286	108.4	**304**	188.7	**301**	202.1	**303**	136.3
364	163.5	**363**	205.9	**365**	240.6	**366**	177.9
462	185.0	**459**	224.0	**457**	256.2	**457**	194.1
544	209.6	**545**	264.0	**552**	307.6	**547**	221.2
642	272.9	**644**	361.0	**638**	399.5	**632**	281.3
727	321.8	**721**	405.4	**720**	467.9	**727**	348.0

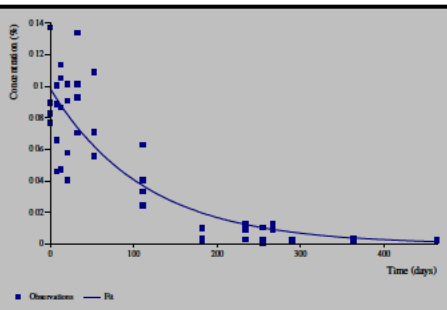
Table B.8.1.2.2.1-29 Degradation rates of triticonazole (time-step normalized) in European field trials - RMS AT assessment (fits shaded in grey are considered most reliable for deriving modelling endpoint)

Study	Field trial	Kinetic model	Par a-met er	Value	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*DegT 50* (d)	*DegT 90* (d)	Fast phase *DegT 50* (d)	Slow phase *DegT 50* (d)	Mod-elling *DegT 50* (d)
Wicks (1996)	Bologna (IT)	**SFO**	***k***	**0.009**	**0.006**	**0.011**	**< 0.01**	**20.7**	**78.9**	**262**	**na**	**na**	**78.9**
		DFOP	k_1	10.070	-30690	30700	0.50	22.2	78.1	262	0.0688	79.1	78.9
			k_2	0.009	0.006	0.012	< 0.01						
			g	0.009	-0.419	0.437	na						
		HS	k_1	0.006	-0.071	0.083	0.44	22.1	80.1	262	115	78.5	78.9
			k_2	0.009	0.006	0.012	< 0.00						
			t_b	5.2	-90.6	101.0	na						
		FOMC	α	64	52	76	na	21.6	54.8	184	na	na	55.5
			β	5030	nd	nd	na						
	Goch (DE)	**SFO**	***k***	**0.010**	**0.006**	**0.014**	**< 0.01**	**28.7**	**66.9**	**222**	**na**	**na**	**66.9**
		DFOP	k_1	0.510	-0.644	1.665	0.19	20.8	21.9	220	1.36	85.3	66.3
			k_2	0.008	0.004	0.012	< 0.01						
			g	0.403	0.211	0.595	na						
		HS	k_1	0.010	0.006	0.015	< 0.01	30.7	66.9	229	66.9	76.8	69.0
			k_2	0.009	-0.016	0.034	0.24						
			t_b	176.7	127.2	226.2	na						
		FOMC	α	0.52	0.20	0.83	na	26.8	17.8	535	na	na	161
			β	6.32	-4.46	17.09	na						
	Manning-tree, spray	SFO	*k*	0.011	0.007	0.016	< 0.01	27.7	61.9	206	na	na	61.9
		DFOP	k_1	**0.101**	**-0.004**	**0.206**	**0.03**	**13.0**	**15.4**	**281**	**6.88**	**140**	**84.6**

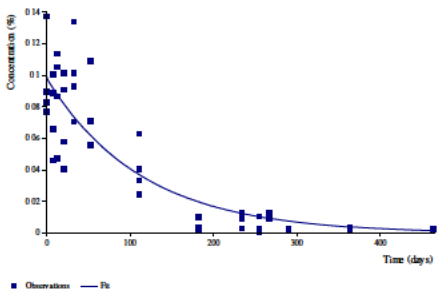
	(UK)		**k_2**	**0.005**	**0.000**	**0.010**	**0.02**						
			g	**0.597**	**0.344**	**0.851**	**na**						
		HS	k_1	0.028	0.014	0.041	< 0.01	23.8	25.1	> 1000	25.1	> 1000	na
			k_2	< 0.001	-0.007	0.007	0.01						
			t_b	64.3	19.7	108.9	na						
		FOMC	α	0.59	0.24	0.94	na	15.2	18.4	392	na	na	118
			β	8.33	-4.57	21.22	na						
	Manning-tree, seed treatment (UK)	**SFO**	**k**	**0.008**	**0.005**	**0.010**	**< 0.01**	**33.2**	**90.4**	**300**	**na**	**na**	**90.4**
		DFOP	k_1	0.008	-0.019	0.034	0.28	35.8	90.4	301	90.3	> 1000	90.7
			k_2	< 0.001	-14.270	14.270	0.50						
			g	0.999	-2.693	4.692	na						
		HS	k_1	0.007	0.005	0.009	< 0.01	34.9	101	216	101	16.5	65.1
			k_2	0.042	-0.347	0.431	0.41						
			t_b	192.4	50.4	334.4	na						
		FOMC	α	28	23	34	na	34.7	64.5	220	na	na	66.3
			β	2620	nd	nd	na						
	Mereville (FR)	SFO	k	0.008	0.005	0.010	< 0.01	20.8	91.4	304	na	na	91.4
		DFOP	k_1	0.034	-0.007	0.075	0.05	13.8	40.6	540	20.6	281	163
			k_2	0.002	-0.003	0.008	0.18						
			g	0.622	0.198	1.046	na						
		HS	**k_1**	**0.019**	**0.008**	**0.031**	**< 0.01**	**13.5**	**35.7**	**441**	**35.7**	**191**	**133**
			k_2	**0.004**	**0.000**	**0.007**	**0.02**						
			t_b	**44.2**	**8.2**	**80.2**	**na**						
		FOMC	α	0.7	0.1	1.3	na	14.2	45.3	663	na	na	200
			β	27.8	-21.4	77.0	na						
Duncan et al. (2003)	Brentwood (UK)	**SFO**	**k**	**0.007**	**0.004**	**0.010**	**< 0.01**	**30.3**	**101**	**337**	**na**	**na**	**101**
		DFOP	k_1	0.013	-0.028	0.055	0.26	32.3	77.4	720	51.5	502	217
			k_2	0.001	-0.024	0.027	0.46						
			g	0.730	-1.422	2.882	na						
		HS	k_1	0.011	0.001	0.021	0.02	31.9	63	450	63	175	136
			k_2	0.004	-0.003	0.011	0.11						
			t_b	73.8	-58.2	205.8	na						
		FOMC	α	1.8	-3.2	6.8	na	31.0	83.3	466	na	na	140
			β	172.9	-517.5	863.2	na						
	St. Trivier sur Moignans (FR)	**SFO**	**k**	**0.014**	**0.004**	**0.023**	**< 0.01**	**16.9**	**51.2**	**170**	**na**	**na**	**51.2**
		DFOP	k_1	2.162	-14150	14200	0.50	18.6	49.8	173	0.321	53.2	52.1
			k_2	0.013	0.001	0.026	0.02						
			g	0.043	-0.322	0.409	na						
		HS	k_1	0.012	-0.010	0.035	0.14	18.7	52.5	161	55.6	46.5	48.5
			k_2	0.015	-0.005	0.034	0.07						
			t_b	36.5	-636.0	709.1	na						
		FOMC	α	117	71	164	na	17.8	31.8	106	na	na	32.0
			β	5360	nd	nd	na						
	Balaguer (ES)	SFO	k	0.037	0.016	0.058	< 0.01	36.7	18.6	61.8	na	na	18.6
		DFOP	k_1	0.102	-0.038	0.242	0.07	29.2	15.9	241	6.78	116	72.6
			k_2	0.006	0.000	0.012	0.02						
			g	0.575	0.194	0.955	na						
		HS	**k_1**	**0.046**	**0.020**	**0.071**	**< 0.01**	**28.5**	**15.2**	**245**	**15.2**	**111**	**73.8**
			k_2	**0.006**	**0.001**	**0.012**	**0.01**						
			t_b[(a)]	**20**	**0**	**39**	**na**						
		FOMC	α	0.75	0.22	1.28	na	30.0	16.6	225	na	na	67.8
			β	10.91	-5.93	27.75	na						
	Goch (DE)	SFO	k	0.046	0.029	0.063	< 0.01	26.1	15.2	50.3	na	na	15.2
		DFOP	**k_1**	**0.095**	**0.021**	**0.168**	**0.01**	**9.4**	**12.2**	**208**	**7.34**	**133**	**62.7**
			k_2	**0.005**	**-0.001**	**0.011**	**0.04**						
			g	**0.705**	**0.456**	**0.953**	**na**						
		HS	k_1	0.053	0.034	0.072	< 0.01	8.0	13.2	210	13.2	118	63.3
			k_2	0.006	0.001	0.010	0.01						
			t_b	22.9	10.3	35.6	na						
		FOMC	α	0.72	0.34	1.09	na	12.1	12.7	186	na	na	56.1
			β	7.76	-1.12	16.64	na						

(a) Initial guess = 20 days (based on visual inspection)

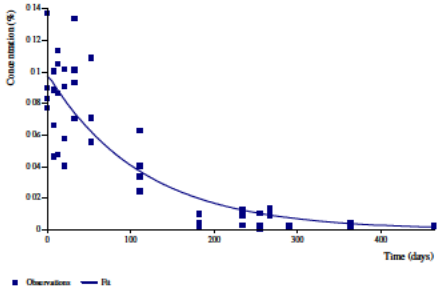
Table B.8.1.2.2.1-30 Fits on degradation rates of triticonazole (time-step normalized) in European field trials - RMS AT assessment (fits considered most reliable are shaded in grey)



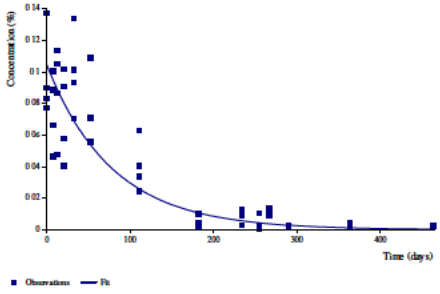
Bologna, Wicks (1996) - SFO



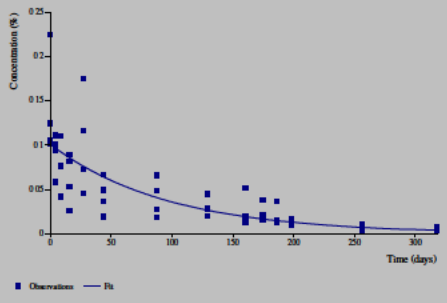
Bologna, Wicks (1996) - DFOP



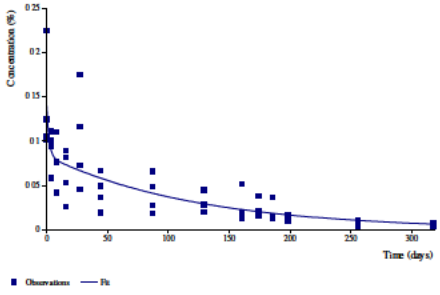
Bologna, Wicks (1996) - HS



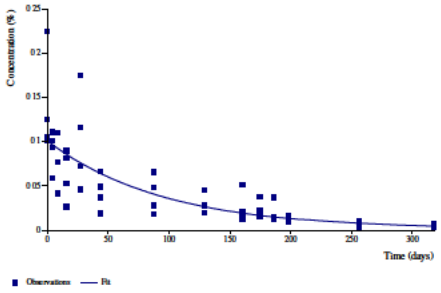
Bologna, Wicks (1996) - FOMC



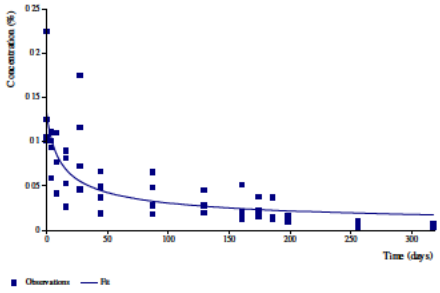
Goch, Wicks (1996) - SFO



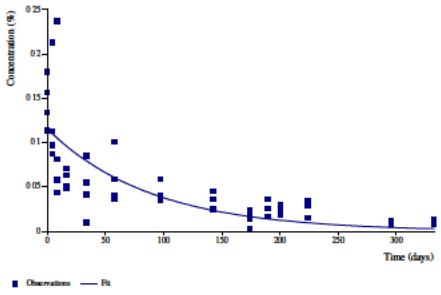
Goch, Wicks (1996) - DFOP



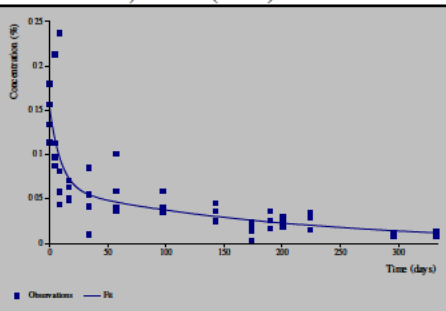
Goch, Wicks (1996) - HS



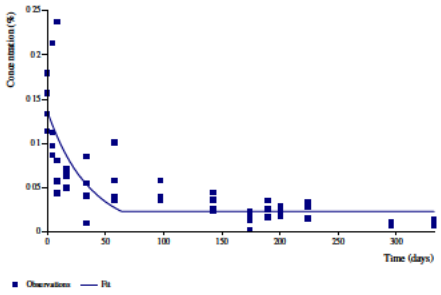
Goch, Wicks (1996) - FOMC



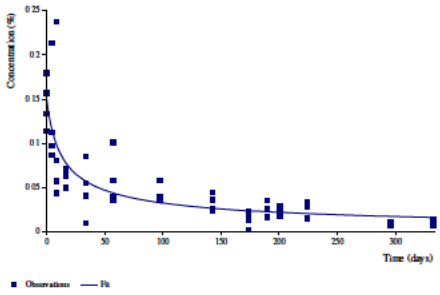
Manningtree (spray), Wicks (1996) - SFO



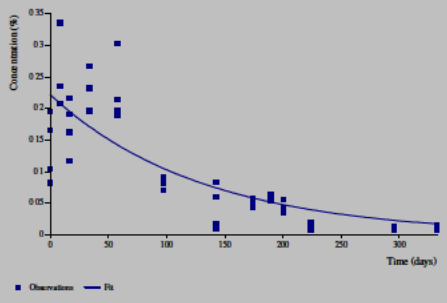
Manningtree (spray), Wicks (1996) - DFOP



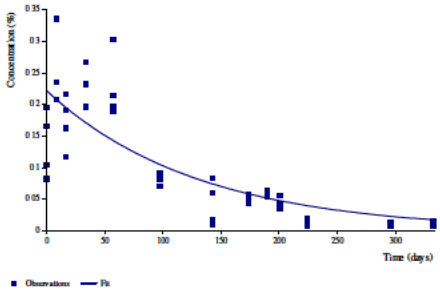
Manningtree (spray), Wicks (1996) - HS



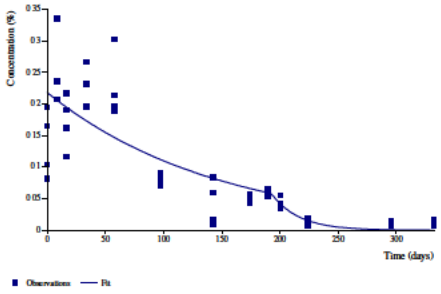
Manningtree (spray), Wicks (1996) - FOMC



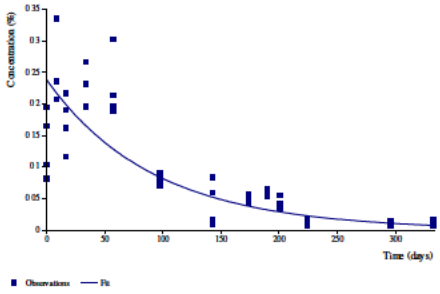
Manningtree (seed treatment), Wicks (1996) - SFO



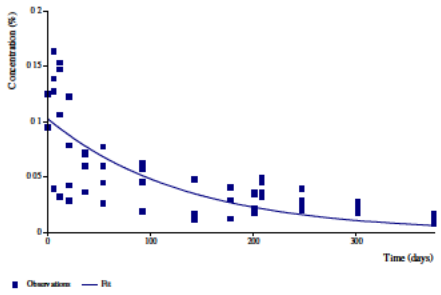
Manningtree (seed treatment), Wicks (1996) - DFOP



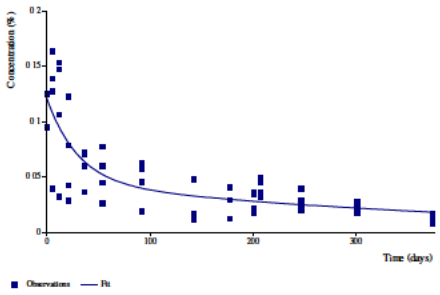
Manningtree (seed treatment), Wicks (1996) - HS



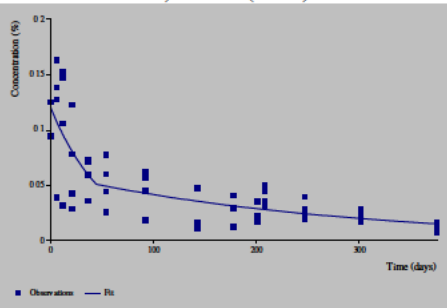
Manningtree (seed treatment), Wicks (1996) - FOMC



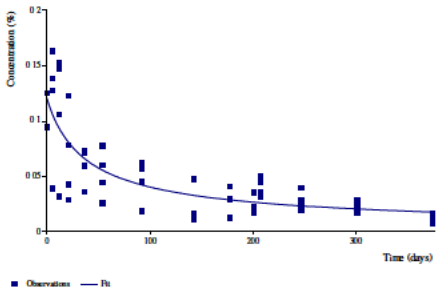
Mereville, Wicks (1996) - SFO



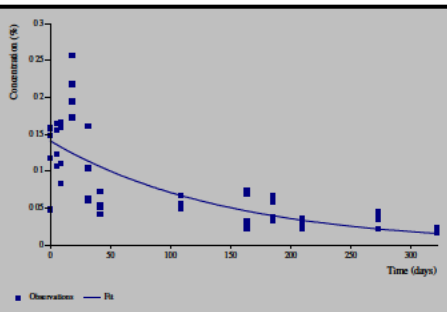
Mereville, Wicks (1996) - DFOP



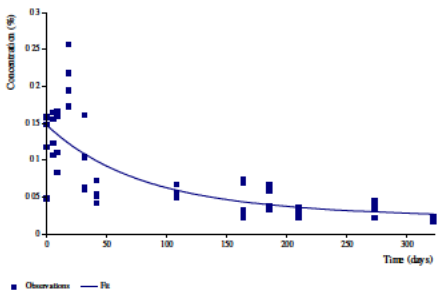
Mereville, Wicks (1996) - HS



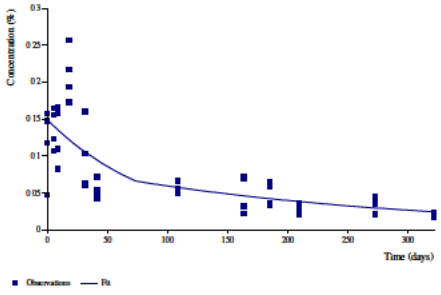
Mereville, Wicks (1996) - FOMC



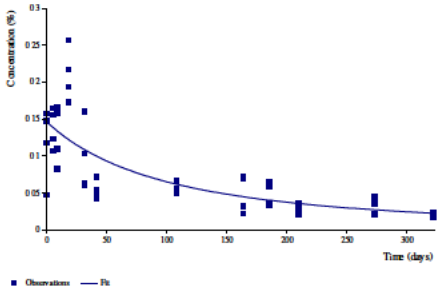
Brentwood, Duncan et al. (2003) - SFO



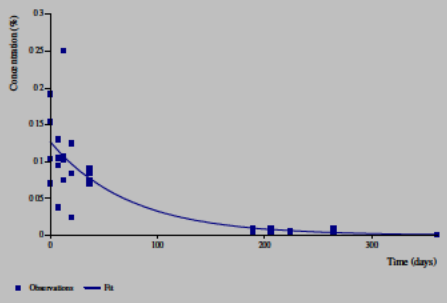
Brentwood, Duncan et al. (2003) - DFOP



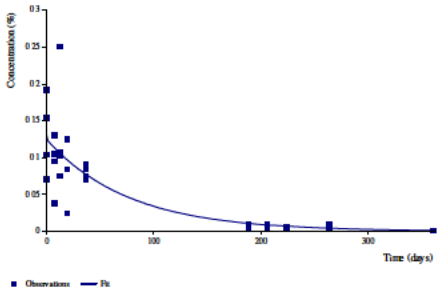
Brentwood, Duncan et al. (2003) - HS



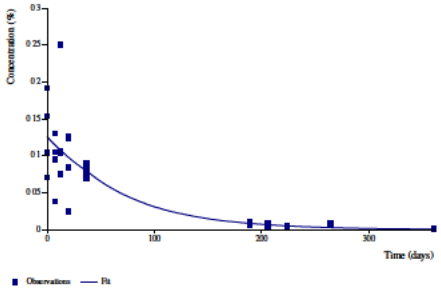
Brentwood, Duncan et al. (2003) - FOMC



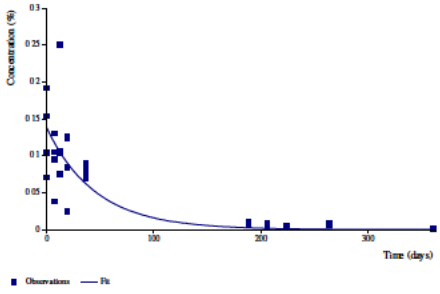
St. Trivier sur Moignans (FR), Duncan et al. (2003) - SFO



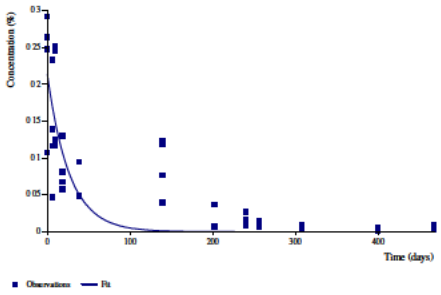
St. Trivier sur Moignans (FR), Duncan et al. (2003) - DFOP



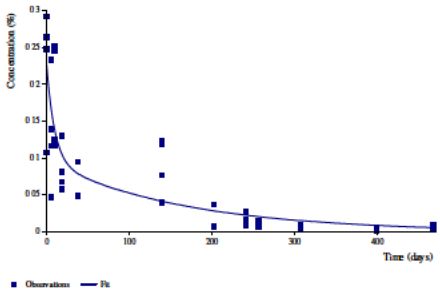
St. Trivier sur Moignans (FR), Duncan et al. (2003) - HS



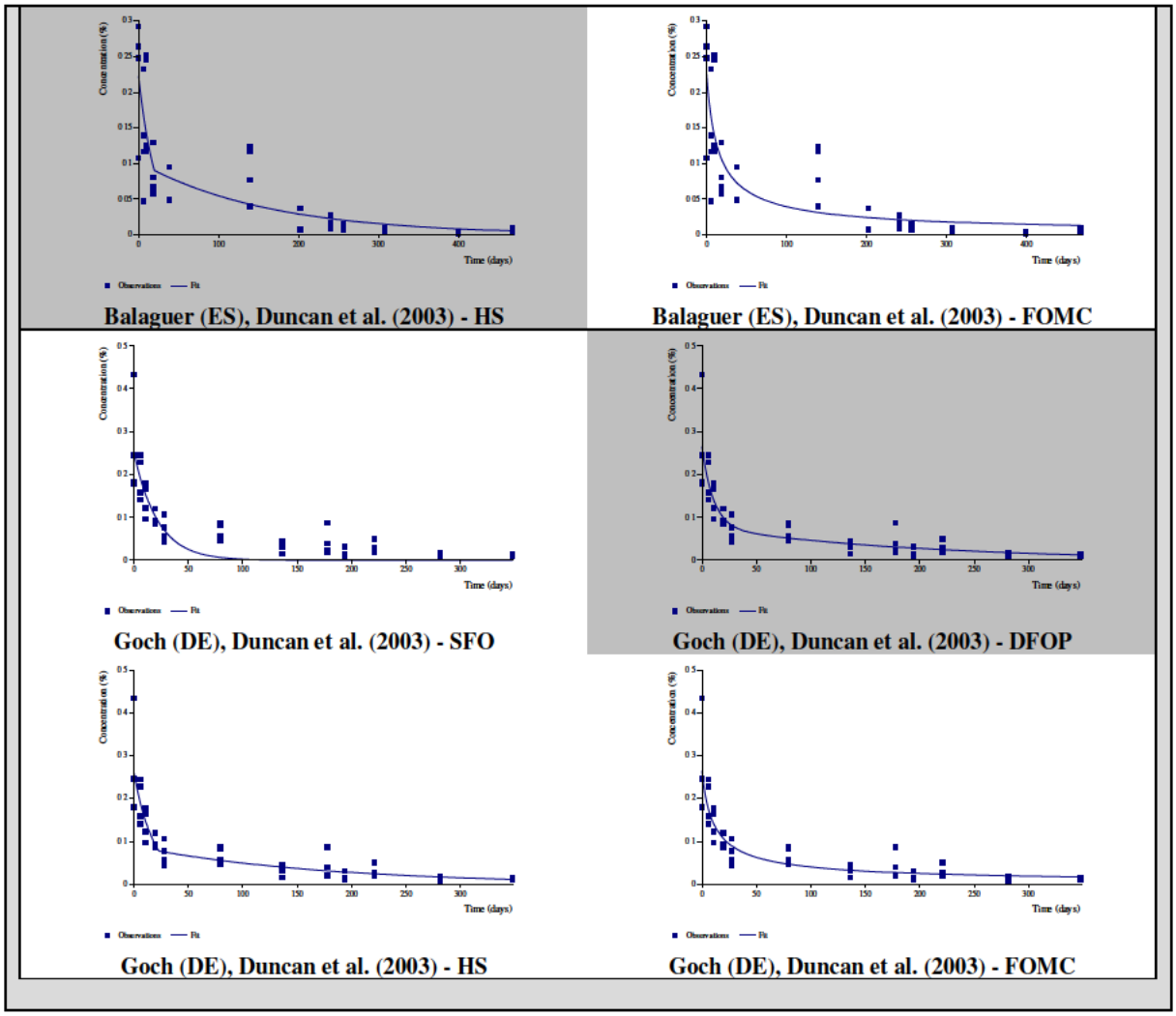
St. Trivier sur Moignans (FR), Duncan et al. (2003) - FOMC



Balaguer (ES), Duncan et al. (2003) - SFO



Balaguer (ES), Duncan et al. (2003) - DFOP



Reference:	**Best-fit analysis and normalization of the field dissipation of the triticonazole (BAS 595 F) metabolite RPA 406341**
Author(s), year:	Huber, S., 2008a
Report/Doc. Number:	2008/1089810
Guideline(s):	FOCUS Kinetics (2006)
GLP:	Not applicable (modelling study)
Validity:	Partly (refer to comment section)
Status:	**New submission**

Material and methods:

The study by Richter (2009) was evaluated according to guidance outlined by FOCUS Kinetics (2006). The goal was to derive best-fit dissipation *DT50* values, as well as to reference conditions (20 °C, Q_{10} = 2.58, *p*F2) normalized single-first-order (SFO) *DT50*.

The kinetic evaluation was based on the interim report for the field study. Thus, report for the kinetic evaluation is dated earlier than the report for the study.

Best-fit models were derived within the software package KinGUI 1.1 according to FOCUS Kinetics guidance on determination of trigger endpoints.

Results:

For all but one site the dissipation behaviour (non-normalized data) could be best described by bi-phasic FOMC models. For those three sites with bi-phasic dissipation kinetics DFOP did not improve the fits.

Table B.8.1.2.2.1-31 Best-fit models for field dissipation (non-normalized data) of RPA 406341 (Trans-diol)

Site	Best-fit *DissT50* (d)	Best-fit *DissT90* (d)	Best fit model	χ^2 error (%)
Goch-Nierswalde (Germany)	36.1	> 1000	FOMC	12.7
Rummen (Belgium)	78.2	260	SFO	20.7
Meauzac (France)	46.9	> 1000	FOMC	13.6
Alberic/Valencia (Spain)	4.6	303	FOMC	24.5

Additionally, normalized endpoints were derived in the study report. However, they do not fulfil latest guidance documents. Thus, a new evaluation was performed by Schwarz and Jarvis (2014b).

Conclusion:

Best-fit dissipation endpoints (trigger endpoints) were derived within this study.

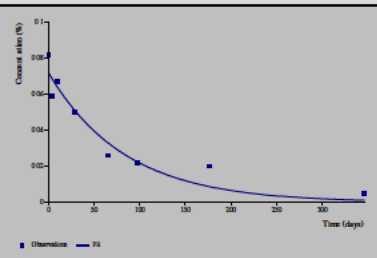
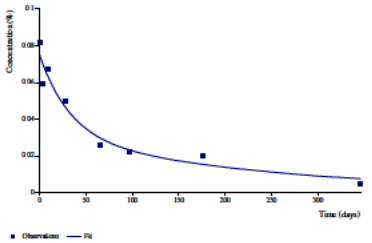
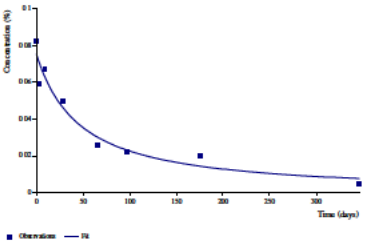
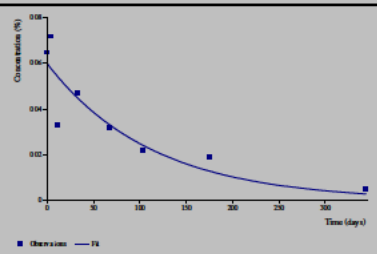
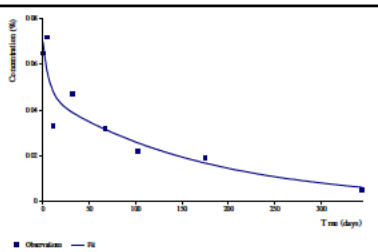
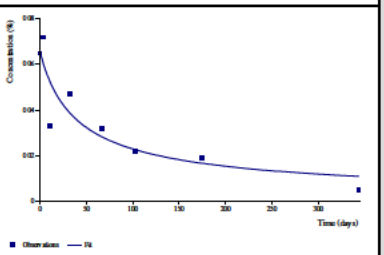
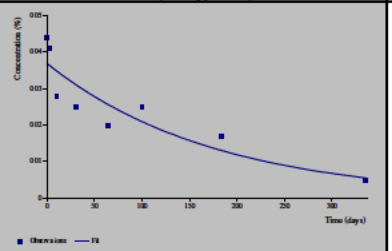
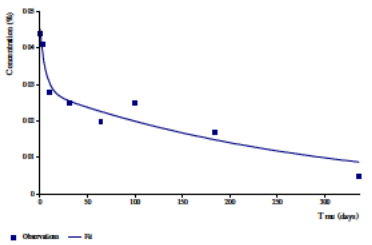
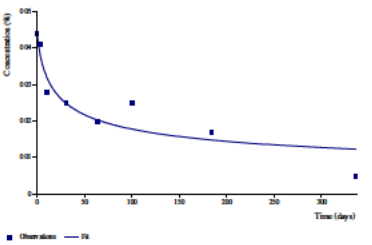
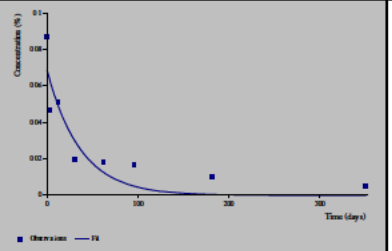
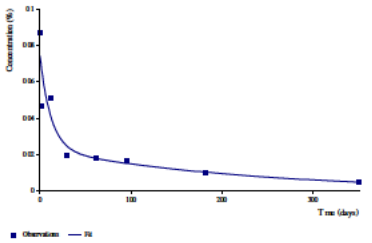
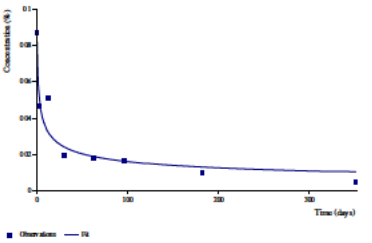
Comments RMS AT:

- The kinetic evaluation was re-done by the RMS AT in line with pertinent guidance applying CAKE 3.3 revealing slightly different values in case of Goch-Nierswalde, Rummen and Meauzac. Results obtained for Valencia are more strongly deviating from the applicant fit. A closer inspection of the residue data used by the applicant in case of Valencia revealed that the 176 DAT sample was set to half of LOQ for unknown reasons (the correct value according to Richter (2009) is 0.01 mg/kg). On overall, the RMS AT considers SFO the only reliable model for the dissipation of RPA 406341 (Trans-diol) in these four field trials from a statistical point of view even if the visual assessment is not always satisfying.

Table B.8.1.2.2.1-32 Best-fit models for field dissipation (non-normalized data) of RPA 406341 (Trans-diol) - RMS AT assessment (fits shaded in grey are considered most reliable)

Site	Kinetic model	Para-meter	Value	Confidence interval (95%) Lower	Confidence interval (95%) Upper	p > t	χ^2 error (%)	*DissT50* (d)	*DissT90* (d)
Goch-Nierswalde (Germany)	**SFO**	**k_1**	**0.012**	**0.006**	**0.018**	**< 0.01**	**13.8**	**58.2**	**193**
	DFOP	k_1	0.031	-0.058	0.120	0.20	12.6	43.7	347
		k_2	0.004	-0.011	0.019	0.24			
		g	0.582	-0.618	1.782	na			
	FOMC	α	1.10	-0.97	3.18	na	11.9	44.6	361
		β	50.95	-105.20	207.20	na			
Rummen (Belgium)	**SFO**	**k_1**	**0.009**	**0.002**	**0.016**	**0.01**	**20.7**	**78.9**	**262**
	DFOP	k_1	0.150	-0.584	0.884	0.30	20.2	50.4	326
		k_2	0.006	-0.005	0.017	0.11			
		g	0.329	-0.360	1.019	na			
	FOMC	α	0.69	-1.05	2.44	na	20.6	48.3	753
		β	27.98	-112.30	168.30	na			
Meauzac (France)	**SFO**	**k_1**	**0.006**	**0.001**	**0.010**	**< 0.01**	**16.3**	**123**	**407**
	DFOP	k_1	0.166	-0.203	0.534	0.14	10.3	64.7	527
		k_2	0.003	0.000	0.007	0.03			
		g	0.374	0.081	0.666	na			
	FOMC	α	0.31	0.03	0.06	na	13.6	47.3	> 1000
		β	5.88	-0.06	0.69	na			
Alberic/ Valencia (Spain)	**SFO**	**k_1**	**0.027**	**0.001**	**0.053**	**0.02**	**28.8**	**25.5**	**84.7**
	DFOP	k_1	0.082	-0.142	0.307	0.18	26.2	14.7	264
		k_2	0.004	-0.016	0.025	0.30			
		g	0.686	-0.083	1.455	na			
	FOMC	α	0.34	0.04	0.64	na	20.3	5.03	672
		β	0.74	-1.67	3.16	na			

Table B.8.1.2.2.1-33 Fits on Best-fit models for field dissipation (non-normalized data) of RPA 406341 (Trans-diol) - RMS AT assessment (fits shaded in grey are considered most reliable)

 Goch-Nierswalde (Germany) - SFO	 Goch-Nierswalde (Germany) - DFOP	 Goch-Nierswalde (Germany) - FOMC
 Rummen (Belgium) - SFO	 Rummen (Belgium) - DFOP	 Rummen (Belgium) - FOMC
 Meauzac (France) - SFO	 Meauzac (France) - DFOP	 Meauzac (France) - FOMC
 Alberic/Valencia (Spain) - SFO	 Alberic/Valencia (Spain) - DFOP	 Alberic/Valencia (Spain) - FOMC

Reference:	**Determination of normalised rates of decline for triticonazole metabolite RPA 406341 from a field dissipation study**
Author(s), year:	Schwarz, N., Jarvis, T., 2014b
Report/Doc. Number:	2014/1083343
Guideline(s):	FOCUS (2006): Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration Sanco/10058/2005 version 2.0 434 pp., FOCUS Kinetics (2011) Generic Guidance v 1.0
GLP:	Not applicable (modelling study)
Validity:	Partly (refer to comment section)
Status:	**New submission**

Material and methods:

The degradation of the triticonazole metabolite RPA 406341 (Trans-diol) on bare soil was investigated under field conditions at four sites situated in different regions of Europe (Germany, Belgium, France and Spain). The nominal application rate was 100 g/ha to bare soil. Following the day 0 sampling, the untreated and treated plots were irrigated with about 10 mm water. Thus, according to EFSA (2014) the influence of surface processes on the degradation of RPA 406341 (Trans-diol) in the study can be excluded. No tillage was performed during the course of the study and no crops were grown throughout any of the trials. Residue data of RPA 406341 (Trans-diol) (in mg/kg) were obtained from the studies and used as input for the kinetic evaluation. Pooled replicates from four subplots per trial site were considered. Residues of RPA 406341 (Trans-diol) were only present in the upper 0 - 10 cm soil layer and degraded to concentrations below the LOQ of 0.01 mg/kg at the last sampling point at all 4 sites (ca. 336 - 346 days after application).

The field data were normalised to 20 °C and *p*F2 using the time-step normalisation approach. The PERSIST model was used to calculate normalised day lengths based on temperature and moisture data which requires that daily average soil moisture and temperature data are either directly available or can be calculated from other data, e.g. daily maximum/minimum air temperatures. Overall, weather data from all sites were provided in the reports and were sufficient for normalisation. However, some data gaps are reported which were filled by adding the average values of the measurements before and/or afterwards.

The modelling was performed using KinGUI Version 2. FOCUS (2006 and 2011) approaches were used to determine the appropriate kinetic fit in each soil for use in determining simulation endpoints.

Findings:

In general, the results showed some variability as would be expected for field data. However, in all cases the χ^2 error values were < 24 %. For all for sites, the SFO model provided an acceptable fit and the SFO *DegT50* was the preferred endpoint. The derived modelling endpoints are summarized in the table below.

Table B.8.1.2.2.1-34 RPA 406341 (Trans-diol) - Modelling endpoints from field studies (time-step normalized data)

Study	Site	Kinetic Model	χ^2 err. (%)	*DegT50* at 20 °C, *p*F2 (d)	*DegT90* at 20 °C, *p*F2 (d)
Richter, 2009	Goch-Nierswalde, Germany	SFO	12.24	35.8	118.9
	Rummen, Belgium	SFO	23.19	33.6	111.5
	Meauzac , France	SFO	14.19	70.0	229.1
	Alberic/Valencia, Spain	SFO	16.76	37.4	124.2

Conclusion:

Modelling endpoints for the field dissipation of RPA 406341 (Trans-diol) were derived within this study.

Comments (RMS AT):

- The RMS AT is not in the positon to fully re-do the time-step normalization provided by the study authors applying the PERSIST model. However, the information provided in the study report is fairly detailed and considered sufficient to conclude on the appropriateness of the time-step normalization performed by the study authors.
- Results on time-step normalized residues not provided in the study summary are given in the table below. For unknown reasons the study authors partly used deviating residue values from those given in Richter (2009). Deviating residue data are indicated in the table below.

Table B.8.1.2.2.1-35 Time-step normalised days after application of triticonazole metabolite RPA 406341 (Trans-diol) and measured residue concentration in mg/kg for all four sites

Goch-Nierswalde (DE)	Rummen (BE)	Meauzac (FR)	Alberic/Valencia (ES)

Normalised day	mg/kg	Normalised day	mg/kg	Normalised day	mg/kg	Normalised day	mg/kg
0.0	0.082	**0.0**	0.065	**0.0**	0.044	**0.0**	0.087
2.5	0.059	**2.6**	0.072	**2.1**	0.041	**1.9**	0.047
7.1	0.067	**6.4**	0.033[a]	**7.4**	0.028	**11.9**	0.051
20.7	0.050	**17.4**	0.047	**21.8**	0.025	**33.1**	0.020
39.9	0.026	**32.7**	0.032	**32.1**	0.020	**63.5**	0.018
50.5	0.022	**42.6**	0.022	**41.5**	0.025	**79.7**	0.017[b]
69.8	0.020	**57.6**	0.019	**65.5**	0.017	**115.4**	0.010[c]
173.1	< 0.01[d]	**168.8**	< 0.01[d]	**180.3**	< 0.01[d]	**290.7**	< 0.01[d]

(a) Erroneously set to 0.034 mg/kg by study authors for unknown reasons (0.033 mg/kg in Richter, 2009)
(b) Erroneously set to 0.011 mg/kg by study authors for unknown reasons (0.017 mg/kg in Richter, 2009)
(c) Erroneously set to < 0.01 mg/kg by study authors for unknown reasons (0.010 mg/kg in Richter, 2009)
(d) LOQ = 0.01 mg/kg (set to 0.005 mg/kg for fitting by RMS AT)

- The kinetic evaluation was re-done by the RMS AT in line with pertinent guidance applying CAKE 3.3 revealing different degradation rates in comparison to the study author's fits for the following reasons:
    - In case of residues < LOQ values where set to LOQ by the study authors. The RMS AT considers 1/2 of LOQ more in line with pertinent guidance.
    - Deviating residue data used for fitting as indicated above.

  On overall the RMS AT agrees with the study authors that from a visual and statistical point of view SFO is the most reliable degradation model for all four field trials. The RMS AT notes that the SFO model may not be considered sufficiently robust in case of the Alberic/Valencia (Spain) field trial as the last sampling point is somehow underestimated. However, as none of the biphasic models give statistically reliable degradation rates the RMS AT recommends staying with the SFO model in this case as well. Being a terminal metabolite the co-RMS UK would consider it an acceptable and conservative approach to derive the endpoint at this site from the DFOP *DegT90* divided by 3.32 (and relax the statistical criteria on the basis of the improved visual fit compared to SFO). However, the RMS AT notes that residues at study end have not reached 10 % of applied, thus it is not considered defendable to calculate a pseudo SFO *DegT50* on basis of the DFOP or HS *DegT90* as is usually done in case of the FOMC model. It may also be noted that the last sampling point is based on a '< LOQ' measurement (set to 1/2 of LOQ for kinetic fitting), thus giving additional uncertainty on the 'true' residue level.

- As irrigation was applied *after* the first application, the RMS AT agrees with the study authors to omit the 0 DAT sample from fitting in line with EFSA guidance on *DegT50* (EFSA, 2014)[4].

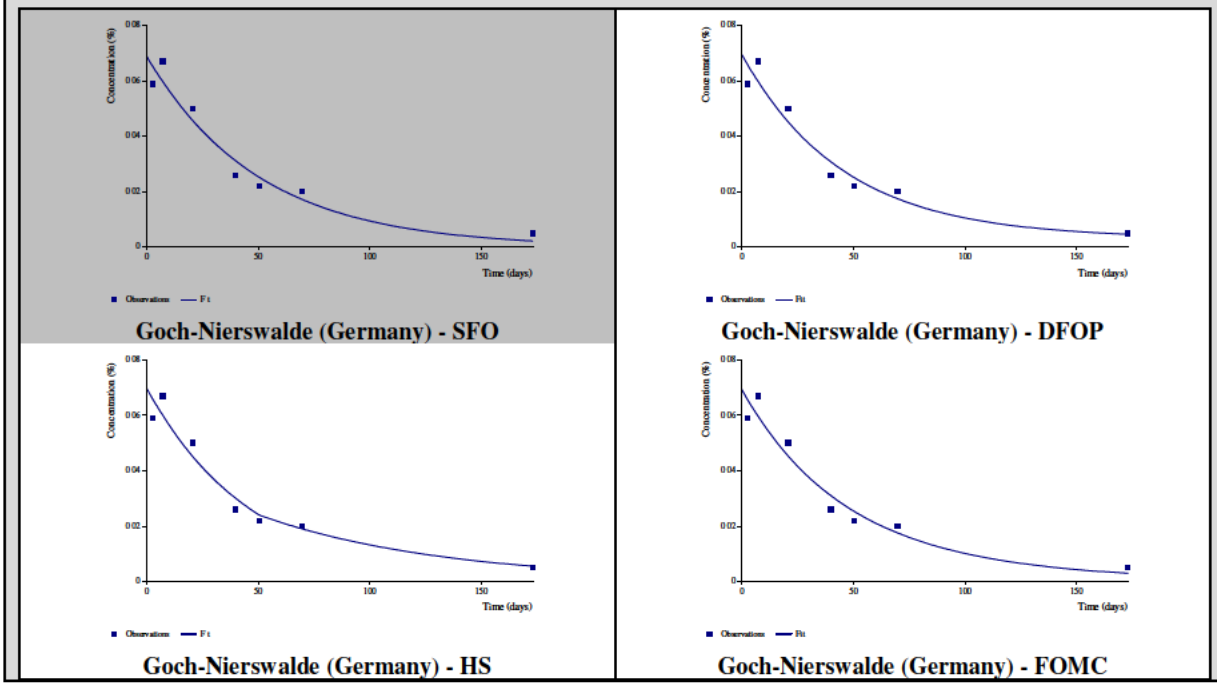
Table B.8.1.2.2.1-36 RPA 406341 (Trans-diol) - Modelling endpoints from field studies (time-step normalized data) - RMS AT assessment (fits shaded in grey are considered most reliable to derive modelling endpoints)

Site	Kinetic model	Para-meter	Value	Confidence interval (95%) Lower	Confidence interval (95%) Upper	p > t	χ^2 error (%)	*DegT50* (d)	*DegT90* (d)	Modelling *DegT50* (d)
Goch-Nierswalde (Germany)	**SFO**	**k_1**	**0.020**	**0.012**	**0.028**	**< 0.01**	**10.9**	**34.8**	**116**	**34.8**
	DFOP	k_1	0.022	-0.092	0.136	0.29	12.7	33.7	130	> 1000
		k_2	< 0.001	-0.487	0.487	0.50				
		g	0.955	-3.286	5.196	na				
	HS	k_1	0.021	0.021	0.021	< 0.01	12.2	32.8	153	57.8
		k_2	0.012	-0.027	0.051	0.20				
		t_b	50.8	-60.2	161.7	na				
	FOMC	α	11.6	-206.6	229.9	na	11.7	34.2	122	36.7
		β	555.1	-10430.0	11500.0	na				
Rummen (Belgium)	**SFO**	**k_1**	**0.021**	**0.001**	**0.041**	**0.02**	**23.5**	**32.7**	**109**	**32.7**
	DFOP	k_1	0.021	-0.013	0.055	0.07	27.9	32.7	109	32.7

[4] EFSA (2014) EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662

		k_2	0.021	-0.007	0.050	0.05				
		g	0.500	-126.700	127.700	na				
	HS	k_1	0.025	-0.070	0.121	0.23				
		k_2	0.017	-0.070	0.105	0.29	27.8	29.4	123	40.4
		t_b	22.9	-279.9	325.6	na				
	FOMC	α	0.40	0.06	0.74	na	23.6	1.38	94.1	28.3
		β	0.30	-2.67	3.26	na				
Meauzac (France)	**SFO**	**k_1**	**0.012**	**0.004**	**0.021**	**< 0.01**	**12.8**	**55.8**	**186**	**55.8**
	DFOP	k_1	0.012	-0.002	0.026	0.03				
		k_2	0.012	0.000	0.025	0.03	15.3	55.8	186	55.9
		g	0.500	-38.170	39.180	na				
	HS	k_1	0.069	-0.077	0.214	0.12				
		k_2	0.009	0.000	0.017	0.02	7.9	28.3	209	77.9
		t_b	7.4	-8.8	23.6	na				
	FOMC	α	1.0	-2.1	4.1	na	12.9	43.2	387	116
		β	43.4	-167.9	254.8	na				
Alberic/ Valencia (Spain)	**SFO**	**k_1**	**0.016**	**0.006**	**0.026**	**< 0.01**	**18.4**	**42.6**	**142**	**42.6**
	DFOP	k_1	0.029	-0.084	0.142	0.24				
		k_2	0.004	-0.034	0.041	0.39	19.7	34.6	274	198
		g	0.740	-1.168	2.648	na				
	HS	k_1	0.023	-0.008	0.055	0.05				
		k_2	0.007	-0.018	0.032	0.22	18.6	29.6	231	98.6
		t_b	41.4	-65.5	148.3	na				
	FOMC	α	1.7	-5.0	8.4	na	18.4	35.6	205	61.8
		β	69.5	-334.2	473.3	na				

Table B.8.1.2.2.1-37 Fits on RPA 406341 (Trans-diol) - Modelling endpoints from field studies (time-step normalized data) - RMS AT assessment (fits shaded in grey are considered most reliable to derive modelling endpoints)

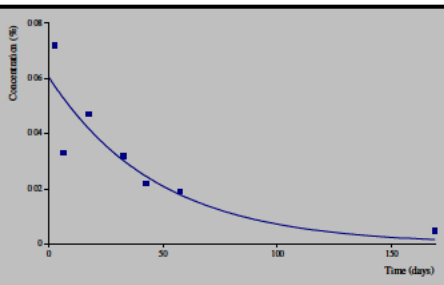


Goch-Nierswalde (Germany) - SFO

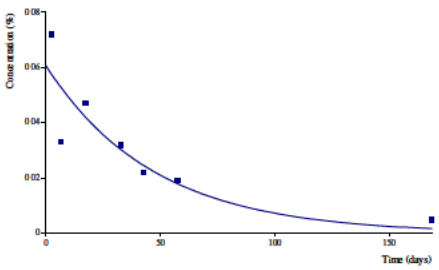
Goch-Nierswalde (Germany) - DFOP

Goch-Nierswalde (Germany) - HS

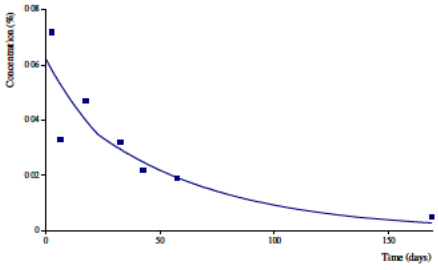
Goch-Nierswalde (Germany) - FOMC



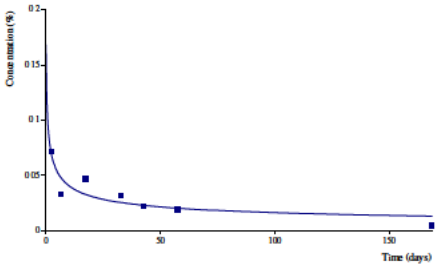
Rummen (Belgium) - SFO



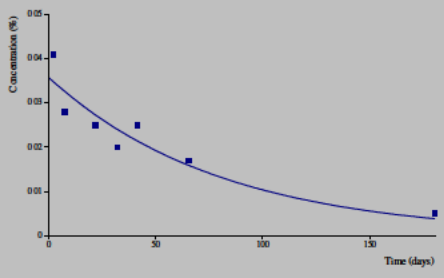
Rummen (Belgium) - DFOP



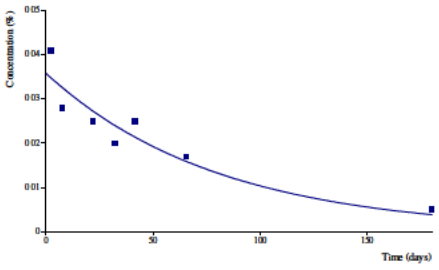
Rummen (Belgium) - HS



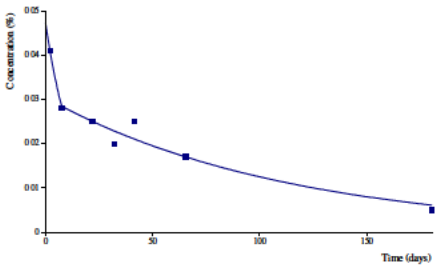
Rummen (Belgium) - FOMC



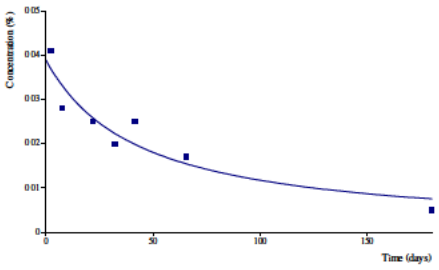
Meauzac (France) - SFO



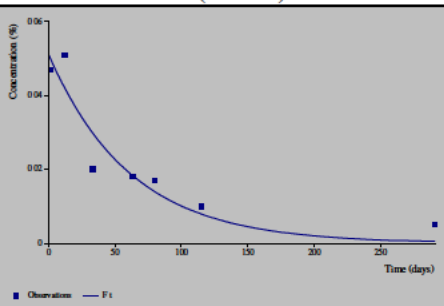
Meauzac (France) - DFOP



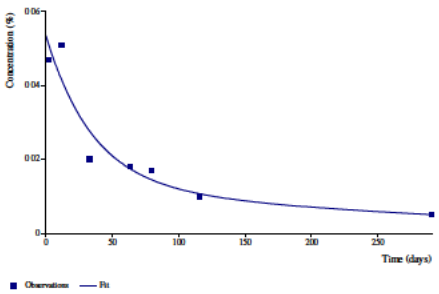
Meauzac (France) - HS



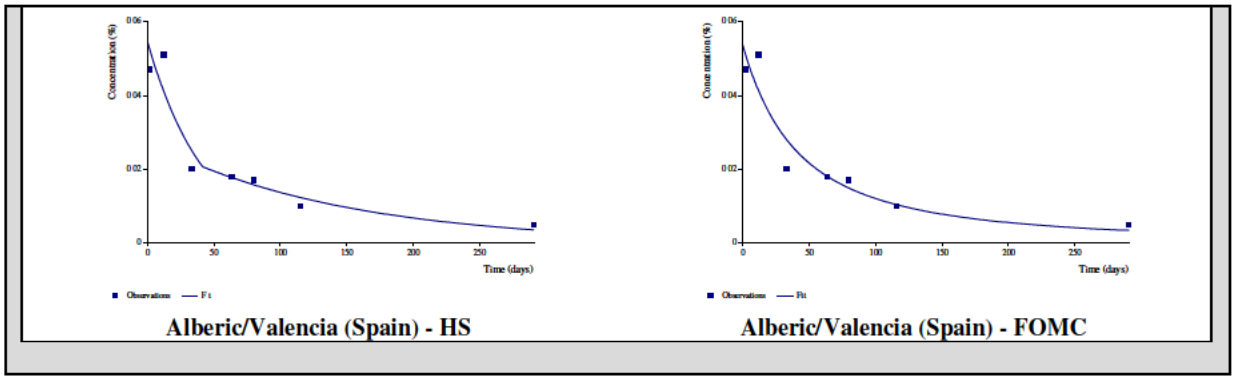
Meauzac (France) - FOMC



Alberic/Valencia (Spain) - SFO



Alberic/Valencia (Spain) - DFOP



B.8.1.2.2.2. Soil accumulation studies

Studies submitted for first Annex I inclusion:

- **Davis (2004)**, investigating accumulation of formulated triticonazole in two field sites

No new studies have been submitted.

Reference:	**Triticonazole - Long term soil dissipation study with repeated applications – Final Report**
Author(s), year:	Davis, H., 2004
Report/Doc. Number:	1849/034-D2149
Guideline(s):	SETAC 1995
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The objective of this study was to investigate the potential for long term accumulation of triticonazole and its soil metabolite RPA 406341 (Trans-diol) following repeated applications of triticonazole. The trials have been being conducted on commercial winter wheat crop sites located on sandy loam and medium loam soil types in Germany and the UK respectively.

A full soil characterisation was conducted on the soil at each site and the results are presented below.

Table B.8.1.2.2.2-1 Soil Characteristics

Location, soil classification	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H (KCl)	CEC (meq/100 g)	Biomass (µg C/g soil)
Goch, DE, sandy loam	19.6	71.6	8.8	1.9	6.2	12.0	436 (Feb. 99) 141 (Nov. 99) 331 (Jan. 01) 153 (Oct. 01) 77 (Nov. 02)
Braham, UK, medium loam	40.7	36.9	22.4	1.4	7.6	15.0	226 (Nov. 99) 294 (Jan. 01) 318 (Oct. 01) 127 (Dec. 02) 145 (Sep. 03)

Each trial plot comprised of two plots with one plot remaining untreated to serve as the control. The second plot has been divided into four sub-plots of equal size. Triticonazole (formulated as a 300 g/L FS) was applied to the

test plot in Germany in November 1998 and in the UK in October 1999 at a nominal rate of 112.5 g/ha (in 400 L/ha). Further applications were made at approximately 12-month intervals such that by finalization of the study the site in Germany has received four applications and the site in the UK has received three applications. Triticonazole formulated was incorporated into the soil to a depth of 5 - 10 cm, the area was drilled with undressed winter wheat seed.

Soil specimens were scheduled for collection pre and post each application and once between April and June, and 12 months after the final treatment. Filter paper specimens were laid onto the bare soil at the time of test application and were collected directly after the test application was complete. At each time the treatments have been applied in good spraying conditions in accordance with Good Agricultural Practice. At each collection for analysis, soil was taken from five pre-assigned collection points within each sub-plot using a bucket auger to a depth of 30 cm. Soil was collected from the control plot at random locations to obtain sufficient material (approximately 1 kg) for the specimen. Following collection soil from each sub-plot was divided into 'Replicate 1' and 'Replicate 2'. 'Replicate 1' samples were analysed whilst 'Replicate 2' samples were sent for storage.

Specimens were stored frozen (< -20 °C) for a maximum of 125 days prior to extraction. Triticonazole and its metabolite RPA 406341 (Trans-diol) have been shown to be stable for a maximum of 22 months under these storage conditions. Extraction from soil was carried out by sonication and shaking with 0.1 M ammonium hydroxide solution and acetone. Extraction was repeated using acetone only. Purification was carried out by solid phase extraction (SPE) using a C18 cartridge. The limit of quantification was 0.002 mg/kg. Final determination was by liquid chromatography with mass spectrometry using tandem mass spectrometric detection (LC/MS/MS).

Findings:

The results from the soil analyses are tabulated below. Recovery of triticonazole and RPA 406341 (Trans-diol) in freshly spiked soils was in the range from 75 - 105 % (at 0.002 and 0.05 mg/kg) in both soils. Filter paper analysis revealed amounts of triticonazole in the range from 78.7 - 125.6 g a.i./ha for DE and 55.4 - 110.3 g a.i./ha for UK.

Table B.8.1.2.2.2-2 Triticonazole and RPA 406341 (Trans-diol) concentrations (mg/kg) in soil samples from the Goch (DE) field site (0 - 30 cm)

Sample Number	Sample Description	Concentration in soil (mg/kg dry weight)			
		Triticonazole		RPA 406341 (Trans-diol)	
		Range	Mean	Range	Mean
0	Pre-study	nd	nd	nd	nd
1	**Yr 1 Post-T1**	**0.011 - 0.058**	**0.029**	**nd**	**nd**
2	Yr 1 Spring	0.006 - 0.018	0.012	nd	nd
3	Yr 1 Pre-T2	0.004 - 0.011	0.006	nd	nd
4	**Yr 2 Post-T2**	**0.026 - 0.059**	**0.039**	**nd**	**nd**
5	Yr 2 Spring	0.013 - 0.019	0.016	nd - 0.002	< 0.002
6	Yr 2 Pre-T3	0.006 - 0.011	0.009	nd	nd
7	**Yr 3 Post-T3**	**0.026 - 0.034**	**0.029**	**nd**	**nd**
8	Yr 3 Spring	0.019 - 0.029	0.024	0.003 - 0.004	0.003
9	Yr 3 Pre-T4	0.008 - 0.012	0.010	nd - 0.003	< 0.002
10	**Yr 4 Post-T4**	**0.029 - 0.047**	**0.037**	**nd**	**nd**
11	Yr 4 Spring	0.017 - 0.046	0.026	0.003 - 0.005	0.004
12	Yr 4 Final	0.007 - 0.013	0.010	nd - 0.004	0.003

nd denotes not detected

Table B.8.1.2.2.2-3 Triticonazole and RPA 406341 (Trans-diol) concentrations (mg/kg) in soil samples from the Braham (UK) field site (0 - 30 cm)

Sample Number	Sample Description	Concentration in soil (mg/kg dry weight)			
		Triticonazole		RPA 406341 (Trans-diol)	
		Range	Mean	Range	Mean
0	Pre-study	nd	nd	nd	nd
1	**Yr 1 Post-T1**	**0.016 - 0.039**	**0.023**	**nd**	**nd**
2	Yr 1 Spring	< 0.002 - 0.033	0.012	nd	nd
3	Yr 1 Pre-T2	< 0.002 - 0.006	0.005	nd	nd

4	**Yr 2 Post-T2**	**0.008 - 0.034**	**0.021**	**nd**	**nd**
5	Yr 2 Spring	0.009 - 0.022	0.013	nd	nd
6	Yr 2 Pre-T3	< 0.002 - 0.011	0.006	nd	nd
7	**Yr 3 Post-T3**	**0.006 - 0.011**	**0.009**	**nd**	**nd**
8	Yr 3 Spring	0.006 - 0.009	0.008	nd	nd
9	Yr 3 Pre-T4	0.005 - 0.009	0.007	nd	nd
10	**Yr 4 Post-T4**	**0.004 - 0.033**	**0.015**	**nd**	**nd**
11	Yr 4 Spring	0.014 - 0.016	0.016	nd	nd
12	Yr 4 Final	0.007 - 0.009	0.008	nd	nd

nd denotes not detected

At 0 days after the first application (T1) mean residues of triticonazole measured 0.029 mg/kg in the German soil and 0.023 mg/kg in the UK soil, declining to 0.006 mg/kg in the German soil and to 0.005 mg/kg in the UK soil at the end of year 1.

At 0 days after the second application (T2) mean residues of triticonazole measured 0.039 mg/kg in the German soil and 0.021 mg/kg in the UK soil, declining to 0.009 mg/kg in the German soil and 0.006 mg/kg in the UK soil at the end of year 2.

At 0 days after the third application (T3) mean residues of triticonazole measured 0.029 mg/kg in the German soil and 0.009 mg/kg in the UK soil, declining to 0.010 mg/kg in the German soil and 0.007 mg/kg in the UK soil at the end of year 3.

At 0 days after the fourth application (T4) mean residues of triticonazole measured 0.037 mg/kg in the German soil and 0.015 mg/kg in the UK soil, declining to 0.010 mg/kg in the German soil and 0.008 mg/kg in the UK soil at the end of year 4.

No measurable residues of the metabolite RPA 406341 (Trans-diol) at or above the limit of quantification (LOQ 0.002 ppm for soil, 8.1 g a.i. equivalents/ha for filter paper) were found in any of the treated soil or filter papers. This is with the exception of certain soil samples taken at the German site. One soil sample taken in spring in year 2, four samples taken in spring in year 3, one sample taken at the end of year 3, four samples taken in spring in year 4 and three samples taken at the final soil collection in the autumn 2002 had residue levels detected above the LOQ of 0.002 mg/kg. In these soil samples the residue levels detected ranged from 0.002 to 0.004 mg/kg.

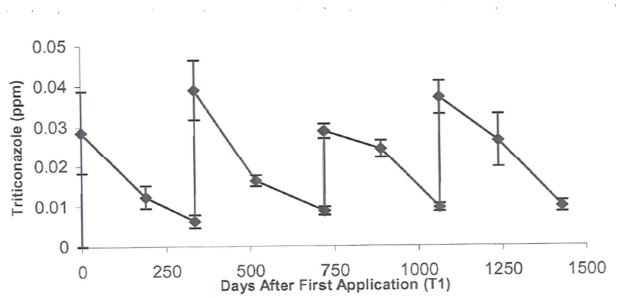


Figure B.8.1.2.2.2-1: Triticonazole concentrations (mg/kg) in soil samples with time after repeated applications from the German test site

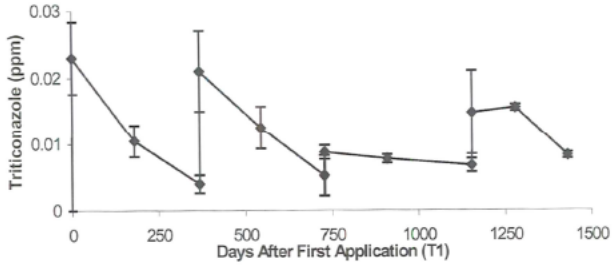


Figure B.8.1.2.2.2-2: Triticonazole concentrations (mg/kg) in soil samples with time after repeated applications from the UK test site

Conclusions:

The data from this study suggests there is no evidence of accumulation of triticonazole or its metabolite RPA 406341 (Trans-diol) in soil following repeated annual application for four years.

Comments (RMS AT):

- The study broadly follows SETAC 1995 and is considered still reliable. With an application rate of 112.5 g a.i./ha the study is clear overdosed.
- In contrast to the study authors the RMS AT is of the opinion that accumulation of triticonazole indeed took place in both field trials with an accumulation plateau of ~ 0.01 mg/kg reached before application in the third year of the DE field trial. In case of the UK field trial an accumulation plateau appears not having been reached by end of the study.

B.8.1.2.3. Summary on field dissipation/degradation (compiled by RMS AT)

The dissipation/degradation of **triticonazole** under realistic outdoor conditions has been assessed in eight field dissipation trials spread all over Europe (IT, DE, UK, FR, ES). Triticonazole was incorporated into bare soils at a nominal application rate of 240 g/ha immediately before planting of winter cereals (in one field trial triticonazole was actually applied as a seed treatment). Notice that all these field trials are clearly overdosed in view of an intended application rate of 12.5 g ai/ha only. In principal, cropping in field trials is not in line with EFSA guidance on *DegT50* (EFSA, 2014)[5] recommending the soil to be kept free from vegetation in order to exclude any possible uptake by plants. However, as the intended use is indeed seed treatment in winter & spring cereals, the RMS AT considers the *DegT50* values obtained in these field trials at least sufficiently robust for the intended use. Notice that plant uptake has to be switched off in exposure models in order to avoid double counting of plant uptake. Using *DegT50* values obtained in these field trials for uses other than winter & spring cereals or at significantly deviating crop stages in winter & spring cereals will be subject to some uncertainties.

Table B.8.1.2.2.2-1 Summary on non-normalized field dissipation rates for triticonazole - trigger endpoints

Field trial	Soil type (USDA)	*p*H ($CaCl_2$)	*DissT50* (d)	*DissT90* (d)	χ^2 err. (%)	Kinetic model	Reference
Bologna (IT)	Loam	8.4[(a)]	169	563	32.5	SFO	Wicks (1996)
Goch (DE)	Sandy loam	6.6[(a)]	183	609	28.5	SFO	
Manningtree (UK) - Spray	Sandy loam	5.3[(a)]	55.0	633	13.5	DFOP	
Manningtree (UK) - Seed treat.	Sandy loam	5.3[(a)]	223	741	38.2	SFO	
Mereville (FR)	Silty clay loam	7.8[(a)]	204	678	17.6	SFO	
Brentwood (UK)	Sandy silt loam	7.3	242	803	27.8	SFO	Duncan et al. (2003)
Saint Trivier sur Moignans (FR)	Sandy silt loam	7.1	118	392	21.1	SFO	
Balaguer (ES)	Clay loam	7.4	99.1	329	31.4	SFO	
Goch (DE)	Sandy silt loam	6.7	36.1	477	8.2	DFOP	
	Maximum (n = 9)		**242**	**803**	**-**	**SFO**	

(a) Measured in water

Table B.8.1.2.2.2-2 Summary on time-step normalized field degradation rates for triticonazole - modelling endpoints

Field trial	Soil type (USDA)	*p*H ($CaCl_2$)	*DegT50* (d)	*DegT90* (d)	χ^2 err. (%)	Kinetic model	Modelling *DegT50* (d)	Ref.
Bologna (IT)	Loam	8.4[(a)]	78.9	262	20.7	SFO	78.9	Wicks (1996)
Goch (DE)	Sandy loam	6.6[(a)]	66.9	222	28.7	SFO	66.9	
Manningtree (UK) - Spray	Sandy loam	5.3[(a)]	15.4	281	13.0	DFOP	84.6[(b)]	
Manningtree (UK) - Seed treat.	Sandy loam	5.3[(a)]	90.4	300	33.2	SFO	90.4	
Mereville (FR)	Silty clay loam	7.8[(a)]	35.7	441	13.5	HS	133[(b)]	
Brentwood (UK)	Sandy silt loam	7.3	101	337	30.3	SFO	101	Duncan et al. (2003)
Saint Trivier sur Moignans (FR)	Silty silt loam	7.1	51.2	170	16.9	SFO	51.2	
Balaguer (ES)	Clay loam	7.4	15.2	245	28.5	HS	73.8[(b)]	
Goch (DE)	Sandy silt loam	6.7	12.2	208	9.4	DFOP	62.7[(b)]	
	Geometric mean (n = 8)[(c)]		**-**	**-**	**-**	**SFO**	**78.7**	
	***p*H-dependency: y/n**		**-**	**-**	**-**	**-**	**n[(d)]**	

(a) Measured in water
(b) Pseudo-SFO *DegT50* based on DFOP or HS overall *DegT90* divided by 3.32 (as residues at study end are clearly below 10 % of initial dose)
(c) Different experiments from Manningtree field site (spray and seed treatment) averaged (geometric mean) before averaging results from different field sites
(d) Refer to text below

The RMS AT investigated field degradation rates of triticonazole in relation to soil *p*H. No such relationship could be established (see figure below).

[5] EFSA (2014) EFSA Guidance Document for evaluating laboratory and field dissipation studies to obtain DegT50 values of active substances of plant protection products and transformation products of these active substances in soil. EFSA Journal 2014;12(5):3662

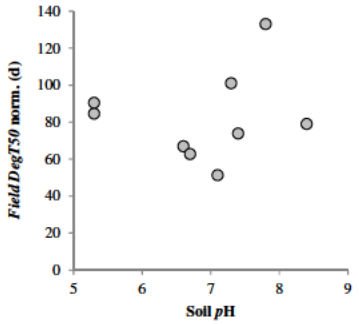


Figure B.8.1.2.2.2-1: Time-step normalized field *DegT50* of triticonazole in relation to soil *p*H

The RMS AT notes that in case of the ground water exposure assessment the obtained geometric *DegT50* of 78.7 days, based on a mixture of SFO *DegT50* values and pseudo *DegT50* values from DFOP and HS fits, is of course conservative for the parent triticonazole but not necessarily conservative for its metabolites. In case of biphasic degradation the FOCUS degradation report 2006 (EC, 2014) gives the option to perform the exposure assessment on basis of two separate runs, the first on basis of the slow DFOP/HS degradation rates and the second on basis of the fast phase DFOP/HS degradation rate. The highest concentration of the two sets may then be used in the risk assessment.

In case of this dataset degradation rates from SFO and DFOP/HS models are mixed making the situation more complicated. As already indicated in a draft guidance document, prepared by CRD in view of supporting the current FOCUS degradation kinetics guidance, this situation may be handled assuming the SFO model a special case of the DFOP model with SFO-k = DFOP-k_1 = DFOP-k_2 and g undefined. In analogy, the SFO may also be considered a special case of the HS model with an undefined split point (t_b). If applied to the time-step normalized triticonazole dataset this gives an overall geometric fast phase *DegT50* of 35.8 days and a geometric slow phase *DegT50* of 98.2 days (see table below). In line with the FOCUS approach mentioned above an additional exposure assessment may therefore be performed on basis of a SFO model with a geometric fast phase *DegT50* of 35.8 days.

Table B.8.1.2.2.2-3 Summary on normalized field degradation rates for triticonazole - alternative approach for deriving modelling endpoints for the fast and slow degradation phase

Field trial	Soil type (USDA)	*p*H ($CaCl_2$)	Fast phase *DegT50* (d)	Slow phase *DegT50* (d)	DFOP-*g*	Kinetic model	Ref.
Bologna (IT)	Loam	8.4[a]	78.9[b]	78.9[b]	na	SFO	Wicks (1996)
Goch (DE)	Sandy loam	6.6[a]	66.9[b]	66.9[b]	na	SFO	
Manningtree (UK) - Spray	Sandy loam	5.3[a]	6.9	140	0.60	DFOP	
Manningtree (UK) - Seed treat.	Sandy loam	5.3[a]	90.4[b]	90.4[b]	na	SFO	
Mereville (FR)	Silty clay loam	7.8[a]	35.7	191	na	HS	
Brentwood (UK)	Sandy silt loam	7.3	101[b]	101[b]	na	SFO	Duncan et al. (2003)
Saint Trivier sur Moignans (FR)	Silty silt loam	7.1	51.2[b]	51.2[b]	na	SFO	
Balaguer (ES)	Clay loam	7.4	15.2	111	na	HS	
Goch (DE)	Sandy silt loam	6.7	7.3	133	0.71	DFOP	
	Geometric mean (n = 8)[c]		**35.8**	**98.2**	-		
	***p*H-dependency: y/n**		**n**	-	-		

(a) In water
(b) SFO model considered as a special case of a DFOP or HS model with $k_1 = k_2$ and g and t_b, respectively, undefined
(c) Data from Manningtree soil (spray and seed treatment) averaged (geometric mean) before averaging different soils

The dissipation/degradation of the metabolite **RPA 406341 (Trans-diol)** under realistic outdoor conditions has been assessed in four field dissipation trials spread all over Europe (DE, BE, FR and ES). RPA 406341 (Trans-diol) was sprayed on bare soils at a nominal application rate of 100 g/ha followed by irrigation to satisfy requirements given in EFSA (2014). Obtained dissipation/degradation rates are given in the tables below. It is noted that application of RPA 306341 (Trans-diol) in these field trials was in late August/early September. This application date may not necessarily be considered representative for the intended use in winter cereals. However, as the peak occurrence of metabolite RPA 406431 (Trans-diol) under real field situation is roughly

around late summer / early autumn in case of application in spring cereals and somewhere in spring in case of application in winter cereals dissipation rates obtained in this study are considered sufficiently robust for trigger endpoints as well as PEC soil calculation.

Table B.8.1.2.2.2-4 Summary on non-normalized field dissipation rates of RPA 406341 (Trans-diol)

Field trial	Soil type[(a)] (USDA)	*p*H[(a)] ($CaCl_2$)	*DissT50* (d)	*DissT90* (d)	χ^2 error (%)	Kinetic model	Reference
Goch-Nierswalde (DE)	Silt loam	4.7	58.2	193	13.8	SFO	Richter (2009)
Rummen (BE)	Silt loam	5.1	78.9	262	20.7	SFO	
Meauzac (FR)	Loam	5.4	123	407	16.3	SFO	
Alberic/Valencia (ES)	Clay	7.6	25.5	84.7	28.8	SFO	
	Maximum (n = 4)		**123**	**407**	**-**	**SFO**	

(a) Top soil

Table B.8.1.2.2.2-5 Summary on time-step normalized (20 °C and *p*F 2) field degradation rates of RPA 406431 (Trans-diol) - modelling endpoints

Field trial	Soil type[(a)] (USDA)	*p*H[(a)] ($CaCl_2$)	*DegT50* (d)	*DegT90* (d)	χ^2 error (%)	Kinetic model	Reference
Goch-Nierswalde (DE)	Silt loam	4.7	34.8	116	10.9	SFO	Richter (2009)
Rummen (BE)	Silt loam	5.1	32.7	109	23.5	SFO	
Meauzac (FR)	Loam	5.4	55.8	186	12.8	SFO	
Alberic/Valencia (ES)	Clay	7.6	42.6	142	18.4	SFO	
	Geometric mean (n = 4)		**40.6**	**135**	**-**	**SFO**	
	***p*H-dependency: y/n**		**n**	**-**	**-**	**-**	

(a) Top soil

The RMS AT notes, that lab *DegT50* values of **RPA 404766 (Cis-diol)** are partly above 60 days thus triggering field dissipation/degradation studies for this metabolite as well. This is currently not the case and considered a data gap from a formal point of view. However, it may be noted that degradation of RPA 404766 (Cis-diol) in laboratory studies was consistently faster than degradation of its isomeric sibling RPA 406341 (Trans-diol) in all soils (with the exception of the US clay soil in Doble, 1996). Therefore, from a scientific point of view, the RMS AT considers field degradation data available for RPA 406341 (Trans-diol) sufficiently robust to serve as conservative estimates of RPA 404766 (Cis-diol) field degradation.

A comparison of the laboratory and field modelling endpoints on basis of the EXCEL sheet **EFSA *DegT50* selector** revealed that field studies with triticonazole show significantly shorter modelling *DegT50* values than laboratory studies (lab and field studies considered as different populations). The same is true for RPA 406431 (Trans-diol). Following EFSA guidance (EFSA, 2014), these results indicate that field degradation rates for triticonazole and RPA 406431 (Trans-diol) are appropriate modelling endpoints for the exposure assessment.

For triticonazole, a **field accumulation study** conducted in DE and UK at an elevated application rate of 112.5 g ai/ha (sprayed) revealed that after correction for the application rate the plateau concentration for triticonazole was in the range of 0.001 mg/kg with peak concentrations ranging from 0.0017 to 0.0043 mg/kg. Concentrations of the major soil metabolite RPA 406341 (Trans-diol) were below LOQ (0.002 mg/kg) except for five sampling points in DE (0.002 – 0.004 mg/kg, uncorrected).

B.8.1.3. Adsorption and desorption in soil

B.8.1.3.1. Adsorption and desorption

B.8.1.3.1.1. Adsorption and desorption of the active substance

Studies submitted for first Annex I inclusion:

- **Burr & Austin (1992)**, investigating phenyl labelled triticonazole in five soils
- **Burr (1998)**, investigating phenyl labelled triticonazole in four soils and one sediment

New studies submitted:

- **Vasques (2015a)**, investigating phenyl labelled triticonazole in five soils
- **Simmonds (2017a)**, investigating phenyl labelled triticonazole in five soils

Reference:	**RPA 400727-^{14}C: Adsorption / desorption on five soils**
Author(s), year:	Burr, C. M., Austin, D. J., 1992
Report/Doc. Number:	R013051, 428632, P91/325
Guideline(s):	US-EPA 163-1, OECD 106
GLP:	Yes
Validity:	None reliable (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The adsorption and desorption characteristics of [phenyl-U-^{14}C]-triticonazole have been studied on five soils. These were a sandy loam, a clay loam, a sand, a loamy sand and a standard Speyer 2.1 sand soil. A preliminary study was carried out to determine the cycle times required for adsorption and desorption. The nominal dosing concentrations to be used were 4.0, 0.8, 0.16 and 0.032 mg/l 0.01 M calcium chloride. One control sample was prepared without soil to check the possible adsorption on the glassware. For adsorption and desorption cycles of 18 hours and 4 hours respectively were chosen. Experiments were done at ambient temperature in the dark. Solvent extraction was carried out with acetonitrile/water (4:1). Adsorbates and selected desorbates were analysed by HPLC.

Adsorption and desorption isotherms and Freundlich coefficients were calculated.

Table B. 8.1.3.1.1-1: Soil Characteristics

Soil[(a)]	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H[(b)]	CEC (meq/100g)
UK sandy loam	73.0	13.5	13.5	1.43	6.30	5.99
UK clay loam	47	21	32	5.65	6.08	28.5
UK loamy sand	79.0	11.5	9.5	29.24	6.24	51.1
UK sand	96.0	1.5	2.5	0.91	6.23	2.30
Speyer 2.1 sand	90.0	4.0	6.0	1.32	6.12	2.95

(a) Texture classification not stated
(b) Matrix not specified

Findings:

The recovery was quantitative varying from 92.38 to 106.76 %. Stability studies showed that triticonazole was stable throughout the study.

K_f values increased from 1.74 in the sand with 0.91 % organic matter to 31.37 in the loamy sand with 29.2 % organic matter. The K_{foc} for the high organic matter soil is significantly lower than the value for the other soils,

there does not appear to be a correlation between soil type and K_{foc}. From the constants obtained using the Freundlich equation triticonazole would be expected to show medium mobility in soil. Details of the results are shown in the tables below.

Table B. 8.1.3.1.1-2: Triticonazole - calculated adsorption constants

Soil	OM (%)	pH[(a)]	K_f (mL/g)	K_{foc} (mL/g)	1/*n* (-)	R^2
UK sandy loam	1.43	6.30	4.10	485	0.925	0.983
UK clay loam	5.65	6.08	12.9	386	0.893	0.999
UK loamy sand	29.24	6.24	31.7	184	0.917	0.999
UK sand	0.91	6.23	1.75	324	0.964	0.999
Speyer 2.1 sand	1.32	6.12	4.39	563	0.862	0.999

(a) Matrix not specified

Correlation coefficients for the observed adsorption isotherms were between 0.983 and 0.999.

Table B. 8.1.3.1.1-3: Triticonazole - calculated desorption coefficients

soil	$K_{f,des}$ (mL/g)	1/*n* (-)	$K_{foc,des}$ (mL/g)
UK sandy loam	1st cycle: 5.53	0.913	654
	2nd cylce: 7.08	0.892	838
	3rd cycle: 9.51	0.902	1225
	4th cycle: 11.54	0.907	1365
	5th cycle: 16.57	0.945	1961
UK clay loam	1st cycle: 14.41	0.901	432
	2nd cycle: 15.10	0.902	452
	3rd cycle: 17.12	0.913	513
	4th cycle: 16.28	0.899	488
	5th cycle: 17.67	0.907	529
UK loamy sand	1st cycle: 36.13	0.916	209
	2nd cycle: 38.52	0.907	223
	3rd cycle: 41.87	0.911	242
	4th cycle: 42.33	0.901	245
	5th cycle: 48.91	0.915	283
UK sand	1st cycle: 2.36	0.933	439
	2nd cycle: 3.12	0.928	580
	3rd cycle: 1.07	0.743	198
	4th cycle: nd	-[(a)]	-
	5th cycle: nd	-	-
Speyer 2.1 sand	1st cycle: 5.55	0.872	711
	2nd cycle: 6.79	0.894	871
	3rd cycle: 9.01	0.926	1156
	4th cycle: 9.24	0.924	1185
	5th cycle: 12.97	0.967	1663

(a) Could not be determined

Conclusions:

According to the K_{foc} values derived in this study (K_{foc} = 184 to 563 mL/g) triticonazole would be classified as having medium mobility in soil. In particular, there was a decrease in mobility with increasing organic carbon content of the soils.

Comments (RMS AT):

- The study broadly follows OECD guideline 106 with major and minor deviations:
  - There is lack of information on a pre-equilibrium phase as requested by OECD guidline106
  - Freundlich sorption is based on 4 rather than 5 test concentrations
  - With an organic carbon content of 17.3 % the UK loamy sand clearly does not fit to soil types recommended in the OECD guideline
  - Calculation of the sorption coefficient is based on the *indirect* method although significant

amounts of none-extractable residues (NER, up to ~ 10 % AR) have been detected after the final desorption step. Applying the *indirect* method in this case, NER are included in the calculation of the sorption coefficient which is not defendable from a scientific point of view (also refer to O'Brien, 2017).

In view of these deficits and keeping in mind that new adsorption studies in line with OECD guideline 106 have been submitted for triticonazole the **study is not considered reliable**.

- The strong increase in $K_{foc,des}$ in the desorption cycles of some soils indicate that triticonazole is prone to aged sorption.

Reference:	**[^{14}C]-Triticonazole: Adsorption/Desorption to and from four soils and a sediment**
Author(s), year:	Burr, C. M., 1998
Report/Doc. Number:	R000496, 201670, 12966
Guideline(s):	US-EPA 163-1, OECD 106
GLP:	Yes
Validity:	None reliable (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The adsorption of phenyl labelled ^{14}C-triticonazole to and desorption from 2 US soils, 2 UK soils and a UK sediment have been investigated. Preliminary studies were carried out to check for adsorption to tubes, to determine the soil/solution ratio to be used and determine the time required for the compound to equilibrate between soil and water. Following preliminary studies an adsorption equilibrium time of 48 hours and a desorption equilibrium time of 1 hour were selected. Degradation was not significant at these times. The treatment solutions were prepared at four nominal concentrations: 4.2, 0.84, 0.17 and 0.03 mg/l 0.01 M calcium chloride. Experiments were done at 20° C in the dark.

Solvent extraction was carried out with acetonitrile/water (50:50 v/v). Selected supernatants were analysed by HPLC.

Adsorption and desorption isotherms and Freundlich coefficients were calculated.

Table B. 8.1.3.1.1-4: Soil Characteristics

Soil (USDA)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/100 g)
US silt loam	35.8	56.0	8.2	0.5	5.1	5.7
US sandy loam	64.2	29.1	6.7	1.2	5.9	6.5
UK loam	33.5	42.6	23.9	2.2	6.5	15.0
UK sand	90.2	4.7	5.1	2.4	6.2	13.2
UK clay[(a)]	20.0	36.4	43.5	3.4	7.5	62.3

(a) Sediment

Findings:

For all soils, the recovery of radioactivity was quantitative with mean recoveries ranging from 93.7 to 97.2 % of applied radioactivity.

The Freundlich adsorption coefficients (K_f) calculated ranged from 4.06 to 14.38 mL/g. When corrected for organic matter content of the soil the K_{foc} values obtained ranged from 344 to 812 mL/g. Triticonazole can therefore be classified as having medium to low mobility in soil.

$K_{f,des}$ values obtained ranged from 8.98 to 141 mL/g depending on the soil and desorption cycle. The $K_{f,des}$ values for the first desorption cycle ranged from 8.98 to 20.7 mL/g with equivalent $K_{foc,des}$ values ranging from 546 to 1795 mL/g. It is indicated that the adsorption was partially reversible.

In the soils the value of 1/*n* ranged from 0.813 to 0.890 suggesting that there was some non-linearity in the relationship between the concentration in the soil and solution for all the soil and the sediment with a relatively higher amount being adsorbed at lower concentrations.

The results are summarised in the tables below.

Table B. 8.1.3.1.1-5: Triticonazole - calculated adsorption coefficients

soil	OC (%)	*p*H ($CaCl_2$)	K_f (mL/g)	K_{foc} (mL/g)	1/*n* (-)	R^2
US silt loam	0.5	5.1	4.06	812	0.857	1.000
US sandy loam	1.2	5.9	5.62	468	0.813	0.999
UK loam	2.2	6.5	8.67	394	0.864	1.000
UK sand	2.4	6.2	14.38	599	0.857	1.000
UK clay sediment	3.4	7.5	11.70	344	0.890	1.000

Table B. 8.1.3.1.1-6: Triticonazole - calculated desorption coefficients

soil	$K_{f,des}$ (mL/g)	1/n (-)	$K_{foc,des}$ (mL/g)
US silt loam	1st cycle: 8.97	0.904	1795
	2nd cycle: 21.90	0.957	4380
	3rd cycle: 47.56	1.002	9511
	4th cycle: 91.90	1.026	18381
	5th cycle: 141.33	1.052	28265
US sandy loam	1st cycle: 9.60	0.837	800
	2nd cycle: 16.97	0.860	1414
	3rd cycle: 28.69	0.889	2391
	4th cycle: 51.72	0.927	4310
	5th cycle: 68.98	0.936	5748
UK loam	1st cycle: 13.12	0.876	596
	2nd cycle: 20.41	0.896	928
	3rd cycle: 31.19	0.921	1418
	4th cycle: 43.04	0.932	1956
	5th cycle: 56.11	0.943	2551
UK sand	1st cycle: 20.74	0.864	864
	2nd cycle: 26.74	0.873	1114
	3rd cycle: 33.48	0.883	1395
	4th cycle: 41.92	0.896	1747
	5th cycle: 50.45	0.909	2102
UK clay sediment	1st cycle: 18.57	0.906	546
	2nd cycle: 27.16	0.929	799
	3rd cycle: 42.87	0.949	1261
	4th cycle: 51.66	0.953	1519
	5th cycle: 67.76	0.972	1993

Conclusions:

According to the K_{foc} values derived in this study (K_{foc} = 334 to 812 mL/g) triticonazole would be classified as having medium to low mobility in soil. K_f values were in the range of 4.1 - 14.4 mL/g.

Comments (RMS AT):

- The study broadly follows OECD guideline 106 with major deviations:
  - There is lack of information on a pre-equilibrium phase as requested by OECD 106.
  - Freundlich sorption is based on 4 rather than 5 test concentrations.

- Calculation of the sorption coefficient is based on the indirect method although high amounts of NER (up to ~ 28 % AR) have been detected after the final desorption step. Applying the indirect method in this case, NER are included in the calculation of the sorption coefficient which is not defendable from a scientific point of view (also refer to O'Brien, 2017).

In view of these deficits and keeping in mind that new adsorption studies in line with OECD guideline 106 have been submitted for triticonazole the **study is not considered reliable**.

- The strong and consistent increase in $K_{foc,des}$ in the desorption cycles indicate that triticonazole is prone to aged sorption.

Reference:	**Adsorption / desorption behaviour of ^{14}C-BAS 595 F on different European soils**
Author(s), year:	Vasques, A. C., 2015a
Report/Doc. Number:	2014/3001242
Guideline(s):	OECD 106, US-EPA 163-1
GLP:	Yes
Validity:	Yes (refer to comments)
Status:	**New submission**

Material and methods:

Radiolabelled test material:	^{14}C-Triticonazole (BAS 595 F)
Batch No.:	866-1401
Label position:	Phenyl-U-^{14}C
Specific Activity:	5.95 MBq/mg
Radiochemical purity:	99.5 %
Molecular weight:	317.82 g/mol (non-radiolabelled)

The study was conducted with five different soils from Europe. The characterisation of the soils is presented in the table below. Soil samples were < 2 mm-mesh sieved and air dried at room temperature. The actual water content of the soils, determined using a halogen moisture analyser, was taken into account for the calculations.

Table B. 8.1.3.1.1-7: Characteristics of the soils used to investigate the adsorption and desorption of ^{14}C-BAS 595 F

Soil designation Origin	La Gironda (Spain)	Li 10 (Germany)	LUFA 2.1 (Germany)	LUFA 2.3 (Germany)	Wildacker (Germany)
USDA textural class:	Sandy clay loam	Loamy sand	Sand	Sandy loam	Silt Loam
Sand [%]	49.2	83.5	90.8	68.6	17.7
Silt [%]	23.0	12.2	6.9	23.1	73.5
Clay [%]	27.7	4.3	2.3	8.3	8.8
Organic carbon [%]	1.22	0.95	0.60	0.99	1.85
CEC [cmol$^+$/kg]	26.3	5.5	-0.7	7.5	3.1
*p*H ($CaCl_2$)	7.4	6.2	5.6	6.7	5.7

Experimental conditions

All tests were carried out in duplicate at room temperature. Test samples were prepared by applying on soil a treatment solution containing test item in a $CaCl_2$ 0.01 mol/L solution. Controls were prepared with only the treatment solution (no soil) in the tube and soil blanks were prepared by weighing soil in the tube and applying $CaCl_2$ 0.01 mol/L solution (no test item). For all tests carried out, the tubes, containing soil or not, after application of the proper solution, were closed and then shaken horizontally on a mechanical shaker at 150 rpm at temperature controlled room (20 ± 2 °C) and dark conditions for the indicated test period.

After test period is reached, the soil/solution suspensions were centrifuged at 3000 rpm for 5 minutes and the supernatants were isolated by pouring to storage flasks.

Both, supernatants and initial solution applied were analysed in order to determine the concentration of the test item in the aqueous solution after adsorption, as well as the initial concentration. The amount of test item adsorbed is indirectly calculated by the depletion of the total applied to the amount determined in the aqueous phase at the end of the test period.

Aliquots of samples were analysed in triplicates by liquid scintillation counter (LSC) for quantification and by radio-HPLC for formation of any degradation products and determination of the nature of the radioactivity.

Extraction procedure for triticonazole consists of a single extraction of 2 g soil (after removal of supernatant) with 20 mL of acetonitrile/water 4/1 (v/v). For each extraction step, the tubes were closed and then shaken horizontally on a mechanical shaker at 250 rpm for 30 minutes, then centrifuged at 3000 rpm for 5 minutes and the extracts were isolated.

The extraction of the soil samples was performed to provide the extraction efficiency, evaluate the nature of items adsorbed to soil and to determine the stability of test item on soil. The total aqueous phase to be considered for the calculations includes the supernatant decanted from soil after centrifugation and the remaining volume of this solution in the soil. In order to determine the volume of the remaining solution on soil just before extraction, soil samples are weighed throughout the experiments at several steps: Before and after treatment and after removal of supernatant. The soils dried weights were used for the calculations.

Preliminary tests
Preliminary experiments revealed that the optimal soil/solution ratio and adsorption equilibrium time for the adsorption/desorption tests were 1/5 and 24 h, respectively. Further preliminary experiments indicated that glass centrifuge tubes are suitable for conducting the adsorption/desorption studies as no significant adsorption on the test vessel surface occurs.

Adsorption-Desorption Isotherm Determination
To determine adsorption isotherms, standard solutions of the test item in 0.01 M $CaCl_2$ were prepared at five concentrations levels (nominal concentrations: from 0.01, 0.05, 0.1, 0.5 and 1.00 µg/mL) and applied directly on the soils (duplicates per concentration level dosed, 2 g soil and 10 mL solution). The experiment was performed by the indirect method. Samples were shaken for 24 hours. Thereafter, the soil/water specimens were centrifuged, decanted, and aliquots of the supernatants were assayed by LSC. Samples with the highest concentration were additionally analysed by radio-HPLC. After adsorption, two desorption steps were performed (24 hours each) by replacing the removed supernatants with an equal volume of 0.01 M $CaCl_2$ solution without test item. After the desorption experiments, the samples from the isotherms determination with the highest concentration were extracted to show the extractability and stability of the test item. A mass balance was calculated for these samples.

Description of analytical procedures
The amounts of radioactivity were determined by radioactivity measurements. Therefore, aliquots of the decanted supernatants were added to scintillation cocktail and radioassayed in a liquid scintillation counter. Radio-HPLC was used to show the purity and stability of the test item during the study.

Results and discussion:

Mass balance
During the main test, acceptable mass balances of the test item for the highest concentration in each soil were achieved with mean mass balances of 97.3, 97.1, 96.5, 95.3 and 95.1 % in soils La Gironda, Li 10, LUFA 2.2, LUFA 2.3 and Wildacker, respectively.

Findings
The stability of the test item in the adsorption/desorption experiments was proven by radio-HPLC analysis of the adsorption, desorption and extraction supernatants from the high dose samples and test item treatment solution fresh and after 48 hours shaking.

Detailed results from the adsorption and desorption tests for triticonazole in all five soils are presented in the tables below.

Table B. 8.1.3.1.1-8: Adsorption isotherms of triticonazole in five soils

Soil	Soil Type (USDA)	K_f (mL/g)	1/n (-)	K_{foc} (mL/g)	R^2
La Gironda	Sandy clay loam	3.97	0.94	325	1.000
Li 10	Loamy sand	4.79	0.91	504	0.999
Lufa 2.1	Sand	5.23	0.93	871	0.999
Lufa 2.3	Sandy loam	3.67	0.89	370	0.997
Wildacker	Silt loam	11.77	0.92	636	0.999

Table B. 8.1.3.1.1-9: Desorption isotherms of triticonazole in five soils

Soil	Desorption 1				Desorption 2			
	$K_{f,des1}$ (mL/g)	1/n (-)	$K_{foc,des1}$ (mL/g)	R^2	$K_{f,des2}$ (mL/g)	1/n (-)	$K_{foc,des2}$ (mL/g)	R^2
La Gironda	5.41	0.92	444	1.000	6.87	0.94	563	0.999
Li 10	6.15	0.92	647	0.999	8.25	0.93	868	0.999
Lufa 2.1	6.20	0.94	1033	0.999	8.62	0.93	1437	0.998
Lufa 2.3	5.13	0.90	518	0.995	8.40	0.92	848	0.995
Wildacker	14.91	0.93	806	1.000	17.99	0.92	973	1.000

Conclusions:

Freundlich adsorption coefficients K_f in the five soils investigated range from 3.7 to 11.8 mL/g, corresponding to K_{foc} values ranging from 325 to 871 mL/g. Freundlich exponents (1/n) varied between 0.89 and 0.94.

Comments (RMS AT):

- The study follows OECD guideline 106 with a major deviation:
  - There is a lack of information about a pre-equilibrium phase as requested by OECD 106.

  In view of the possibly missing pre-equilibrium phase the study may not be considered fully reliable from a regulatory point of view. The pre-equilibration phase is considered to disrupt soil aggregates and to increase sorption surface. This may have an impact on the definitive sorption phase of the experiment particularly if the adsorption phase is short (a few hours). However, as sorption data obtained in this study (with an adsorption phase of 48 hrs) are not significantly different from results obtained in the next study (Simmonds, 2017a) using the same soils (albeit different batches), sorption result of this study are considered equally reliable. Nevertheless applicants and study authors are encouraged to adequately follow this basic OECD guideline 106 requirement. **The RMS AT recommends re-emphasising this issue in EFSA's OECD 106 checklist.**

  Concentrations of the test item adsorbed to the soil were determined by the *indirect* method which makes the calculation susceptible to possible degradation and formation of NER. Although not measured by dedicated combustion techniques, NER were in the range of 2.7 - 4.9 % AR if calculated on basis of data provided for the mass balance (test concentration of 1.0 µg/L including extractable residues after the final desorption step). In view of these low amounts of NER and as no degradation of the test item was observed the *indirect* method is considered sufficiently robust.

- The strong and consistent increase in $K_{foc,des}$ in the desorption cycles indicate that triticonazole is prone to aged sorption.

Reference:	**[^{14}C]-BAS 595F: Adsorption to and desorption from five soils**
Author(s), year:	Simmonds, R., 2017a
Report/Doc. number:	2017/1142046
Guideline(s):	OECD 106 (2000)
GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Radiolabelled test material:	[Phenyl-U-^{14}C]-triticonazole (BAS 595 F)
Batch No.:	866-1701
Specific Activity:	5.63 MBq/mg
Radiochemical purity:	96.2 %
Molecular weight:	317.81 g/mol (non-radiolabelled)

Soils

The study was conducted with five different soils from Europe. The characterisation of the soils is presented in the table below. Soil samples were < 2 mm mesh sieved. The actual water content of the soils was determined by comparison of weights of soil before and after oven-drying at ca. 100 °C.

Table B. 8.1.3.1.1-10: Characteristics of the soils used to investigate the adsorption and desorption of triticonazole

Soil designation Origin	Wildacker (Germany)	LUFA 2.3 (Germany)	LUFA 2.1 (Germany)	Li 10 (Germany)	La Gironda (Spain)
USDA textural class:	Silt Loam	Sandy Loam	Sand	Loamy Sand	Silty Clay Loam
Sand [%]	21.4	63.4	89.8	82.3	16.1
Silt [%]	69.2	28.1	7.7	12.2	49.3
Clay [%]	9.4	8.5	2.5	5.5	34.6
Organic carbon [%]	2.01	0.66	0.72	0.89	1.92
CEC [cmol$^+$/kg]	6.1	4.5	1.7	3.5	30.7
*p*H ($CaCl_2$)	5.8	5.3	5.6	6.1	7.1

Experimental conditions of preliminary tests

Preliminary studies were carried out to check for adsorption to the tubes, to determine any potential background radioactivity in the soil, to determine the soil to solution ratio to be used, to check stability of [^{14}C]-triticonazole in 0.01 M calcium chloride solutions and to determine the time required for the test item to equilibrate between soil and water under adsorption and desorption conditions.

Controls for testing adsorption to the tubes were prepared with only the treatment solution (no soil) using PTFE and glass tubes. The tubes were shaken for 48 hours and aliquots analysed by LSC.

Soil blanks (background radioactivity) were prepared by weighing 10 g of each soil in a glass tube (in duplicates) and applying 0.01 M $CaCl_2$ solution (without test item). The tubes were shaken for 48 hours. After this period, the soil/solution suspensions were centrifuged at 2500 rpm for 10 minutes. The supernatants were analysed by LSC.

Test samples (determination of soil to solution ratios) were prepared by applying test item in a 0.01 M $CaCl_2$ solution on each soil. First, calcium chloride was added to 1, 2 and 4 g of soil to give soil/solution ratios of approximately 1:20, 1:10 and 1:5. The tubes were shaken overnight to pre-equilibrate (ca. 16 hrs) prior to treatment. Following pre-equilibration, 1 mL of the application solution was added to each tube (final nominal treatment concentration of 0.1 mg/L). The tubes were shaken for a further 24 hours, centrifuged at 4600 rpm for 10 minutes, the supernatants transferred to pre-weighed plastic bottles and analysed by LSC and Radio-HPLC.

Stability of the test item in 0.01 M $CaCl_2$ was tested by periodically (4, 24 and 96 hours) analysing a sample of calcium chloride treated with the test item by HPLC.

For determination of the adsorption equilibrium time, ten tubes for each soil with either a 1:20 (Wildacker soil) or 1:10 (all remaining soils) soil/solution ratio were shaken for 16 hours to equilibrate. After equilibration, the tubes were treated with test item to achieve a final nominal treatment concentration of 0.1 mg/L and were again put on a shaker. Two tubes from each soil were removed after 4, 8, 24, 32 and 48 hrs. At each time point, the tubes were centrifuged at 4600 rpm for 10 minutes, the supernatants removed and analysed by LSC. The soils were extracted and analysed as described below.

The preliminary desorption experiment (to determine desorption equilibrium time) followed a similar regime with 1:20 and 1:10 soil:solution ratio, 16 h pre-equilibration, 24 h adsorption and 1, 2, 24 and 48 h desorption.

At each time point, the tubes were centrifuged at 4600 rpm for 10 minutes, the supernatants removed and analysed by LSC. The soils were extracted and analysed as described below.

Extraction of the soil samples was performed to provide extraction efficiency, evaluate the nature of items adsorbed to soil and to determine the stability of test item on soil. The extraction procedure for [^{14}C]-triticonazole consisted of an extraction of 1 or 2 g of soil (depending on soil type and appropriate soil/solution ratio) with 20 mL of acetonitrile/water 80:20 (v/v), followed by 20 mL with acetonitrile:methanol 70:30 (v/v). For each extraction step, the tubes were placed on a flat-bed shaker for 30 minutes, centrifuged at 4600 rpm for 10 minutes and the extracts isolated. Each extract supernatant removed to determine the radioactivity by LSC. All adsorption supernatants and combined acetonitrile/water extracts were further analysed by HPLC. As there was negligible radioactivity associated with the last acetonitrile/methanol extracts, no further analysis of these samples was undertaken.

The extraction regime was confirmed by a supplementary test of a modified extraction. Following pre-equilibration for 16 hours, 24 hour shaking and centrifugation (adsorption phase), soils were extracted using consecutively acetonitrile, acetonitrile/methanol (70:30 v/v), acetonitrile/water (70:30 v/v) and methanol/water (70:30 v/v). After each extraction step, tubes were horizontally shaken for 30 minutes, centrifuged at 4600 rpm for 10 minutes and supernatants transferred. Each supernatant was weighed, and weighed aliquots were then removed for quantification. Following counting by LSC, the four solvent extracts were combined and concentrated before analysis by HPLC.

To determine the mass balance of extraction samples, the soil samples were air-dried, weighed and ground to a fine powder. Triplicate aliquots (approximately 0.2g) were weighed and combusted. The combustion products were absorbed in Carbosorb E and mixed with Permafluor E+ prior to quantification.

Preliminary tests (conclusions for definitive test)
Both, screw capped PTFE tubes and plastic-coated screw capped glass tubes were used for the preliminary check. Following the findings, PTFE tubes were selected for use throughout the remainder of the study. Background radioactivity detected was negligible and no correction necessary. Preliminary experiments revealed that the optimal soil/solution ratio for the adsorption/desorption tests were 1/20 for the Wildacker soil and 1/10 for all remaining soils. Stability of the test item in calcium chloride was verified for up to 96 hours, indicating stability for longer than the duration of the intended definitive phase of the study. A pre-equilibration time of 16 hours, followed by an adsorption equilibrium time of 24 hours was chosen for all soils, followed by two desorption cycles of 2 hours each. The modified extraction regime using acetonitrile, followed by acetonitrile/methanol, acetonitrile/water and methanol/water was chosen for the definitive test. The chosen treatment range was 0.01-1.0 mg/L, i.e. less than half the aqueous solubility of the test item.

Adsorption-Desorption Isotherm Determination (definitive test)
All tests were carried out in duplicate at room temperature (20 ± 2 °C), with shaking periods in the dark.

In the definitive test, approx. 1 g or 2 g soil (resulting in 1/20 soil/solution ratio for Wildacker and 1/10 soil/solution ratio for the remaining soils) were weighed into pre-weighed tubes and an appropriate volume of 0.01 M calcium chloride solution was added (20 mL minus soil moisture and 1mL for treatment solution volume added later). Samples were shaken for approx. 16 hours to pre-equilibrate prior to treatment. Following pre-equilibration, 1 mL of standard solutions of [^{14}C]-triticonazole in 0.01 M $CaCl_2$, prepared at five concentrations levels (nominal concentrations: 0.01, 0.05, 0.1, 0.5 and 1.0 mg/L), were added. Soil solutions were mixed for 24 hours on an end-over-end shaker. Tubes were weighed and centrifuged at 4600 rpm for 10 minutes. Supernatant was removed and weight of the supernatant and remnant soil pellets were recorded.

After adsorption, two desorption steps were performed (2 hours each) by replacing the removed supernatants with an equal volume of 0.01 M $CaCl_2$ solution without test item.

Aliquots of supernatants of the adsorption step and desorption step as well as the four extraction steps were analysed by liquid scintillation counter (LSC) for quantification. Adsorption supernatants, desorption supernatants and solvent extracts of each soil were further analysed by Radio-HPLC for formation of any degradation products and determination of the nature of the radioactivity as well as stability of the test items.

Material balance was assayed by LSC to determine total recovery of radioactivity. Stability and parental mass balance were determined by HPLC. Calculations of test item concentrations in supernatants and solvent extracts

with the indirect and direct calculation method are based on results measured by LSC, however with the direct method, the measured values are additionally corrected for purity in respective HPLC measurements.

Description of analytical methodology
The amounts of radioactivity were determined by radioactivity measurements. Therefore, aliquots of the decanted supernatants were added to scintillation cocktail and radioassayed in a liquid scintillation counter. Radio-HPLC (Luna C18 5µm 250 x 4.6 mm) was used to show the purity and stability of the test item during the study.

For the LSC measurements, an LOD of 0.03 ng (9 dpm) and an LOQ of 0.09 ng (30 dpm) applied. For HPLC, the LOQ was determined at 0.1 % AR for most treatment rates, and 0.5 % AR for the lowest treatment rate.

Results and discussion:

Mass balance
During the main test, overall mean mass balances (expressed as % AR) for individual samples was 96.6, 96.5, 96.3, 97.0 and 97.1 % in soils Wildacker, LUFA 2.3, LUFA 2.1, Li10 and La Gironda, respectively.

Mass balance (HPLC-based) for Wildacker, LUFA 2.3, LUFA 2.1, Li10 and La Gironda resulted in mean values of parental mass balance of 92.8, 93.1, 92.9, 93.1 and 89.7 %.

For La Gironda, the parental mass balance was < 90 % triticonazole, therefore, the direct calculation method (test item in soil determined by solvent extraction and all test item concentrations corrected for purity found with HPLC measurement) was applied for La Gironda soil, while an indirect calculation method (amount of test item in soil determined by difference of test item in solution) was applied for the other four soils as indicated by OECD 106.

Findings
The stability of the test item in the definitive test (adsorption/desorption experiments) was proven by radio-HPLC analysis of the adsorption, desorption and extraction supernatants from all dose samples and test item treatment solutions.

Detailed results from the adsorption and desorption tests for triticonazole in all five soils are presented in the tables below.

Table B. 8.1.3.1.1-11: Adsorption isotherms of triticonazole in five soils

Soil	Soil Type (USDA)	K_f (mL/g)	1/*n*	R^2	K_{foc} (mL/g)
Wildacker	Silt Loam	13.37	0.893	0.999	665
LUFA 2.3	Sandy Loam	4.52	0.898	0.999	685
LUFA 2.1	Sand	5.60	0.889	0.999	778
Li10	Loamy Sand	5.11	0.888	0.999	574
La Gironda[(a)]	Silty Clay Loam	5.56	0.848	0.998	290

(a) As HPLC-based parental mass balance was slightly below 90 % (average of 89.37 %), adsorption and desorption isotherms were calculated based on the direct method using HPLC-corrected quantification to account for any degradation.

Table B. 8.1.3.1.1-12: Desorption isotherms of triticonazole in five soils

Soil	Desorption 1				Desorption 2			
	$K_{f,des1}$ (mL/g)	1/*n*	R^2	$K_{foc,des1}$ (mL/g)	$K_{f,des2}$ (mL/g)	1/*n*	R^2	$K_{foc,des2}$ (mL/g)
Wildacker	31.33	0.961	1.000	1559	57.13	0.996	1.000	2842
LUFA 2.3	10.96	0.965	0.999	1660	25.49	1.016	0.999	3863
LUFA 2.1	12.45	0.946	0.999	1729	24.19	0.995	0.998	3360
Li10	9.73	0.934	0.999	1094	19.13	0.982	0.999	2149
La Gironda[(a)]	8.45	0.849	1.000	440	13.31	0.883	0.999	693

(a) As HPLC-based parental mass balance was slightly below 90 % (average of 89.37 %), adsorption and desorption isotherms were calculated based on the direct method using HPLC-corrected quantification to account for any degradation.

Conclusion:

Freundlich adsorption coefficients K_f of triticonazole ranged from 4.5 to 13.4 mL/g in the five soils, which corresponded to K_{foc} values ranging from 290 to 778 mL/g. Freundlich exponents 1/*n* varied between 0.848 and 0.898. The desorption coefficients $K_{f,des1}$ and $K_{f,des2}$ ranged from 8.5 to 31.3 mL/g and 13.3 to 57.1 mL/g in the five soils, respectively, with $K_{foc,des}$ values between 440 and 1660 mL/g, and 693 to 3863 mL/g.

Comments (RMS AT):

- The study follows OECD guideline 106 and is considered reliable. It is noted that soils properties (texture, OC and *p*H) are not necessarily fully in line with recommendations given in the OECD guideline. However, this is not considered to invalidate the study or parts of it.

- The RMS AT notes that combustion data (i.e. non-extractable residues, NER) observed in this study after the second desorption step where on average ≤ 1.1 % AR in all soils with the exception of the La Gironda soil (≤ 3.7 % AR) thus considered negligible in sense of OECD guideline 106 (*'extraction efficiency should be at least 95 %'*). Nevertheless, in case of La Gironda soil, NER were accounted for by the study author (i.e. excluded in the calculation of the sorption coefficient).

- The strong and consistent increase in $K_{foc,des}$ in the desorption cycles indicate that triticonazole is prone to aged sorption.

B.8.1.3.1.2. Adsorption and desorption of metabolites, breakdown and reaction products

Studies submitted for first Annex I inclusion:

- **Simmonds & Lowden (2000a)**, investigating RPA 406341 (Trans-diol) in four soils and one sediment
- **Simmonds & Lowden (2001)**, investigating RPA 404766 (Cis-diol) in four soils and one sediment
- **Simmonds & Lowden (2000b)**, investigating RPA 407922 in four soils and one sediment

New studies submitted:

- **Vasques (2015b)**, investigating RPA 406341 (Trans-diol), RPA 404766 (Cis-diol) and RPA 407922 in five soils
- **O'Brian (2017)**, investigating RPA 404766 (Cis-diol) in five soils
- **Kingman (2017)**, investigating RPA 406341 (Trans-diol) in five soils
- **Simmonds (2017b)**, investigating RPA 407922 in five soils
- **Szegedi (2018)**, investigating adsorption of the metabolite fractions 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' observed > 5 % AR at two consecutive sampling points in Ayliffe & Austin (1993)

Reference:	**Adsorption to and desorption from four soils and a sediment (^{14}C) RPA 406341**
Author(s), year:	Simmonds, M., Lowden, P., 2000a
Report/Doc. Number:	C010431, GOoD16714, 202662, 16714
Guideline(s):	US-EPA 163-1, OECD 106
GLP:	Yes
Validity:	None reliable (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The objective of the study was to determine the adsorption/desorption characteristics of [phenyl-U-^{14}C]-RPA 406341 (Trans-diol) in four soil types (two American and two European) and one sediment (UK). Following preliminary studies an adsorption equilibrium time of 48 hours was selected for two of the soils and an adsorption equilibrium time of 24 hours was selected for the remaining three soils. A desorption equilibrium time of 2 hours was selected for all soils. Preliminary studies were also carried out to check for adsorption to tubes and to determine the soil/solution ratio to be used as well as the stability of the compound under the test conditions. The treatment solutions were prepared at four nominal concentrations: 4.39, 0.878, 0.176 and 0.035 mg/l 0.01M calcium chloride. Experiments were done at 20 °C in the dark.

Solvent extraction was carried out with methanol. Selected supernatants were analysed by HPLC.

Adsorption and desorption isotherms and Freundlich coefficients were calculated.

Table B. 8.1.3.1.2-1: Soil Characteristics

Soil (USDA)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/100 g)
US silt loam	39.4	55.1	5.5	0.5	6.0	6.3
US sandy loam	69.1	24.4	6.6	1.3	5.2	5.0
UK loam	33.4	41.5	25.1	1.9	6.4	10.0
UK clay loam	22.3	41.7	36.0	4.1	7.4	51.9
UK sandy clay loam[(a)]	52.5	21.5	26.0	2.6	7.7	43.8

(a) Sediment

Findings:

The recovery was quantitative varying from 98.3 to 99.6 %. No adsorption to glass tubes or significant degradation of RPA 406341 (Trans-diol) was observed. Correlation coefficients for the observed adsorption isotherms were between 0.999 and 1.000. The values of 1/*n* ranged from 0.840 to 0.877 indicating a high degree of non-linear adsorption with concentration. The K_{oc} values ranged from 61 to 163 mL/g, RPA 406341 (Trans-diol) would be expected to have high mobility in soil. K_f and K_{oc} values obtained did not display any trend related to the soil *p*H, organic carbon content, cation exchange capacity or clay content.

The desorption isotherms do not follow the adsorption isotherm in any soil suggesting that once adsorbed the compound would be increasingly less readily desorbed. The pattern of the desorption isotherms suggests that the adsorption is only partially reversible in all the soils. From the K_f values obtained it can be concluded that RPA 406341 (Trans-diol) was adsorbed to soil to a limited extent. The results are detailed in the tables below.

Table B. 8.1.3.1.2-2: RPA 406341 (Trans-diol) - calculated adsorption coefficients

soil	OC (%)	*p*H ($CaCl_2$)	K_f (mL/g)	1/*n* (-)	K_{foc} (mL/g)	R^2
US silt loam	0.5	6.0	0.82	0.849	163	1.000
US sandy loam	1.3	5.2	1.64	0.840	126	0.999
UK loam	1.9	6.4	2.65	0.868	140	1.000
UK clay loam	4.1	7.4	2.50	0.861	61	1.000
UK sandy clay loam[(a)]	2.6	7.7	3.31	0.877	127	1.000

(a) Sediment

Table B. 8.1.3.1.2-3: RPA 406341 (Trans-diol) - calculated desorption coefficients

soil	$K_{f,des}$ (mL/g)	1/*n* (-)	$K_{foc,des}$ (mL/g)
US silt loam	1st cycle: 1.71	0.895	343
	2nd cycle: 4.85	0.948	970
	3rd cycle: 14.87	1.042	2956
	4th cycle: 49.98	1.112	9995
	5th cycle: 143.77	1.173	28754
US sandy loam	1st cycle: 2.79	0.866	214
	2nd cycle: 4.22	0.896	324
	3rd cycle: 6.91	0.897	532
	4th cycle: 13.24	0.925	1019
	5th cycle: 23.31	0.947	1793
UK loam	1st cycle: 4.78	0.896	252
	2nd cycle: 8.15	0.911	429
	3rd cycle: 12.95	0.925	681
	4th cycle: 19.16	0.937	1008
	5th cycle: 27.18	0.948	1430
UK clay loam	1st cycle: 3.06	0.877	75
	2nd cycle: 3.78	0.885	92
	3rd cycle: 5.23	0.901	128
	4th cycle: 7.42	0.914	181
	5th cycle: 11.02	0.920	269
UK sandy clay loam[(a)]	1st cycle: 4.27	0.895	164
	2nd cycle: 5.62	0.911	216
	3rd cycle: 7.56	0.926	291
	4th cycle: 10.40	0.939	400
	5th cycle: 14.80	0.953	569

(a) Sediment

Conclusions:

According to the K_{foc} values obtained in this study (K_{foc} in the range of 61 - 163 mL/g) the metabolite RPA 406341 (Trans-diol) would be classified as having high mobility in soil.

Comments (RMS AT):

- The study broadly follows OECD guideline 106 with some deviations:

- There is lack of information on a pre-equilibrium phase as requested by OECD guideline 106.
- Freundlich sorption is based on 4 rather than 5 test concentrations.
- Calculation of the sorption coefficient is based on the *indirect* method although significant amounts of NER (up to ~ 14 % AR) have been detected after the final desorption step. Applying the *indirect* method in this case, NER are included in the calculation of the sorption coefficient which is not defendable from a scientific point of view (also refer to O'Brien, 2017).

In view of these deficits and keeping in mind that new adsorption studies in line with OECD guideline 106 have been submitted for RPA 406341 (Trans-diol) the **study is not considered reliable**.

- The strong and consistent increase in $K_{foc,des}$ in the desorption cycles indicate that RPA 406341 (Trans-diol) is prone to aged sorption.

Reference:	**Adsorption to and desorption from four soils and a sediment (^{14}C) RPA 404766**
Author(s), year:	Simmonds, M., Lowden, P., 2001
Report/Doc. Number:	C012304, GOoD16953
Guideline(s):	US-EPA 163-1, OECD 106
GLP:	Yes
Validity:	None reliable (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The objective of the study was to determine the adsorption/desorption characteristics of [phenyl-U-^{14}C]-RPA 404766 (Cis-diol) in four soil types (two American and two European) and one sediment (UK). Following preliminary studies an adsorption equilibrium time of 24 hours and a desorption equilibrium time of 2 hours was selected for all soils. Preliminary studies were also carried out to check for adsorption to tubes and to determine the soil/solution ratio to be used as well as the stability of the compound under the test conditions. The treatment solutions were prepared at four nominal concentrations: 5, 1, 0.2 and 0.04 mg/l 0.01M calcium chloride. Experiments were done at 20 ± 1 °C in the dark. Solvent extraction was carried out with methanol. Selected supernatants were analysed by HPLC.

Adsorption and desorption isotherms and Freundlich coefficients were calculated.

Table B. 8.1.3.1.2-4: Soil Characteristics

Soil (USDA classif.)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/100g)
US silt loam	39.4	55.1	5.5	0.5	6.0	6.3
US sandy loam	69.1	24.4	6.6	1.3	5.2	5.0
UK loam	33.4	41.5	25.1	1.9	6.4	10.0
UK clay loam	22.3	41.7	36.0	4.1	7.4	51.9
UK sandy clay loam[(a)]	52.5	21.5	26.0	2.6	7.7	43.8

(a) Sediment

Findings:

The recovery was good with mean recoveries ranging from 98.3 % to 99.3 % of applied radioactivity.

No adsorption to the glass tubes or significant degradation of RPA 404766 (Cis-diol) was observed. The K_f values ranged from 0.67 mL/g in the US sandy silt loam to 1.62 mL/g in the sediment, indicating low adsorption to soil. The high degree of non-linearity as shown by the values of 1/*n* which ranged from 0.825 to 0.884

demonstrates very specific interactions and saturation of the adsorption sites. The K_{foc} values ranged from 35 to 133 mL/g. RPA 404766 (Cis-diol) can be classified as highly mobile in soil.

The desorption isotherms do not follow the adsorption isotherm in any soil, showing a clear hysteresis in the adsorption/desorption curve, suggesting that once adsorbed RPA 404766 (Cis-diol) would be increasingly less readily desorbed.

Table B. 8.1.3.1.2-5: RPA 404766 (Cis-diol) - calculated adsorption coefficients

soil	OC (%)	*p*H ($CaCl_2$)	K_f (mL/g)	1/*n* (-)	K_{foc} (mL/g)	R^2
US silt loam	0.5	6.0	0.67	0.825	133	0.999
US sandy loam	1.3	5.2	1.09	0.850	84	1.000
UK loam	1.9	6.4	1.51	0.884	79	1.000
UK clay loam	4.1	7.4	1.43	0.854	35	1.000
UK sandy clay loam[(a)]	2.6	7.7	1.62	0.877	62	1.000

(a) Sediment

Table B. 8.1.3.1.2-6: RPA 404766 (Cis-diol) - calculated desorption coefficients

soil	$K_{f,des}$ (mL/g)	1/*n* (-)	$K_{foc,des}$ (mL/g)
US silt loam	1st cycle: 1.30	0.824	259
	2nd cycle: 3.47	0.849	693
	3rd cycle: 10.70	0.894	2139
	4th cycle: 7.55	0.940	5509
	5th cycle: 56.81	0.973	11361
US sandy loam	1st cycle: 2.27	0.846	175
	2nd cycle: 5.89	0.899	453
	3rd cycle: 14.39	0.931	1107
	4th cycle: 29.27	0.962	2251
	5th cycle: 62.04	1.023	4772
UK loam	1st cycle: 2.49	0.902	155
	2nd cycle: 5.86	0.915	309
	3rd cycle: 10.74	0.924	565
	4th cycle: 17.62	0.932	928
	5th cycle: 26.34	0.936	1386
UK clay loam	1st cycle: 1.95	0.864	48
	2nd cycle: 2.87	0.856	70
	3rd cycle: 5.24	0.899	128
	4th cycle: 9.21	0.904	225
	5th cycle: 20.03	0.957	488
UK sandy clay loam[(a)]	1st cycle: 2.15	0.871	83
	2nd cycle: 3.10	0.873	119
	3rd cycle: 4.83	0.882	186
	4th cycle: 8.27	0.895	318
	5th cycle: 15.29	0.923	588

(a) Sediment

Conclusions:

From the K_f values obtained (0.67 - 1.62 mL/g) it can be concluded that RPA 404766 (Cis-diol) shows only low adsorption to soil. 1/*n* values ranged from 0.825 to 0.844 showing a high degree of non-linearity. On the basis of K_{foc} values which ranged from 35 to 133 mL/g, with a mean of 79 mL/g, RPA 404766 (Cis-diol) can be classified as highly mobile in soils within a range of *p*H values.

Comments (RMS AT):

- The study broadly follows OECD guideline 106 with some major and minor deviations:
  - There is a lack of information about a pre-equilibrium phase as requested by OECD 106
  - Freundlich sorption is based on 4 rather than 5 test concentrations
  - Calculation of the sorption coefficient is based on the *indirect* method although significant

amounts of NER (up to ~ 7 % AR) have been detected after the final desorption step. Applying the *indirect* method in this case, NER are included in the calculation of the sorption coefficient which is not defendable from a scientific point of view (also refer to O'Brien, 2017).

In view of these deficits and keeping in mind that new adsorption studies (fully in line with OECD 106) have been submitted for RPA 404766 (Cis-diol) the **study is not considered reliable**.

- The strong and consistent increase in $K_{foc,des}$ in the desorption cycles indicate that RPA 404766 (Cis-diol) is prone to aged sorption.

Reference:	**Adsorption to and desorption from four soils and a sediment (^{14}C) RPA 407922**
Author(s), year:	Simmonds, M., Lowden, P., 2000b
Report/Doc. Number:	C010432, GOoD16952, 202633
Guideline(s):	US-EPA 163-1, OECD 106
GLP:	Yes
Validity:	Not essential (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The objective of the study was to determine the adsorption/desorption characteristics of [triazole-3(5)-^{14}C]-RPA 407922 in four soil types (two American and two European) and one sediment (UK). Following preliminary studies an adsorption equilibrium time of 48 hours was selected for four of the soils and an adsorption equilibrium time of 24 hours was selected for the sandy loam soil. A desorption equilibrium time of 2 hours was selected for all soils. Preliminary studies were also carried out to check for adsorption to tubes and to determine the soil/solution ratio to be used as well as the stability of the compound under the test conditions. The treatment solutions were prepared at four nominal concentrations: 5, 1, 0.2 and 0.04 mg/l 0.01M calcium chloride. Experiments were done at 20° C in the dark. Solvent extraction was carried out with methanol. Selected supernatants were analysed by HPLC.

Adsorption and desorption isotherms and Freundlich coefficients were calculated.

Table B. 8.1.3.1.2-7: Soil Characteristics

Soil (USDA classif.)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)	CEC (meq/100g)
US silt loam	39.4	55.1	5.5	0.5	6.0	6.3
US sandy loam	69.1	24.4	6.6	1.3	5.2	5.0
UK loam	33.4	41.5	25.1	1.9	6.4	10.0
UK clay loam	22.3	41.7	36.0	4.1	7.4	51.9
UK sandy clay loam[(a)]	52.5	21.5	26.0	2.6	7.7	43.8

(a) Sediment

Findings:

The recovery was quantitative varying from 97.4 to 100.2 %.

No adsorption to glass tubes or significant degradation of RPA 407922 was observed. Correlation coefficients for the observed adsorption isotherms were between 0.987 and 0.999. The values of 1/*n* ranged from 0.708 to 0.865 indicating a high degree of non-linear adsorption with concentration. The K_{foc} values ranged from 407 to 1305 mL/g, RPA 407922 would be expected to have low to medium mobility in soils. The K_{foc} values obtained showed a *p*H related trend with higher values obtained in the lower *p*H soils. Excluding the US sandy loam, the soil which demonstrated the lowest *p*H and the greatest degradation, a trend was observed with higher K_f values obtained with increasing organic carbon content, cation exchange capacity and clay content. The desorption

isotherms do not follow the adsorption isotherm in any soil suggesting that once adsorbed the compound would be increasingly less readily desorbed. The pattern of the desorption isotherms suggests that the adsorption is only partially reversible in all the soils. From the K_f values obtained it can be concluded that RPA 407922 was highly adsorbed to soil.

Table B. 8.1.3.1.2-8: RPA 407922 - calculated adsorption coefficients

soil	OC (%)	*p*H ($CaCl_2$)	K_f (mL/g)	1/*n* (mL/g)	K_{foc} (mL/g)	R^2
US silt loam	0.5	6.0	3.88	0.755	775	0.987
US sandy loam	1.3	5.2	16.96	0.825	1305	0.998
UK loam	1.9	6.4	9.44	0.825	497	0.998
UK clay loam	4.1	7.4	19.13	0.708	467	0.993
UK sandy clay loam[(a)]	2.6	7.7	10.57	0.865	407	0.999

(a) Sediment

Table B. 8.1.3.1.2-9: RPA 407922 - calculated desorption coefficients

soil	$K_{f,des}$ (mL/g)	1/*n* (-)	$K_{foc,des}$ (mL/g)
US silt loam	1st cycle: 11.25	0.774	2250
	2nd cycle: 32.59	0.825	6518
	3rd cycle: 76.55	0.872	15311
	4th cycle: 143.71	0.904	28741
	5th cycle: 241.41	0.935	48282
US sandy loam	1st cycle: 53.40	0.859	4108
	2nd cycle: 178.85	1.031	13758
	3rd cycle: 240.67	0.946	18513
	4th cycle: 400.56	0.985	30812
	5th cycle: 546.66	0.998	42051
UK loam	1st cycle: 19.72	0.858	1038
	2nd cycle: 36.78	0.889	1936
	3rd cycle: 58.97	0.907	3104
	4th cycle: 86.90	0.928	4573
	5th cycle: 121.93	0.943	6417
UK clay loam	1st cycle: 30.56	0.628	745
	2nd cycle: 48.54	0.640	1184
	3rd cycle: 79.80	0.683	1946
	4th cycle: 131.40	0.737	3205
	5th cycle: 228.39	0.800	5571
UK sandy clay loam[(a)]	1st cycle: 14.91	0.872	574
	2nd cycle: 21.14	0.886	813
	3rd cycle: 28.96	0.892	1114
	4th cycle: 41.44	0.909	1594
	5th cycle: 60.36	0.921	2321

(a) Sediment

Conclusions:

From the K_{fOC} values obtained in this study (K_{foc} in the range from 407 - 1305 mL/g) the metabolite RPA 407922 would be classified as having medium to low mobility in soil. The K_{foc} values showed a *p*H related trend with higher values obtained in the lower *p*H soils. K_f values were in the range of 3.9 - 19.1 mL/g, pending on the organic carbon content and clay content in soil.

Comments (RMS AT):

- The study broadly follows OECD guideline 106 with some major and minor deviations:
  - There is lack of information on a pre-equilibrium phase as requested by OECD guideline 106.
  - Freundlich sorption is based on 4 rather than 5 test concentrations
  - Calculation of the sorption coefficient is based on the *indirect* method although significant amounts of NER (up to ~ 90 % AR!) have been detected after the final desorption step. Applying the indirect method in this case, NER are included in the calculation of the sorption

coefficient which is not defendable from a scientific point of view (also refer to O'Brien, 2017).

- No exposure assessment is triggered for RPA 407922. Consequently, this study is **considered not essential**.

Reference:	**Adsorption/desorption behavior of ^{14}C-RPA404766/M595F001 (Reg. 5079295), ^{14}C-RPA 406341/M595F002 (Reg. 5059144) and ^{14}C-RPA407922 (Reg. 5079288) (metabolites of ^{14}C-BAS 595 F) on different European soils**
Author(s), year:	Vasques, A. C., 2015b
Report/Doc. Number:	2015/3000503
Guideline(s):	OECD 106 (2000)
GLP:	Yes
Validity:	Yes (refer to comments)
Status:	**New submission**

Material and methods:

Radiolabelled test item:	^{14}C-RPA 406341(Trans-diol)
Batch No.:	1102-1002
Label position:	Triazole-3(5)-^{14}C
Specific Activity:	6.33 MBq/mg
Radiochemical purity:	98.5 %
Molecular weight:	333.82 g/mol (non-radiolabelled)
Radiolabelled test item:	^{14}C-RPA 404766 (Cis-diol)
Batch No.:	1104-1056
Label position:	Triazole-3(5)-14C
Specific Activity:	6.65 MBq/mg
Radiochemical purity:	98.5 %
Molecular weight:	333.82 g/mol (non-radiolabelled)
Radiolabelled test item:	^{14}C-RPA 407922
Batch No.:	1103-1028
Label position:	Triazole-3(5)-14C
Specific Activity:	5.66 MBq/mg
Radiochemical purity:	97.4 %
Molecular weight:	333.82 g/mol (non-radiolabelled)

Soils

The study was conducted with five different European soils. The characterisation of the soils is presented in the table below. Soil samples used were < 2 mm-mesh sieved and air dried at room temperature. The actual water content of the soils, determined using a halogen moisture analyser, was taken into account for the calculations.

Table B. 8.1.3.1.2-10: Characterisation of the soils used to investigate the adsorption and desorption of ^{14}C-RPA404766 (Cis-diol), ^{14}C-RPA 406341 (Trans-diol) and ^{14}C-RPA407922

Soil designation Origin	La Gironda (Spain)	Li 10 (Germany)	LUFA 2.1 (Germany)	LUFA 2.3 (Germany)	Wildacker (Germany)
DIN textural class	Sandy clay loam	Silty sand	Sand	Loamy sand	Clay silt
Sand [%]	48.0	82.2	89.5	66.9	17.7
Silt [%]	24.3	13.5	8.2	24.8	72.9
Clay [%]	27.7	4.3	2.3	8.3	9.4
Organic carbon [%]	1.3	0.6	0.6	0.7	1.97
CEC [mmolc/kg][a] or [cmol$^+$/kg][b]	452[a]	67[a]	28[a]	72[a]	7.6[b]
*p*H ($CaCl_2$)	7.7	5.5	6.0	7.1	5.8

Experimental conditions
All tests were carried out in duplicate at room temperature. Test samples were prepared by applying a treatment solution containing the test item in a 0.01 mol/L $CaCl_2$ solution on soil.

Controls were prepared with only the treatment solution (no soil) in the tube and soil blanks were prepared by weighing soil in the tube and applying 0.01 mol/L $CaCl_2$ solution (no test item). For all tests carried out, the tubes, containing soil or not, after application of the proper solution, were closed and then shaken horizontally on a mechanical shaker at 150 rpm at temperature controlled room (20 ± 2°C) and at dark conditions for the indicated test period. After the test period is reached, suspensions were centrifuged at 3000 rpm for 5 minutes and the supernatants were isolated by pouring to storage flasks.

Aliquots of the supernatant are analysed in triplicates by liquid scintillation counter (LSC) for quantification and by radio-HPLC, for formation of any degradation products and determination of the nature of the radioactivity. At adsorption equilibrium test, at least the sampling of interest (equilibrium time) or longer test period samples were analysed by radio-HPLC. At isotherms determination test, only supernatants from samples treated with the treatment solution of the highest dose were analysed by radio-HPLC.

The extraction procedure for ^{14}C-RPA 404766 (Cis-diol) consisted of two consecutive extractions conducted with a 5 g soil sample (after removal of the supernatant), one with 20 mL acetone, and one with 20 mL acetonitrile/water 1/1 (v/v). At each extraction step, the tubes were closed and then shaken horizontally on a mechanical shaker at 250 rpm for 30 minutes, then centrifuged at 3000 rpm for 5 minutes. The extracts were then combined and made up to a volume of 50 mL with acetone.

The extraction procedure for ^{14}C-RPA 406341 (Trans-diol) consisted of four consecutive extraction step conducted with a 5 g soil sample (after removal of supernatant): two extractions steps with methanol and two extraction steps with acetonitrile/water 1/1 (v/v) solution. Each extraction step was conducted by adding 20 mL of the respective solution. At each extraction step, the tubes were closed and then shaken horizontally on a mechanical shaker at 250 rpm for 30 minutes, then centrifuged at 3000 rpm for 5 minutes. The extracts were then combined and brought to a volume of 100 mL with methanol. 15 mL aliquots of extracts were concentrated at turbovap down to almost dryness and brought to 1 mL with methanol.

The extraction procedure for ^{14}C-RPA 407922 consisted of two consecutive extractions conducted with a 5 g soil sample (after removal of supernatant) with 20 mL of methanol each. At each step, the tubes were closed and then shaken horizontally on a mechanical shaker at 250 rpm for 30 minutes, then centrifuged at 3000 rpm for 5 minutes. The extracts were then combined and made up to a volume of 50 mL with methanol. 15 mL aliquots of the extracts were concentrated at turbovap down to almost dryness and brought to 1 mL with methanol.

For the indirect method, both supernatants and initial solution applied were analysed in order to determine the concentration of the test item in the aqueous solution after adsorption, as well as the initial concentration. The amount of test item adsorbed is indirectly calculated by the depletion of the total applied amount to the amount determined in the aqueous phase at the end of the test period. The extraction of the soil samples provides the extraction efficiency, enables to evaluate the nature of the items adsorbed to soil and to determine the stability of the test item in soil. For the adsorption equilibrium test, at least the sampling of interest (equilibrium time) or longer test period samplings were extracted, for determination of the extraction method. For the determination of isotherms, only the supernatants from samples originally treated with the treatment solution of the highest dose, were extracted. The total aqueous phase considered for the calculations included the supernatant decanted from soil after centrifugation and the remaining volume of this solution in the soil. In order to determine the volume of the remaining solution in soil right before extraction, soil samples were weighed throughout the experiments at several steps: before and after treatment as well as after removal of the supernatant.

For the direct method, the amount adsorbed onto soil is given by the amount of test item extracted, considering the volume of the supernatant remaining in the soil after decantation. Therefore, the extraction of the soil samples enables the direct determination of the amount adsorbed onto soil and the determination of the nature of items adsorbed to soil. Besides the information of concentration on both, aqueous phase and extracts, soil sample weights throughout the experiments at several steps are needed: before and after treatment as well as after removal of the supernatant, for determination of the volume of the solution remaining in the soil right before extraction. The extraction efficiency may be demonstrated by the mass balance. Aliquots of the extracts were analysed in triplicates by liquid scintillation for quantification and by radio-HPLC, for formation of any

degradation products and determination of the nature of the radioactivity. The soil dry weights were used for the calculation.

Preliminary tests
Preliminary experiments revealed that the optimal soil / solution ratio for metabolites RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) in the main test is 1/1 with adsorption in the range of 27.5 to 80.8 % in the two soils tested. For the metabolite RPA 407922, a ratio of 1/10 was chosen. The adsorption equilibrium test revealed that the appropriate equilibrium times for metabolites RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) were 24 and 48 hours, respectively. For metabolite RPA 407922 an equilibration time of 48 hours was chosen for the La Gironda soil and an equilibration time of 24 hours was chosen for the other four soils.

Adsorption-Desorption Isotherm Determination
The adsorption isotherm determination was performed with all five concentration levels nominal 1.0, 0.50, 0.10, 0.050 and 0.010 µg/mL) and all five soils. For RPA404766 (Cis-diol) and RPA 406341 (Trans-diol), centrifuge Teflon tubes were used. For RPA 407922, centrifuge glass tubes were used.

Appropriate volumes of application solutions were applied directly to the soils. The test with RPA 404766 (Cis-diol) was conducted with the direct method, due to presence of unknown peaks in the treatment solution with the highest concentration, summering around 8 % (radio purity checked before tests 92.0 %). The test with RPA 406341 (Trans-diol) was also conducted with the direct method, due to formation of unknown peaks in the $CaCl_2$ supernatant of preliminary tests. Subsequent extractions with 0.01 mol/aqueous $CaCl_2$, inherent from indirect method, could lead to higher degradation of test item.

The test with RPA 407922 was conducted with the indirect method. The method was chosen due to formation of unknown peaks on solvent extract chromatograms of preliminary tests samples. The indirect method was expected to reduce the amount available for solvent extraction due to the subsequent aqueous $CaCl_2$ 0.01 mol/L and, consequently, reach a higher mass balance at Freundlich isotherm determination tests.

Desorption experiments were not conducted for test items RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol). The soil was extracted right after the adsorption phase with organic solvent. For RPA 407922, the Freundlich desorption isotherms test was conducted with the same soil samples used for the determination of adsorption isotherms after removal of the supernatant. The test was performed with all the five soils and at five concentration levels. Desorption step 1 was performed as follows: The removed supernatant was replaced by an equal volume of 0.01 mol/L $CaCl_2$ solution without test item. The new mixture was gently agitated for the same test period and conditions. The volumes of the supernatants were measured gravimetrically. Desorption step 2 was performed with the soil samples left from desorption step 1 as described above.

Description of analytical procedures
The concentrations of the ^{14}C-test items were determined by radioactivity measurements. Therefore, aliquots of the decanted supernatants were added to scintillation cocktail and radioassayed in a liquid scintillation counter.

Radio-HPLC was used to demonstrate the purity and stability of the test item during the study.

When recovery of radioactivity fell below 90 %, the extracted soil was combusted. Therefore, the extracted soil was air dried and homogenized. Aliquots were weighed in triplicates and submitted to combustion in an oxidizer. The gases formed in the combustion were trapped in a scintillation solution and analysed with LSC.

Results and discussion:

Mass balance
The mass balance determination was carried out for all samples at the end of the isotherm experiments. The mass balance of ^{14}C-RPA 404766 (Cis-diol) ranged from 86.3 % to 98.7 %, with radioactivity recoveries ranging from 91.2 to 98.7 %.The mass balance of ^{14}C-RPA 406341 (Trans-diol) ranged from 95.1 to 102.7 %, with radioactivity recovery from 95.6 to 104.0 % and the mass balance of ^{14}C-RPA 407922 ranged from 90.4 to 97.2 %, with radioactivity recovery from 94.8 % to 98.5 %. Unknown compounds observed during the tests in both phases, accounted only for a maximum of 1.2 % of total applied radioactivity (average of duplicates) for all soils.

Transformation of parent products

The purity of test substance in the treatment solution at the beginning of the study was 92.0 % for ^{14}C-RPA 404766 (Cis-diol) and 100.0 % for ^{14}C-RPA 406341 (Trans-diol) and ^{14}C-RPA 407922.

From the control run in parallel to tests, it was inferred that the test item was stable in 0.01 mol/L $CaCl_2$ solution in absence of soil during 48 h, compared to original solution applied. Also, the test solution of the highest concentration samples and of the samples which were analysed for formation of degradation products or test item, was considered stable during the test period, by recovery of test item higher or equal to 90 %, except for ^{14}C-RPA 404766 (Cis-diol) recoveries from one soil (Wildacker), due to formation of bound residues.

Detailed results from the adsorption and desorption tests for the three metabolites in all five soils are presented in the tables below.

Table B. 8.1.3.1.2-11: Adsorption isotherms of RPA 404766 (Cis-diol) in five soils

Soil	Soil Type (DIN)	K_f (mL/g)	1/n (-)	K_{foc} (mL/g)	R^2
La Gironda	Sandy clay loam	0.68	0.99	52.6	1.000
Li 10	Silty sand	0.83	0.98	139	1.000
Lufa 2.1	Sand	0.28	0.97	46.1	0.999
Lufa 2.3	Loamy sand	0.34	0.90	49.0	0.999
Wildacker	Clay silt	3.17	0.95	161	0.999

Table B. 8.1.3.1.2-12: Adsorption isotherms of RPA 406341 (Trans-diol) in five soils

Soil	Soil Type (DIN)	K_f (mL/g)	1/n (-)	K_{foc} (mL/g)	R^2
La Gironda	Sandy clay loam	1.38	0.94	106	0.999
Li 10	Silty sand	1.94	1.00	324	0.995
Lufa 2.1	Sand	0.68	0.98	114	1.000
Lufa 2.3	Loamy sand	0.80	0.96	114	0.997
Wildacker	Clay silt	2.59	0.95	132	0.997

Table B. 8.1.3.1.2-13: Adsorption isotherms of RPA 407922 in five soils

Soil	Soil Type (DIN)	K_f (mL/g)	1/n (-)	K_{foc} (mL/g)	R^2
La Gironda	Sandy clay loam	3.57	0.93	275	1.000
Li 10	Silty sand	4.46	0.94	743	0.999
Lufa 2.1	Sand	1.89	0.98	315	0.999
Lufa 2.3	Loamy sand	1.59	0.92	228	1.000
Wildacker	Clay silt	8.70	0.89	442	0.995

Table B. 8.1.3.1.2-14: Desorption isotherms of RPA 407922 in five soils

Soil	Desorption 1				Desorption 2			
	$K_{f,des1}$ (mL/g)	1/*n* (-)	$K_{foc,des1}$ (mL/g)	R^2	$K_{f,des2}$ (mL/g)	1/*n* (-)	$K_{foc,des2}$ (mL/g)	R^2
La Gironda	7.94	0.92	611	0.997	16.29	0.95	1253	0.996
Li 10	8.82	0.96	1471	0.999	14.96	0.96	2493	0.997
Lufa 2.1	4.89	0.96	815	0.999	11.27	0.94	1878	0.992
Lufa 2.3	4.88	0.94	697	0.995	25.92	1.02	3702	0.995
Wildacker	18.73	0.92	951	0.999	36.92	0.97	1874	0.996

Conclusion:

The Freundlich adsorption coefficients K_f for ^{14}C-RPA 404766 (Cis-diol) ranged from 0.3 to 3.2 mL/g. The K_{foc} values ranged from 46 to 161 mL/g and 1/*n* values ranged from 0.90 to 0.99.

The Freundlich adsorption coefficients K_f for ^{14}C-RPA 406341 (Trans-diol) ranged from 0.7 to 2.6 mL/g. The K_{foc} values ranged from 106 to 324 mL/g and 1/*n* values ranged from 0.94 to 1.00.

The Freundlich adsorption coefficients K_f for ^{14}C-RPA 407922 ranged from 1.6 to 8.7 mL/g. The K_{foc} values ranged from 228 to 743 mL/g and 1/*n* values ranged from 0.89 to 0.98.

Freundlich desorption isotherms were established for ^{14}C-RPA407922 and $K_{f,des}$ values ranged from 4.9 to 18.7 mL/g for desorption step 1 and from 11.3 to 36.9 mL/g for desorption step 2. The corresponding $K_{foc,des}$ values ranged from 611 to 1471 mL/g for desorption step 1 and from 1253 to 3702 mL/g for desorption step 2.

Comments (RMS AT):

- The study follows OECD guideline 106 with a major deviations:
    - There is a lack of information about a pre-equilibrium phase as requested by OECD 106.

  In view of the possibly missing pre-equilibrium phase the study may not be considered fully reliable from a regulatory point of view. However, as sorption data obtained in this study are very close to results obtained in O'Brien (2017) and Kingman (2017) using the same soils (albeit different batches), sorption result for RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) in this study are considered equally reliable. Nevertheless applicants and study authors are encouraged to adequately follow this basic OECD guideline 106 requirement.

- The study authors adequately applied the *direct* method for RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) adequately accounting for (insignificant) degradation of the test items and formation of NER. As the *indirect* method was used for RPA 407922, significant amounts of NER (7.9 % AR on average at a test concentration of 1 mg/L) found in the Wildacker soil have been incorrectly attributed to the amount of test item 'adsorbed'. However, as no exposure assessment is triggered for RPA 407922 adsorption and desorption data for RPA 407922 are not considered further.

Reference:	**[^{14}C]-M595F001 (RPA 404766, metabolite of BAS 595 F): Adsorption on five European soils**
Author(s), year:	O'Brien, L. B. S., 2017
Report/Doc. Number:	2017/7013112
Guideline(s):	OECD 106 (2000)
GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Radiolabelled test material	[Triazole-3(5)-^{14}C]-RPA404766 (Cis-diol) (M595F001)
Batch No.:	1104-1102 (L67-148)
Specific Activity of test item:	6.44 MBq/mg
Radiochemical purity:	99.4 %
Molecular weight:	333.8 g/mol (non-radiolabelled)
Expiry date:	July 01, 2020

Soils

The study was conducted with five different soils from Europe. The characterization of the soils is presented in the table below. Soil samples were < 2 mm mesh sieved. Soil moisture content was determined by drying aliquots to constant weight in an oven at 105 °C.

Table B.8.1.3.1.2-15 Characteristics of the soils used to investigate the adsorption of RPA 404766 (Cis-diol)

Soil designation Origin	Wildacker (Germany)	LUFA 2.3 (Germany)	LUFA 2.1 (Germany)	Li 10 (Germany)	La Gironda (Spain)

USDA textural class	Silt Loam	Sandy Loam	Sand	Loamy Sand	Silty Clay Loam
Sand [%]	21.4	63.4	89.8	82.3	16.1
Silt [%]	69.2	28.1	7.7	12.2	49.3
Clay [%]	9.4	8.5	2.5	5.5	34.6
Organic carbon [%]	2.01	0.66	0.72	0.89	1.92
CEC [$cmol^+/kg$]	6.1	4.5	1.7	3.5	30.7
*p*H ($CaCl_2$)	5.8	5.3	5.6	6.1	7.1

Experimental conditions of preliminary tests
Preliminary studies were carried out to check for adsorption to the tubes, to determine any potential background radioactivity in the soil, to determine the soil to solution ratio to be used and to check stability of [^{14}C]-RPA 404766 (Cis-diol) in 0.01 M calcium chloride solutions.

Controls for testing adsorption to the tubes were prepared with only the treatment solution in a final nominal concentration of 1 µg/mL (no soil) using polypropylene, glass and Teflon tubes. The tubes were shaken for 24 hours and aliquots analysed by LSC.

Soil blanks (background radioactivity) were run in duplicate with each sample set and average background values were automatically subtracted from each sample after measurement. The supernatants were analysed by LSC.

Test samples (determination of soil to solution ratios) were prepared by applying test item in a 0.01 M $CaCl_2$ solution in Wildacker and LUFA 2.3 soils (representing the soils with highest and lowest organic carbon content). Two replicates of both soils were treated at soil/solution ratios of 1:10, 1:5 and 1:1 (at nominal concentrations of 1 µg/mL). The tubes were shaken overnight to pre-equilibrate (at least 12 h) prior to treatment. Following pre-equilibration, soils were dosed with a final nominal treatment concentration of 10 µg/mL. The tubes were shaken for a further 48 hours, centrifuged at 6000 G for approx. 15 minutes and analysed by LSC (indirect method).

Preliminary stability of the test item in 0.01 M $CaCl_2$ solution that had been in contact with all five soils was tested. Hereby, a 0.01 M $CaCl_2$ solution was pre-equilibrated for at least 12 hours in each soil and then centrifuged. Supernatants were dosed to achieve a nominal concentration of 1 µg/mL and shaken for 48 hours. Samples were then analysed by HPLC coupled to a radiodetector.

An adsorption kinetics test was conducted using a 1 µg/mL test item concentration in 0.01 M $CaCl_2$ with a 1:1 soil/solution ratio in the dark at 20 ± 2 °C. Following a pre-equilibration period overnight (soil in 0.01 M $CaCl_2$), test substance was added and samples were taken at 4, 6, 16, 24 and 48 hours to determine the optimum contact time of the test substance on each of the five soils. Samples were centrifuged (6000 G for 15 minutes) and supernatant, combined extracts and post-extracted soil (description below) analysed by LSC and radio-HPLC. Determination of concentrations in the adsorption kinetics test (Tier 2) was calculated by direct method.

For the extraction, the soil for each sample after the adsorption step was extracted once with 20 mL acetone followed by extraction with 20 mL acetonitrile/water 1:1 (v/v). Both extracts remained on the soil for 30 minutes on a horizontal shaker followed by centrifugation (6000 G for 15 minutes). The two extracts were then combined and radioactivity determined by LSC and radio-HPLC. For determination by HPLC, samples (depending on concentration) were prepared by concentration under nitrogen gas (water bath at 35 °C) and by filtration through a 0.22 µm nylon mesh prior to analysis.

The post-extracted soil was air-dried, mixed well and non-extracted residues determined by oxidative combustion analysis. Samples were stored in a freezer and thawed before analysis.

Preliminary tests (conclusions for definitive test)
Polypropylene tubes, glass tubes and Teflon tubes were used for the preliminary adsorption check. Following the findings, polypropylene tubes were selected for use throughout the remainder of the study. Background radioactivity was low and average background values were subtracted from each sample after measurement. Preliminary experiments revealed that the optimal soil/solution ratio for the adsorption kinetics test was 1/1 for the two soils with lowest and highest organic carbon content. Stability of the test item in calcium chloride was verified for 48 hours. A pre-equilibration time of at least 12 hours, followed by an adsorption equilibrium time of 48 hours was chosen for all soils. The extraction regime using acetone, followed by acetonitrile/water (1:1) was successful and chosen for the definitive test. The treatment range was 0.01 - 1.0 mg/L.

Adsorption isotherm determination (definitive test)
All tests were carried out in duplicate at room temperature (20 ± 2 °C), with shaking periods in the dark.

For the determination of the adsorption isotherms, five different test item concentrations were used. A soil/test solution ratio of 1/1 was used for all soils. Following pre-equilibration of at least 12 hours, application solutions were added to the soil samples to achieve the required test concentrations (nominal 0.01, 0.05, 0.1, 0.5 and 1.0 mg/L of [^{14}C]-RPA 404766 (Cis-diol) in 0.01 M $CaCl_2$). The adsorption equilibrium time for the duplicate samples was 48 hours. Samples were centrifuged at 6000 G for 15 minutes and supernatants were removed. The soil after adsorption step was extracted once with 20 mL acetone, followed by extraction with 20 mL acetonitrile/water 1:1 (v/v), with each extraction on a horizontal shaker for 30 minutes (300 cycles per minute), followed by centrifugation (6000 G for 15 minutes). The post-extracted soils were air-dried, mixed well and the non-extracted residues (NER) were determined by oxidative combustion analysis.

Supernatants and combined soil extracts were determined by LSC on the same day as sample collection.

Process recovery was determined in representative samples. HPLC analysis of aqueous supernatants was performed within 35 days of sample collection, and of soil extracts within 22 days after sample collection. Samples were stored in a freezer and thawed before work-up and analysis. The aqueous samples were (1 µg/mL test concentration samples) were directly analysed after filtration through a 0.22 µm nylon mesh. The 0.01 µg/mL test concentrations were reduced in volume under nitrogen gas in a TurboVap (bath set to 35 °C) and then filtered. The soil samples were reduced (1 µg/mL under nitrogen gas using TurboVap (bath set to 35 °C), 0.01 µg/mL samples under nitrogen using N-Evap nitrogen evaporator. All samples were filtered through a 0.22 µm nylon mesh.

In parallel to the treated samples, blank (untreated soil samples with $CaCl_2$ solution) and control samples at the highest test concentration of 1 µg/mL (treated 0.01 M $CaCl_2$ solution) was also incubated. Stability was assessed in the adsorption supernatant and combined soil extracts for both sample replicates of lowest and highest test concentrations by radio-HPLC.

Description of analytical methodology
All samples prepared LSC were analysed for 5 minutes in a Beckman LS 6500 Liquid Scintillation Counter. The NER samples were air-dried, homogenised and combusted for four minutes. The generated $^{14}CO_2$ was collected into a Harvey scintillation cocktail and assayed by LSC for 5 minutes.

Radio-HPLC (Phenomenex Luna C18, 5µm, 250 x 4.6 mm) was used to show the purity and stability of the test item during the study.

For the LSC measurements, the LOD (limit of detection) was considered twice the background activity and therefore 70 dpm. The LOQ was considered twice the background radioactivity and therefore 105 dpm. For RPA 404766, the LOD and LOQ correspond to 0.18 ng and 0.27 ng, respectively.

For HPLC, the LOQ was determined at 0.4 % of AR for soils treated at 0.01 µg/mL. LOD was considered approximately one-half the limit of quantification (0.2 % AR).

Results and discussion:

Mass balance
During the main test, the mean material balance (overall recovery expressed as % AR) of [^{14}C]-RPA 404766 (Cis-diol) for the test soils during determination of adsorption isotherms ranged from 90.7 to 98.7 % of the total of test item applied in five different soils at five different concentrations. Purity (HPLC-based) of RPA 404766 (Cis-diol) for Wildacker, LUFA 2.3, LUFA 2.1, Li10 and La Gironda resulted in values ranging from 95.7 to 100.0 % in adsorption supernatants expressed as percentage region of interest (% ROI).

For all soils, the *direct* method for calculation of the sorption parameters was applied.

Findings
The stability of the test item in the definitive test (adsorption isotherm test) was proven by radio-HPLC analysis of the adsorption and extraction supernatants from all dose samples and test item treatment solutions.

Detailed results from the adsorption tests for [^{14}C]-RPA 404766 (Cis-diol) in all five soils are presented in the table below.

Table B.8.1.3.1.2-16 Adsorption isotherms of RPA 404766 (Cis-diol) in five soils (based on the *direct* method)

Soil	Soil Type (USDA)	K_f (mL/g)	1/*n* (-)	R^2	K_{foc} (mL/g)
Wildacker	Silt Loam	1.95	0.903	0.999	96.8
LUFA 2.3	Sandy Loam	0.48	0.920	1.000	72.6
LUFA 2.1	Sand	0.68	0.946	0.999	94.0
Li10	Loamy Sand	0.67	0.922	0.999	74.8
La Gironda	Silty Clay Loam	1.30	0.874	0.996	67.6

Conclusion:

Freundlich adsorption coefficients K_f of RPA 404766 (Cis-diol) ranged from 0.48 to 1.95 mL/g in the five soils, which corresponded to K_{foc} values ranging from 67.6 to 96.8 mL/g. Freundlich exponents 1/*n* varied between 0.874 and 0.946. The average partition coefficients K_d ranged from 0.59 to 2.74 mL/g with the corresponding average K_{oc} of 90 to 137 mL/g.

Comments (RMS AT):

- The study follows OECD guideline 106 and is considered reliable. It is noted that soils properties (texture, OC and *p*H) are not necessarily fully in line with recommendations given in the OECD guideline. However, this is not considered to invalidate the study or parts of it.

- Significant amounts of non-extractable residues (NER) were observed in the Wildacker and La Gironda soil after the 48-hrs adsorption step (on average 7.4 and 12.0 % AR, respectively, below 5 % AR in the other soils, see tables below). Most study authors conducting sorption experiments according to OECD guidline106 consider NER to be part of the parental mass balance, which is, strictly speaking, not in line with OECD guideline 106 (refer to Eq. 10 in the guidance document). Unfortunately, OECD guideline 106 is indeed not clear on how to proceed in case of significant NER formation. It may be noted that OECD guideline 106 requires extraction efficiency of at least 95 % (bullet point 64 in OECD guideline 106), which implies that NER should be negligible in most cases. On overall, the RMS AT welcomes **further guidance** on how to account for NER in OECD 106 batch experiments (**preferable as a clarification in EFSA's 'OECD 106 evaluators checklist'**).

  As no or only insignificant degradation of the test item was observed in the soil extracts the study author came to the conclusion that NER can be included in the calculation of the sorption coefficient. In view of the RMS AT sorption coefficients should only be based on extractable amounts of the test item, otherwise NER are considered to equally contribute to the sorption equilibrium which is not defendable from a scientific point of view. It is also worthwhile to notice that NER are already taken into account for degradation. From a conceptual point of view, both, degradation as well as sorption, have to equally account for NER (which also implies that the extraction procedure used in both experimental systems should be ideally the same). Otherwise, sorption is overestimated in the exposure assessment.

  As extraction efficiency is clearly below the requested 95 % in the Wildacker and La Gironda soils, the RMS AT recommends reassessing sorption coefficients on basis of extractable amount at least for these two soils. To do so, a correction factor (f_{corr}) was calculated by the RMS AT on basis of extractable and non-extractable residues following the 48-hrs adsorption experiment (see tables below). Next, the concentration of the test item adsorbed to the soil (including NER as proposed by the study authors) at each test concentration was reduced by this correction factor to exclude NER. Finally, the Freundlich isotherms were calculated on basis of the corrected test concentrations in the soil as usual. Notice that the numbers given in the tables below do not account for slight degradation observed in some samples (recovery of test item ≥ 97.5 % in the liquid phase and organic extract based

on HPLC).

It may be noted that NER observed in Lufa 2.3, Lufa 2.1 and Li10 soil are well in line with formation of NER observed at early stage (1-3 DAT) in dedicated soil degradation experiments with RPA 404766 (Cis-diol), NER in Wildacker and La Gironda are indeed somewhat higher than observed in Crowe (2002).

Table B.8.1.3.1.2-17 Total mass balance (% AR) of the definitive test (48 hrs adsorption) in the Wildacker and Lufa 2.3 soil as well as sorption correction factor in the Wildacker soil - RMS AT assessment based on study raw data

Conc. (µg/ml)	Wildacker						Lufa 2.3					
	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]
0.01	20.7	71.4	7.8	99.9	92.1	0.90	53.8	36.5	3.7	93.9	90.2	nc
0.01	21.7	68.0	7.8	97.5	89.7	0.90	55.1	38.4	2.5	96.0	93.5	nc
0.05	23.3	64.2	6.1	93.6	87.5	0.91	55.4	34.4	2.9	92.7	89.8	nc
0.05	22.7	67.8	6.1	96.6	90.4	0.92	55.6	34.6	2.2	92.4	90.2	nc
0.1	24.3	56.6	8.5	89.3	80.9	0.87	57.7	32.6	4.1	94.5	90.4	nc
0.1	24.0	61.7	8.5	94.2	85.7	0.88	57.7	32.4	3.7	93.8	90.2	nc
0.5	27.2	59.1	7.4	93.7	86.3	0.89	63.3	31.3	3.2	97.8	94.6	nc
0.5	28.0	59.8	7.7	95.5	87.8	0.89	63.0	31.2	3.4	97.6	94.2	nc
1	26.6	60.6	7.2	94.5	87.2	0.89	62.6	30.3	3.3	96.1	92.8	nc
1	29.1	58.8	7.3	95.2	87.9	0.89	64.5	28.8	2.4	95.7	93.3	nc
Mean	**24.7**	**62.8**	**7.4**	**95.0**	**87.6**	**0.89**	**58.8**	**33.1**	**3.1**	**95.0**	**91.9**	**nc**

nc denotes not calculated (NER < 5 % AR)
(a) Mass balance (according to OECD 106) = aqueous phase + extractables (no degradation of test item)
(b) Correction factor = extractables / (extractables + NER)

Table B.8.1.3.1.2-18 Total mass balance (% AR) of the definitive test (48 hrs adsorption) in the Lufa 2.1 and Li10 soil - RMS AT assessment based on study raw data

Conc. (µg/ml)	Lufa 2.1						Li10					
	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]
0.01	47.4	39.4	2.3	89.2	86.8	nc	44.5	46.2	3.3	94.0	90.7	nc
0.01	47.5	42.0	2.7	92.2	89.4	nc	47.0	43.7	3.2	93.9	90.7	nc
0.05	48.0	41.8	2.4	92.2	89.8	nc	48.1	42.7	2.5	93.2	90.8	nc
0.05	48.2	38.8	3.5	90.4	87.0	nc	48.2	43.6	2.2	94.0	91.8	nc
0.1	51.0	39.7	2.6	93.2	90.7	nc	51.6	39.8	3.2	94.6	91.4	nc
0.1	50.5	37.7	3.0	91.2	88.2	nc	53.2	39.6	2.8	95.6	92.8	nc
0.5	53.8	40.6	2.3	96.7	94.4	nc	54.1	39.7	2.5	96.3	93.8	nc
0.5	53.1	37.7	2.1	92.9	90.8	nc	52.5	42.6	3.3	98.4	95.1	nc
1	55.3	38.2	1.6	95.2	93.5	nc	55.2	38.3	2.0	95.5	93.5	nc
1	55.1	35.7	2.7	93.5	90.8	nc	56.0	37.3	2.3	95.5	93.2	nc
Mean	**51.0**	**39.1**	**2.5**	**92.7**	**90.2**	**nc**	**51.0**	**41.3**	**2.7**	**95.1**	**92.4**	**nc**

nc denotes not calculated (NER < 5 % AR)
(a) Mass balance (according to OECD 106) = aqueous phase + extractables (no degradation of test item)
(b) Correction factor = extractables / (extractables + NER)

Table B.8.1.3.1.2-19 Mass balance (% AR) of the definitive test (48 hrs adsorption) as well as sorption correction factor in the La Gironda soil - RMS AT assessment based on study raw data

Conc. (µg/ml)	La Gironda					
	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]
0.01	28.0	51.5	11.2	90.7	79.5	0.82
0.01	22.3	57.5	13.6	93.4	79.8	0.81
0.05	27.2	55.0	10.6	92.9	82.3	0.84
0.05	27.3	54.2	11.3	92.9	81.5	0.83
0.1	30.1	50.3	13.9	94.3	80.4	0.78
0.1	32.7	48.4	13.2	94.3	81.2	0.79

0.5	35.2	46.3	11.5	93.0	81.5	0.80
0.5	36.1	48.1	11.5	95.6	84.2	0.81
1	38.4	44.0	11.3	93.7	82.4	0.80
1	37.4	46.2	11.7	95.3	83.6	0.80
Mean	**31.5**	**50.2**	**12.0**	**93.6**	**81.6**	**0.81**

(a) Mass balance (according to OECD 106) = aqueous phase + extractables (no degradation of test item)
(b) Correction factor = extractables / (extractables + NER)

Table B.8.1.3.1.2-20 Re-calculated adsorption isotherms of RPA 404766 (Cis-diol) in the Wildacker and La Gironda soil (based on the *direct* method) - RMS AT assessment based on extractable amounts

Soil	Soil Type (USDA)	K_f (mL/g)	1/*n* (-)	R^2	K_{foc} (mL/g)
Wildacker	Silt Loam	1.71	0.889	0.999	85.3
La Gironda	Silty Clay Loam	1.03	0.868	0.996	53.6

Reference:	**[^{14}C]-M595F002 (RPA 406341, metabolite of BAS 595 F): Adsorption on five European soils**
Author(s), year:	Kingman, A. M. S., 2017
Report/Doc. Number:	2017/7013113
Guideline(s):	OECD 106 (2000), EPA 835.1230
GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Radiolabelled test material	[Triazole-3(5)-^{14}C]- RPA 406341 (Trans-diol, M595F002)
Batch No.:	1102-1101 (L85-198)
Specific Activity of test item:	6.60 MBq/mg
Radiochemical purity:	98.3 %
Molecular weight:	333.8 g/mol (non-radiolabelled)
Expiry date:	July 01, 2018

Soils
The study was conducted with five different soils from Europe. The characterization of the soils is presented in the table below. Soil samples were < 2 mm mesh sieved. Soil moisture content was determined by drying aliquots to constant weight in an oven at 105 °C.

Table B.8.1.3.1.2-21 Characteristics of the soils used to investigate the adsorption of [^{14}C]-RPA 406341 (Trans-diol)

Soil designation Origin	Wildacker (Germany)	LUFA 2.3 (Germany)	LUFA 2.1 (Germany)	Li 10 (Germany)	La Gironda (Spain)
USDA textural class	Silt Loam	Sandy Loam	Sand	Loamy Sand	Silty Clay Loam
Sand [%]	21.4	63.4	89.8	82.3	16.1
Silt [%]	69.2	28.1	7.7	12.2	49.3
Clay [%]	9.4	8.5	2.5	5.5	34.6
Organic carbon [%]	2.01	0.66	0.72	0.89	1.92
CEC [cmol$^+$/kg]	6.1	4.5	1.7	3.5	30.7
*p*H ($CaCl_2$)	5.8	5.3	5.6	6.1	7.1

Experimental conditions of preliminary tests
Preliminary studies were carried out to check for adsorption to the tubes, to determine any potential background radioactivity in the soil, to determine the soil to solution ratio to be used and to check stability of [^{14}C]-RPA 406341 (Trans-diol) in 0.01 M calcium chloride solutions.

Controls for testing adsorption to the tubes were prepared with only the treatment solution in a final nominal concentration of 1 µg/mL (no soil) using polypropylene, glass and Teflon tubes. The tubes were shaken for 24 hours and aliquots assayed by LSC.

Soil blanks (background radioactivity) were run in duplicate with each sample set and average background values were automatically subtracted from each sample after measurement. The supernatants were analysed by LSC.

Test samples (determination of soil to solution ratios) were prepared by applying test item in a 0.01 M $CaCl_2$ solution in Wildacker and LUFA 2.3 soils (representing the soils with highest and lowest organic carbon content). Two replicates of both soils were treated at soil/solution ratios of 1:10, 1:5 and 1:1 (at nominal concentrations of 1 µg/mL). The tubes were shaken overnight to pre-equilibrate (at least 12 h) prior to treatment. Following pre-equilibration, soils were dosed with a final nominal treatment concentration of 10 µg/mL. The tubes were shaken for a further 48 hrs (in the dark), centrifuged at 6000 G for approx. 15 minutes and analysed by LSC (indirect method).

Preliminary stability of the test item in 0.01 M $CaCl_2$ solution that had been in contact with all five soils was tested. Hereby, a 0.01 M $CaCl_2$ solution was pre-equilibrated for at least 12 hours in each soil and then centrifuged. Supernatants were dosed with 10 µg/mL test item to achieve a nominal treated concentration of 1 µg/mL and shaken for 48 hours. Samples were then analysed by HPLC coupled to a radiodetector (radio-HPLC).

An adsorption kinetics test was conducted using a 1 µg/mL test item concentration in 0.01 M $CaCl_2$ with a 1:1 soil/solution ratio in the dark at 20 ± 2°C. Following a pre-equilibration period overnight (soil in 0.01 M $CaCl_2$), test substance was added and samples were taken at 4, 6, 16, 24 and 48 hours to determine the optimum contact time of the test substance on each of the five soils. Samples were centrifuged (6000 G for 15 minutes) and supernatant, combined extracts and post-extracted soil (description below) analysed by LSC and radio-HPLC. Determination of concentrations in the adsorption kinetics test was calculated by direct method.

For the extraction, the soil for each sample after the adsorption step was extracted twice with 20 mL acetone followed by two extractions with 20 mL acetonitrile/water 1:1 (v/v). The four extracts each remained on the soil for 30 minutes on a horizontal shaker followed by centrifugation (6000 G for 15 minutes). The four extracts were then combined and radioactivity determined by LSC and radio-HPLC. For determination by HPLC, samples (depending on concentration) were prepared by concentration under nitrogen gas (water bath at 35 °C) and by filtration through a 0.22 µm nylon mesh prior to analysis.

The post-extracted soil was air-dried, mixed well and non-extracted residues determined by oxidative combustion analysis. Samples were stored in a freezer and thawed before analysis.

Preliminary tests (conclusions for definitive test)
Polypropylene tubes, glass tubes and Teflon tubes were used for the preliminary adsorption check. Following the findings, polypropylene tubes were selected for use throughout the remainder of the study. Background radioactivity was low and average background values were subtracted from each sample after measurement. Preliminary experiments revealed that the optimal soil/solution ratio for the adsorption isotherm test was 1/1 for the two soils with lowest and highest organic carbon content. Stability of the test item in calcium chloride was verified for 48 hours. A pre-equilibration time of at least 12 hours, followed by an adsorption equilibrium time of 48 hours was chosen for all soils. The extraction regime using two extractions with acetone, followed by two extractions with acetonitrile/water (1:1) was successful and chosen for the definitive test. The treatment range was 0.01 - 1.0 mg/L.

Adsorption Isotherm Determination (definitive test)
All tests were carried out in duplicate at room temperature (20 ± 2 °C), with shaking periods in the dark.

For the determination of the adsorption isotherms, five different test item concentrations were used. A soil/test solution ratio of 1/1 was used for all soils. Following pre-equilibration of at least 12 hours, application solutions were added to the soil samples to achieve the required test concentrations (nominal 0.01, 0.05, 0.1, 0.5 and 1.0 mg/L of [^{14}C]-RPA 406341 (Trans-diol) in 0.01 M $CaCl_2$). The adsorption equilibrium time for the duplicate samples was 48 hours. Samples were centrifuged at 6000 G for 15 minutes and supernatants were removed. The soil after adsorption step was extracted twice with 20 mL acetone, followed by two extractions with 20 mL acetonitrile/water 1:1 (v/v), with each extraction on a horizontal shaker for 30 minutes (300 cycles per minute),

followed by centrifugation (6000 G for 15 minutes). The four soil extracts were combined. The post-extracted soils were air-dried, mixed well and the non-extracted residues (NER) were determined by oxidative combustion analysis.

Supernatants and combined soil extracts were determined by LSC on the same day as sample collection.

Process recovery was determined in representative samples. HPLC analysis of aqueous supernatants was performed within 45 days of sample collection, and of soil extracts within 41 days after sample collection. Samples were stored in a freezer and thawed before work-up and analysis. The aqueous samples were (1 µg/mL test concentration samples) were directly analysed after filtration through a 0.22 µm nylon mesh. The 0.01 µg/mL test concentrations were reduced in volume under nitrogen gas in a TurboVap (bath set to 35 °C) and then filtered. The 1 µg/mL soil samples were reduced under nitrogen gas using TurboVap (bath set to 35 °C) and filtered through a 0.22 µm nylon mesh. The 0.01 µg/mL samples were concentrating using a rotary evaporator with a water bath at 35°C. The sample containing flasks were rinsed, the rinse combined with the samples and centrifuged at 10000 rpm for 10 minutes.

In parallel to the treated samples, blank (untreated soil samples with $CaCl_2$ solution) and control samples at the highest test concentration of 1 µg/mL (treated 0.01 M $CaCl_2$ solution) was also incubated. Stability was assessed in the adsorption supernatant and combined soil extracts for both sample replicates of lowest and highest test concentrations by radio-HPLC.

Description of analytical methodology
All samples prepared LSC were analysed for 5 minutes in a Beckman LS 6500 Liquid Scintillation Counter. The NER samples were air-dried, homogenised and combusted for four minutes. The generated $^{14}CO_2$ was collected into a Harvey scintillation cocktail and assayed by LSC for 5 minutes.

Radio-HPLC (Phenomenex Luna C18, 5µm, 250 x 4.6 mm) was used to show the purity and stability of the test item during the study.

For the LSC measurements, the LOD (limit of detection) was considered twice the background activity and therefore 70 dpm. The LOQ was considered twice the background radioactivity and therefore 105 dpm. For [^{14}C]-RPA 406341, the LOD and LOQ correspond to 0.18 ng and 0.27 ng, respectively.

For HPLC, the LOQ was determined at 0.4 % of AR for soils treated at 0.01 µg/mL. The LOD was considered approximately one-half the limit of quantification (0.2 % AR).

Results and discussion:

Mass balance
During the main test, the mean material balance (overall recovery expressed as % AR) of [^{14}C]-RPA 406341 (Trans-diol) for the test soils during determination of adsorption isotherms ranged from 93.4 to 97.8 % of the total of test item applied in five different soils at five different concentrations. Purity (HPLC-based) of RPA 406341 (Trans-diol) for Wildacker, LUFA 2.3, LUFA 2.1, Li10 and La Gironda resulted in values ranging from 85.3 to 100.0 % in adsorption supernatants expressed as percentage region of interest (% ROI).

For all soils, the *direct* method for calculation of the sorption parameters was applied.

Findings
The stability of the test item in the definitive test (adsorption isotherm test) was proven by radio-HPLC analysis of the adsorption and extraction supernatants from all dose samples and test item treatment solutions.

Detailed results from the adsorption tests for [^{14}C]-RPA 406341 (Trans-diol) in all five soils are presented in the table below.

Table B.8.1.3.1.2-22 Adsorption Isotherms of [^{14}C]-RPA 406341(Trans-diol) in five soils (based on the *direct* method)

Soil	Soil Type (USDA)	K_f (mL/g)	1/*n* (-)	R^2	K_{foc} (mL/g)

Wildacker	Silt Loam	3.72	0.919	0.999	185
LUFA 2.3	Sandy Loam	1.02	0.945	0.999	154
LUFA 2.1	Sand	1.35	0.937	1.000	188
Li10	Loamy Sand	1.31	0.932	1.000	148
La Gironda	Silty Clay Loam	1.93	0.868	0.997	100

Conclusion:

Freundlich adsorption coefficients K_f of RPA 406341 (Trans-diol) ranged from 1.02 to 3.72 mL/g in the five soils, which corresponded to K_{foc} values ranging from 100 to 188 mL/g. Freundlich exponents $1/n$ varied between 0.868 and 0.945. The average partition coefficients K_d ranged from 1.2 to 5.1 mL/g with the corresponding average K_{oc} of 164 to 256 mL/g.

Comments (RMS AT):

- The study follows OECD guideline 106 and is considered reliable. It is noted that soils properties (texture, OC and *p*H) are not necessarily fully in line with recommendations given in the OECD guideline. However, this is not considered to invalidate the study or parts of it.

- Similar to O'Brien (2017) significant amounts of NER were found in the La Gironda soil as well (8.8 % AR on average, refer to tables below) which have been included by the study author in the calculation of the sorption coefficient as no or only insignificant degradation was observed. In line with the approach given in O'Brien (2017) the sorption coefficient in the La Gironda soil was therefore re-calculated by the RMS AT on basis of extractable amounts only (thus excluding NER). Notice that the numbers given in the tables below do not account for slight degradation observed in some samples (recovery of test item ≥ 97.8 % in the liquid phase and organic extract based on HPLC).

  It may be noted that NER observed in Wildacker, Lufa 2.3. Lufa 2.1 and Li10 soil are well in line with formation of NER observed at early stage in dedicated soil degradation experiments with RPA 406341 (Trans-diol), NER in the La Gironda soil are indeed somewhat higher than observed in McGhee (2000).

Table B.8.1.3.1.2-23 Total mass balance (% AR) of the definitive test (48 hrs adsorption) in the Wildacker and Lufa 2.3 soil - RMS AT assessment based on study raw data

Conc. (µg/ml)	Wildacker						Lufa 2.3					
	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]
0.01	15.0	77.5	3.5	96.1	92.6	nc	42.0	51.4	1.7	95.1	93.4	nc
0.01	14.2	78.0	3.4	95.6	92.1	nc	43.4	49.0	1.6	93.9	92.3	nc
0.05	15.5	76.2	3.2	94.9	91.7	nc	43.1	51.2	3.0	97.3	94.2	nc
0.05	15.7	79.0	3.5	98.2	94.7	nc	43.7	53.3	2.6	99.6	97.0	nc
0.1	16.0	78.6	3.6	98.3	94.7	nc	44.0	49.3	1.5	94.7	93.2	nc
0.1	15.7	76.4	3.9	96.0	92.1	nc	44.2	47.8	1.9	93.8	91.9	nc
0.5	18.2	74.7	3.4	96.4	93.0	nc	46.5	49.7	1.8	97.9	96.1	nc
0.5	18.7	73.6	3.0	95.3	92.3	nc	48.3	47.4	2.0	97.7	95.7	nc
1	19.6	72.8	4.0	96.4	92.3	nc	48.5	45.9	1.9	96.3	94.4	nc
1	19.5	73.4	4.0	96.9	92.9	nc	49.3	46.6	1.6	97.5	95.8	nc
Mean	**16.8**	**76.0**	**3.6**	**96.4**	**92.8**	**nc**	**45.3**	**49.1**	**1.9**	**96.4**	**94.4**	**nc**

nc denotes not calculated (NER < 5 % AR)
(a) Mass balance (according to OECD 106) = aqueous phase + extractables (no degradation of test item)
(b) Correction factor = extractables / (extractables + NER)

Table B.8.1.3.1.2-24 Total mass balance (% AR) of the definitive test (48 hrs adsorption) in the Lufa 2.1 and Li10 soil - RMS AT assessment based on study raw data

Conc. (µg/ml)	Lufa 2.1						Li10					
	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]	Aqu.	Extr.	NER	Total	Mass bal.[a]	f_{corr}[b]
0.01	34.9	62.0	1.0	97.8	96.8	nc	34.5	60.7	1.6	96.7	95.2	nc

0.01	35.3	59.9	1.0	96.1	95.2	nc	34.8	58.7	0.8	94.3	93.5	nc
0.05	36.1	56.0	1.4	93.5	92.1	nc	36.3	58.8	1.7	96.8	95.1	nc
0.05	35.4	58.0	1.6	95.0	93.4	nc	35.6	60.1	1.7	97.4	95.7	nc
0.1	36.4	55.9	1.2	93.5	92.2	nc	37.2	53.8	1.4	92.4	91.0	nc
0.1	35.8	56.4	1.1	93.3	92.2	nc	36.5	57.0	1.2	94.7	93.5	nc
0.5	38.8	55.9	1.1	95.8	94.8	nc	39.6	54.1	1.3	94.9	93.7	nc
0.5	39.4	54.3	1.0	94.7	93.7	nc	41.0	55.0	1.1	97.0	95.9	nc
1	39.5	54.4	1.3	95.1	93.9	nc	40.5	55.1	1.1	96.8	95.7	nc
1	40.5	53.2	1.2	95.0	93.7	nc	41.9	53.2	1.1	96.2	95.1	nc
Mean	**37.2**	**56.6**	**1.2**	**95.0**	**93.8**	**nc**	**37.8**	**56.7**	**1.3**	**95.7**	**94.4**	**nc**

nc denotes not calculated (NER < 5 % AR)
(a) Mass balance (according to OECD 106) = aqueous phase + extractables (no degradation of test item)
(b) Correction factor = extractables / (extractables + NER)

Table B.8.1.3.1.2-25 Total mass balance (% AR) in the definitive test (48 hrs adsorption) as well as sorption correction factor in the La Gironda soil - RMS AT assessment based on study raw data

Conc. (µg/ml)	La Gironda					
	Aqu.	Extr.	NER	Total	Mass bal.[(a)]	f_{corr}[(b)]
0.01	20.6	65.6	9.8	96.0	86.2	0.87
0.01	19.1	66.8	8.6	94.5	85.9	0.89
0.05	23.5	62.9	9.8	96.1	86.4	0.87
0.05	23.0	63.2	9.7	95.9	86.2	0.87
0.1	22.7	63.6	8.4	94.7	86.2	0.88
0.1	20.7	66.1	8.2	95.0	86.8	0.89
0.5	31.7	57.3	7.9	97.0	89.1	0.88
0.5	30.4	58.3	8.2	96.8	88.6	0.88
1	30.3	58.8	9.0	98.0	89.0	0.87
1	30.6	56.1	8.6	95.2	86.6	0.87
Mean	**25.3**	**61.8**	**8.8**	**95.9**	**87.1**	**0.88**

(a) Mass balance (according to OECD 106) = aqueous phase + extractables (no degradation of test item)
(b) Correction factor = extractables / (extractables + NER)

Table B.8.1.3.1.2-26 Re-calculated adsorption isotherms of RPA 406341 (Trans-diol) in the La Gironda soil (based on the *direct* method) - RMS AT assessment based on extractable amounts

Soil	Soil Type (USDA)	K_f (mL/g)	1/*n* (-)	R^2	K_{foc} (mL/g)
La Gironda	Silty Clay Loam	1.57	0.839	0.996	81.6

Reference:	**[^{14}C]-RPA 407922: Adsorption to and Desorption from Five Soils**
Author(s), year:	Simmonds, R., 2017b
Report/Doc. Number:	2017/114204
Guideline(s):	OECD 106 (2000)
GLP:	Yes
Validity:	Not essential (refer to comment section)
Status:	**New submission**

Material and methods:

Radiolabelled test material	[Triazole-3(5)-^{14}C]-RPA 407922
Batch No.:	1103-1101
Specific Activity:	5.55 MBq/mg
Radiochemical purity:	97.7 %
Molecular weight:	333.8 g/mol (non-radiolabelled)

Soils

The study was conducted with five different soils from Europe. The characterization of the soils is presented in the table below. Soil samples were < 2 mm mesh sieved. The actual water content of the soils was determined by comparison of weights of soil before and after oven-drying at ca. 100 °C.

Table B.8.1.3.1.2-27 Characteristics of the soils used to investigate the adsorption and desorption of [^{14}C]-RPA 407922

Soil designation Origin	Wildacker (Germany)	LUFA 2.3 (Germany)	LUFA 2.1 (Germany)	Li 10 (Germany)	La Gironda (Spain)
USDA textural class	Silt Loam	Sandy Loam	Sand	Loamy Sand	Silty Clay Loam
Sand [%]	21.4	63.4	89.8	82.3	16.1
Silt [%]	69.2	28.1	7.7	12.2	49.3
Clay [%]	9.4	8.5	2.5	5.5	34.6
Organic carbon [%]	2.01	0.66	0.72	0.89	1.92
CEC [cmol$^+$/kg]	6.1	4.5	1.7	3.5	30.7
*p*H ($CaCl_2$)	5.8	5.3	5.6	6.1	7.1

Experimental conditions of preliminary tests

Preliminary studies were carried out to check for adsorption to the tubes, to determine any potential background radioactivity in the soil, to determine the soil to solution ratio to be used, to check stability of [^{14}C]-RPA 407922 in 0.01 M calcium chloride solutions and to determine the time required for the test item to equilibrate between soil and water under adsorption and desorption conditions.

Controls for testing adsorption to the tubes were prepared with only the treatment solution (no soil) using PTFE and glass tubes. The tubes were shaken for 48 hours and aliquots analysed by LSC.

Soil blanks (background radioactivity) were prepared by weighing 10 g of each soil in tubes (in duplicates) and applying 0.01 M $CaCl_2$ solution (without test item). The tubes were shaken for 48 hours. After this period, the soil/solution suspensions were centrifuged at 4600 rpm for 10 minutes. The supernatants were analysed by LSC.

Test samples (determination of soil to solution ratios) were prepared by applying test item in a 0.01 M $CaCl_2$ solution in each soil. First, calcium chloride was added to 1, 2 and 4 g of soil to give soil/solution ratios of approximately 1:20, 1:10 and 1:5. The tubes were shaken overnight to pre-equilibrate (ca. 16 h) prior to treatment. Following pre-equilibration, 1 mL of the application solution was added to each tube (final nominal treatment concentration of 0.1 mg/L). The tubes were shaken for a further 24 hours, centrifuged at 4600 rpm for 10 minutes, the supernatants transferred to pre-weighed plastic bottles and analysed by LSC and Radio-HPLC.

Stability of the test item in 0.01 M $CaCl_2$ was tested by periodically (4, 24 and 100 hours) analysing a sample of calcium chloride treated with the test item by HPLC.

For determination of the adsorption equilibrium time, ten tubes for each soil with either a 1:10 (Wildacker and La Gironda soil) or 1:5 (all remaining soils) soil:solution ratio were shaken for 16 hours to equilibrate. After equilibration, the tubes were treated with test item to achieve a final nominal treatment concentration of 0.1 mg/L and were again put on a shaker. Two tubes from each soil were removed after 4, 8, 24, 32 and 48 hours. At each time point, the tubes were centrifuged at 4600 rpm for 10 minutes, the supernatants removed and analysed by LSC. The soils were extracted and analysed as described below.

For the preliminary adsorption experiment, tubes with 1:10 and 1:5 soil/solution ratio were shaken for 16 hours to equilibrate. After equilibration, the tubes were treated with test item to achieve a final nominal treatment concentration of 0.1 mg/L and were again put on a shaker. Two tubes from each soil were removed after 4, 8, 24, 32 and 48 hours. At each time point, the tubes were centrifuged at 4600 rpm for 10 minutes, the supernatants removed and analysed by LSC. The soils were extracted and analysed as described below.

The preliminary desorption experiment (to determine desorption equilibrium time) followed a similar regime with 1:10 and 1:5 soil:solution ratio, 16 h pre-equilibration, 24 h or 48 adsorption (depending on soil) and 1, 2, 24 and 48 h desorption. At each time point, the tubes were centrifuged at 4600 rpm for 10 minutes, the supernatants removed and analysed by LSC. The soils were extracted and analysed as described below.

Extraction of the soil samples was performed to provide extraction efficiency, evaluate the nature of items adsorbed to soil and to determine the stability of test item on soil. The extraction procedure for [^{14}C]-

RPA 407922 consisted of an extraction of 2 or 4 g of soil (depending on soil type and appropriate soil/solution ratio) with 20 mL of acetonitrile, followed by acetonitrile/methanol 70:30 (v/v), acetonitrile/water 70:30 (v/v) and methanol/water 70:30 (v/v). For each extraction step, the tubes were placed on a flat-bed shaker for 30 minutes, centrifuged at 4600 rpm for 10 minutes and the extracts isolated. Each extract supernatant removed to determine the radioactivity by LSC. All adsorption supernatants and combined acetonitrile/water extracts were further analysed by HPLC.

To determine the mass balance of extraction samples, the soil samples were air-dried, weighed and ground to a fine powder. Triplicate aliquots (approximately 0.2 g) were weighed and combusted. The combustion products were absorbed in Carbosorb E and mixed with Permafluor E+ prior to quantification.

Preliminary tests (conclusions for definitive test)
Both, screw capped PTFE tubes and plastic-coated screw capped glass tubes were used for the preliminary check. Following the findings, PTFE tubes were selected for use throughout the remainder of the study. Background radioactivity detected was negligible and no correction necessary. Preliminary experiments revealed that the optimal soil/solution ratio for the adsorption/desorption tests were 1/10 for the Wildacker and La Gironda soil and 1/5 for all remaining soils. Stability of the test item in calcium chloride was verified for up to 100 hours, indicating stability for longer than the duration of the intended definitive phase of the study.

A pre-equilibration time of 16 hours, followed by an adsorption equilibrium time of 24 hours for LUFA 2.3, Li10 and La Gironda soils and 48 hours for the Wildacker and LUFA 2.1 soils were chosen for all soils, followed by two desorption cycles of 2 hours each. The extraction regime using acetonitrile, followed by acetonitrile/methanol, acetonitrile/water and methanol/water was successful and chosen for the definitive test. The treatment range was 0.01-1.0 mg/L, i.e. highest concentration well below half the aqueous solubility of the test item.

Adsorption-desorption isotherm determination (definitive test)
All tests were carried out in duplicate at room temperature (20 ± 2 °C), with shaking periods in the dark.

In the definitive test, approx. 1 g or 2 g soil (resulting in 1/10 soil/solution ratio for Wildacker and La Gironda and 1/5 soil/solution ratio for the remaining soils) were weighed into pre-weighed tubes and an appropriate volume of 0.01 M calcium chloride solution was added (20mL minus soil moisture and 1mL for treatment solution volume added later). Samples were shaken for approx. 16 hours to pre-equilibrate prior to treatment. Following pre-equilibration, 1 mL of standard solutions of [^{14}C]-RPA 407922 in 0.01 M $CaCl_2$, prepared at five concentrations levels (nominal concentrations: 0.01, 0.05, 0.1, 0.5 and 1.0 mg/L), were added. Soil solutions were mixed for 24 or 48 hours (24 hours for LUFA 2.3, Li10 and La Gironda soils and 48 hours for the Wildacker and LUFA 2.1) on an end-over-end shaker. Tubes were weighed and centrifuged at 4600 rpm for 10 minutes. Supernatant was removed and weight of the supernatant and remnant soil pellets were recorded.

After adsorption, two desorption steps were performed (2 hours each) by replacing the removed supernatants with an equal volume of 0.01 M $CaCl_2$ solution without test item.

Aliquots of supernatants of the adsorption step and desorption step as well as the four extraction steps were analysed by liquid scintillation counter (LSC) for quantification. Adsorption supernatants, desorption supernatants and solvent extracts of each soil were further analysed by Radio-HPLC for formation of any degradation products and determination of the nature of the radioactivity as well as stability of the test items.

Material balance was assayed by LSC to determine total recovery of radioactivity. Stability and parental mass balance were determined by HPLC. Calculations of test item concentrations in supernatants and solvent extracts with the indirect and direct calculation method are based on results measured by LSC, however with the direct method, the measured values are additionally corrected for purity in respective HPLC measurements.

Description of analytical methodology
The amounts of radioactivity were determined by radioactivity measurements. Therefore, aliquots of the decanted supernatants were added to scintillation cocktail and radioassayed in a liquid scintillation counter. Radio-HPLC (Luna C18 5µm 250 x 4.6 mm) was used to show the purity and stability of the test item during the study.

For the LSC measurements, an LOD of 0.03 ng (9 dpm) and an LOQ of 0.09 ng (30 dpm) applied. For HPLC, the LOQ was determined at 0.1 % AR for most treatment rates, and 0.5 % AR for the lowest treatment rate.

Results and discussion:

Mass balance
During the main test, overall mass balances (expressed as % AR) for individual samples was 96.9, 97.0, 95.9, 96.2 and 95.7 % in soils Wildacker, LUFA 2.3, LUFA 2.1, Li10 and La Gironda, respectively.

Parental mass balance (HPLC-based) for Wildacker, LUFA 2.3, LUFA 2.1, Li10 and La Gironda resulted in respective mean values of RPA 407922 mass balance of 79.5, 92.9, 89.3, 88.6 and 73.9 %.

For all soils, the *direct* method for calculation of the sorption parameters was applied as degradation was observed in all soils and values are then corrected for HPLC purity.

Findings
The stability of the test item in the definitive test (adsorption/desorption experiments) was proven by Radio-HPLC analysis of the adsorption, desorption and extraction supernatants from all dose samples and test item treatment solutions.

Detailed results from the adsorption and desorption tests for [^{14}C]-RPA 407922 in all five soils are presented in the tables below.

Table B.8.1.3.1.2-28 Adsorption Isotherms of [^{14}C]-RPA 407922 in five soils (based on the *direct* method)

Soil	Soil Type (USDA)	K_f (mL/g)	1/*n* (-)	R^2	K_{foc} (mL/g)
Wildacker	Silty Clay Loam	10.18	0.909	1.000	506
LUFA 2.3	Sandy Loam	2.46	0.907	1.000	373
LUFA 2.1	Sand	3.27	0.909	0.998	454
Li10	Loamy Sand	3.34	0.880	0.999	375
La Gironda	Silty Clay Loam	4.33	0.839	0.999	226

Table B.8.1.3.1.2-29 Desorption Isotherms of [^{14}C]-RPA 407922 in five soils (based on the *direct* method)

Soil	Desorption 1				Desorption 2			
	$K_{f,des1}$ (mL/g)	1/*n* (-)	R^2	$K_{foc,des1}$ (mL/g)	$K_{f,des2}$ (mL/g)	1/*n* (-)	R^2	$K_{foc,des2}$ (mL/g)
Wildacker	25.36	0.967	0.999	1262	36.36	0.951	0.999	1809
LUFA 2.3	4.90	0.935	0.999	742	8.85	0.964	0.998	1341
LUFA 2.1	5.80	0.930	1.000	806	9.96	0.941	0.999	1383
Li10	5.68	0.917	1.000	638	8.86	0.933	0.999	996
La Gironda	8.20	0.865	0.999	427	14.61	0.89	0.999	761

Conclusion:

Freundlich adsorption coefficients K_f of [^{14}C]-RPA 407922 ranged from 2.5 to 10.2 mL/g in the five soils, which corresponded to K_{foc} values ranging from 226 to 506 mL/g. Freundlich exponents 1/n varied between 0.839 and 0.909. The desorption coefficients $K_{f,des1}$ and $K_{f,des2}$ ranged from 4.9 to 36.4 mL/g in the five soils, with $K_{foc,des1}$ and $K_{foc,des2}$ values between 427 mL/g and 1809 mL/g.

Comments (RMS AT):

- The study follows OECD guideline 106 and is considered reliable. It is noted that soils properties (texture, OC and *p*H) are not necessarily fully in line with recommendations given in the OECD guideline. However, this is not considered to invalidate the study or parts of it.
- In this study, the study authors adequately calculated sorption coefficients on basis of extractable

amounts only (thus excluding NER) corrected for degradation of the test item observed.

- No exposure assessment is triggered for RPA 407922. Subsequently, this study is **considered not essential**.

Reference:	**Statement - Exposure assessment for "Met 6" and "Met 7", potential degradation products of BAS 595F triticonazole**
Author(s), year:	Szegedi, K., 2018
Report/Doc. Number:	2018/1091281
Guideline(s):	None
GLP:	Not applicable (statement)
Validity:	Partly (refer to comment section)
Status:	**New submission**

Adsorption coefficients (K_{oc}) were estimated for 'Met 6 (MWT 333)' and for 'Met 7 (MWT 315)' using QSAR methods implemented in the KocWIN 2.00 (EPISuite) tool. Values obtained based on log(K_{ow}) are reported. Details on the calculation are provided in the manual of the software tool.

Smiles codes for 'Met 6 (MWT 333)' and for 'Met 7 (MWT 315)' are presented in the table below.

Table B.8.1.3.1.2-30 Unknown metabolite fractions of triticonazole in soil degradation experiments

Metabolite	Mass (g/mol)	Smiles code
'Met 6 (MWT 333)'	333.8	CC1(C)CC\C(=C/c2ccc(Cl)cc2O)\C1(O)Cn3cncn3
'Met 7 (MWT 315)'	315.5	CC1(C)C=C/C(=C/c2ccc(Cl)cc2)\C1(O)Cn3cncn3

Obtained K_{oc} values are presented in the table below.

Table B.8.1.3.1.2-31 Estimated K_{oc} values for unknown metabolite fractions of triticonazole

Metabolite	K_{oc} (mL/g)
'Met 6 (MWT 333)'	577.1
'Met 7 (MWT 315)'	547.3

Comments (RMS AT):

- The RMS AT notes that the structure of the metabolite fraction 'Met 6 (MWT 333)' proposed by the applicant is uncertain (also refer to 'route of degradation)'. Therefore it is not considered defendable to base the QSAR on the SMILES notation as given in the study.

- Based on HPLC retention times estimated K_{oc} values obtained by KocWIN 2.00 (EPISuite) are considered too high. Notice that triticonazole has a measured mean K_{foc} value of 537 mL/g. On basis of the relative retention time of 'Met 6 (MWT 333)' (rRT = 0.63) and 'Met 7 (MWT 315)' (rRT = 0.70) it can be concluded that soil sorption of these two metabolite fractions is probably much lower than for triticonazole. Indeed, the RMS AT recommends to estimate sorption values for these two metabolite fractions on basis of their retention time observed in Ayliffe & Austin (1993) set into context with the retention time and measured mean K_{foc} values of triticonazole (geomean K_{foc} = 537 mL/g, rRT = 1.00), RPA 306341 (Trans-diol) (K_{foc} = 144 mL/g, rRT = 0.45) and RPA 404766 (Cis-diol) (K_{foc} = 75.7 mL/g, rRT = 0.33). This gives the regression function K_{foc} (mL/g) = 697 × rRT - 161 (r^2 = 0.999). On basis of this regression function the K_{foc} values of the metabolite fractions 'Met 6 (MWT 333)' and 'Met 7 (MWT 315)' are approx. 278 mL/g and 327 mL/g, respectively.

B.8.1.3.2. Aged sorption

Studies on aged sorption were not performed for the active substance triticonazole since they are not required under Commission Regulation (EU) No 283/2013 in accordance with Regulation (EC) No 1107/2009.

B.8.1.4. Mobility in soil

B.8.1.4.1. Column leaching studies

B.8.1.4.1.1. Column leaching of the active substance

Studies submitted for first Annex I inclusion:

- **John et al. (1993)**, investigating leaching of fresh and aged triticonazole in five soils

No new studies have been submitted.

Reference:	**Fungicides: RPA 400727-^{14}C (Phenyl label): Fresh & aged leaching study with five soils (final report)**
Author(s), year:	John, A. E., Lowden, P., Austin, D. J., 1993 (amended 1998)
Report/Doc. Number:	R012972, P91/357 & amendment R012973, 200173
Guideline(s):	US-EPA 163-1, BBA IV, 4-2
GLP:	Yes
Validity:	Supportive information (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The leaching of [phenyl-U-^{14}C]-triticonazole (called RPA 400727 in the report) freshly applied and after ageing for 30 days under aerobic conditions has been studied in five soils. Segmented glass columns (36 cm height) were packed with air-dried sieved soil and prewetted with water. Following treatment with triticonazole (fresh or aged) at a rate nominally equivalent to 360 g ai/ha, calcium chloride solution (0.005 M) was allowed to percolate through the columns (total 1040 ml) at a rate which did not exceed its infiltration at the soil surface. Leachate collected was equivalent to 500 mm of precipitation with leaching times varying from 3 to 12 days.

During the 30 day ageing period soil samples were adjusted to 75 % of their moisture holding capacity at 1/3 bar. For the four agricultural soils ageing was conducted in the sandy loam soil, for the German Speyer 2.1 soil the ageing was carried out in the Speyer soil itself. Samples were kept at 22 ± 2 °C in the dark. Moist air was continuously drawn over the soil surface. The air was subsequently passed through ethylene glycol and potassium hydroxide to trap possible volatiles and any carbon dioxide evolved. The fate of the triticonazole at the end of the incubation period was examined by extraction (acetonitrile/water, 4:1) and HPLC analysis.

Table B. 8.1.4.1.1-1: Soil Characteristics

Soil (USDA	Sand (%)	Silt (%)	Clay (%)	OM (%)	*p*H[(a)]	CEC (meq/100 g)	Biomass (µg C/g)	Water capacity at 0.33 bar (%)
UK sandy loam	73	13.5	13.5	1.43	6.3	6.0	118	12.0
UK clay loam	47	21	32	5.65	6.1	28.5	na	30.0
UK loamy sand	79	11.5	9.5	29.2	6.2	> 50.0	na	38.5
UK sand	96	1.5	2.5	0.91	6.2	2.3	na	2.8
Speyer 2.1 sand	90	4	6	1.32	6.1	3.0	58	11.5

(a) Matrix not specified

Findings:

For the non-aged part of the study the recovery of radioactivity after leaching of triticonazole ranged between 90.0 and 105.2 % of applied radioactivity. A summary of the distribution of radioactivity recovered is given in the tables below.

Table B. 8.1.4.1.1-2: Distribution of radioactivity following leaching of non-aged triticonazole through soil columns (% AR, duplicate samples)

Soil	Soil section						Leachate	Total
	Top segment	2	3	4	5	6		
UK Sandy loam	56.5	35.4	1.2	0.3	0.1	0.2	0.6	94.2
	22.6	50.6	15.5	0.6	0.4	0.2	0.2	90.0
UK Clay loam	50.9	46.7	2.3	0.8	0.5	0.3	0.4	101.8
	48.0	45.3	2.2	0.8	0.5	0.5	0.3	97.6
UK Loamy sand	98.9	1.1	0.3	0.2	0.1	0.1	0.1	100.8
	103.6	1.0	0.3	0.2	0.1	0.1	0.1	105.4
UK Sand	3.4	3.2	4.3	5.9	6.7	9.8	66.0	99.2
	2.9	1.7	2.5	3.9	6.4	10.2	75.1	102.7
Speyer 2.1 sand	24.6	26.3	51.9	1.0	0.5	0.3	0.7	105.2
	36.6	54.8	7.2	0.6	0.4	0.3	0.4	100.3

Table B.8.2.2.1-3: Distribution of radioactivity following leaching of 30 day aged triticonazole through soil columns (% AR, duplicate samples)

Soil	Soil section						Leachate	Total
	Top segment	2	3	4	5	6		
UK Sandy loam	31.3	45.1	15.4	1.4	1.2	0.5	1.5	96.4
	45.1	31.8	9.4	2.1	0.8	0.5	1.2	93.8
UK Clay loam	82.7	12.9	2.4	1.3	0.6	0.2	0.6	100.7
	76.9	15.1	2.6	1.1	0.5	0.4	0.7	97.2
UK Loamy sand	92.4	1.9	0.4	0.1	0.1	0.0	0.5	95.3
	85.7	4.3	0.7	0.1	0.0	0.0	0.4	91.3
UK Sand	19.0	5.6	8.1	12.5	18.2	15.5	21.9	100.8
	19.0	4.8	6.9	10.2	12.5	13.7	32.2	99.3
Speyer 2.1 sand	47.3	39.3	9.3	0.9	0.7	0.6	2.0	100.4
	55.4	35.5	5.0	1.0	0.8	0.6	1.6	99.8

With sandy loam, clay loam, loamy sand and the German standard soil Speyer 2.1 less than 1 % of AR emerged in the leachate. However with the sand approximately 70 % AR emerged. HPLC analysis of the extracted segments showed predominantly triticonazole with small amounts of the metabolites RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol). When triticonazole is leached after ageing under aerobic conditions for 30 days there was very little metabolism of the pesticide with approximately 95 % AR remaining as parent material. The percentages of radioactivity found in the leachate of these columns was less than 1 % for the clay loam and loamy sand, less than 2 % for the sandy loam and the Speyer 2.1 and 27 % for the sand. In the leachates of the aged columns di-hydroxylated metabolites were found.

Conclusions:

The results of the column leaching study with the active substance show that the mobility of triticonazole is dependent on the soil type. With the sand up to 75 % AR emerged into the leachate. With the other soils the amount was less than 1 % AR.

After 30 days ageing period the vast majority of the material present was unchanged triticonazole (95 % AR). The rest consisted of small amounts of RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol). For all the soils except the sand the amount of radioactivity in the leachate was low (≤ 2 % AR) but slightly higher than in the non-aged column leachates. In the sand soil up to 32 % AR were found. During ageing of the soil small amounts of more polar metabolites (RPA 406341 (Trans-diol), RPA 404766 (Cis-diol)) which leached to a higher degree were formed. The smaller amount of radioactivity in the leachate of the sand (compared to the non-aged column leachate) was explained by an increase in the binding of triticonazole during the ageing period and retardation of the movement through the soil column.

Comments (RMS AT):

- The study broadly follows OECD guideline 312 with some deviations:
    - For irrigation 1040 mm of 0.005 M $CaCl_2$ was used, at an application rate close to the hydraulic conductivity of the columns, homogeneously applied over a time period of 3 - 12 days. OECD guideline 312 recommends 200 mm of 0.01 M $CaCl_2$ over a timer period of 2 days.
    - Selected soils do not fulfil all selection criteria given in the OECD guideline 312
    - With a nominal application rate of 360 g a.i./ha the study is clearly overdosed (intended use rate is 12.5 g a.i./ha)

  On overall, the study is still considered reliable and may be used for **supportive information**.

- The comparison of the non-aged and aged experiments (leachate as well as residues in soil) indicates that triticonazole is prone to aged sorption in soil. This is also evident from the OECD 106 batch experiments conducted with triticonazole with sorption coefficients consistently increasing with the number of desorption cycles. In view of the RMS AT aged sorption of triticonazole in soil is also most probably responsible for the bi-phasic decline behaviour observed in many laboratory degradation experiments.

B.8.1.4.1.2. Column leaching of metabolites, breakdown and reaction products

Studies submitted for first Annex I inclusion:

- **Voelkel (1995)**, investigating the leaching behaviour RPA 406780, RPA 406341 (Trans-diol) and RPA 407922 in three soils

No new studies have been provided

Reference:	**Leaching Characteristics of three Metabolites of triticonazole (RPA 406780, RPA 406341, RPA 407922) in three Soils**
Author(s), year:	Voelkel, W., 1995 (amended 1995)
Report/Doc. Number:	R012040, 201160 & amendment R012041, 201160a
Guideline(s):	BBA IV, 4-2
GLP:	Yes
Validity:	None reliable (refer to comment section)
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The leaching behaviour of the unlabelled test substances RPA 406780, RPA 406341 (Trans-diol) and RPA 407922, metabolites of triticonazole, was investigated in three German standard soils. The test substances were dissolved in water (pre-dissolved in acetone) and applied dropwise onto the top of untreated soil columns at an amount equivalent to the field rate of 0.2 kg triticonazole/ha (39.22 µg RPA 406780, 39.23 µg RPA 406341 (Trans-diol) and 39.22 µg RPA 407922). The inner diameter of the glass columns was 5 cm, the length was 40 cm. The leaching experiment was performed at room temperature with deionized water which was added dropwise at a rate of about 0.14 ml/minute. The artificial rainfall was applied over two days and amounted to a total simulated precipitation of about 200 mm.

Leachate samples were extracted with ethyl acetate and analysed by GC.

Table B. 8.1.4.1.2-1: Soil Characteristics

Soil (DIN classification)[(b)]	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H[(a)]	CEC (meq/100 g)

Speyer 2.1, sand	87.4	9.1	3.5	0.70	6.1	4.9
Speyer 2.2, loamy sand	82.0	12.9	5.1	2.29	6.0	9.7
Speyer 2.3, silty sand	64.0	27.7	8.3	1.34	6.9	9.5

(a) Matrix not specified
(b) Sand: > 0.063 mm

Findings:

The volumes of leachates for each soil column were between 375 and 415 ml. None of the three metabolites were detected in the leachates with the limit of quantification being 0.125 µg/L.

Conclusion:

Under the conditions of the test, none of the triticonazole metabolites were found to constitute a leaching risk.

Comments (RMS AT):

- The study broadly follows OECD guideline 312. However, deionized water was used for irrigation instead of a 0.01 M $CaCl_2$ solution. In view of this major deviation the study is **not considered reliable**.

B.8.1.4.2. Lysimeter studies

Studies submitted for first Annex I inclusion:

- **Schnoeder (2003)**, investigating the leaching behaviour of phenyl labelled triticonazole in an outdoor lysimeter
- **Schnoeder (2004)**, investigating the leaching behaviour of triazole labelled triticonazole in an outdoor lysimeter

No new studies have been submitted.

Reference:	**Triticonazole[benzene ring-U-^{14}C]: Outdoor Lysimeter Study (Final Report)**
Author(s), year:	Schnoeder, F., 2003
Report/Doc. Number:	C032148, 1756-1849-009
Guideline(s):	BBA IV, 4-3, 1990
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

A lysimeter study has been conducted at Covance Laboratories GmbH near Münster, Germany. Two square lysimeters were involved in this study with columns of 110 cm undisturbed soil in depth and 1 m^2 soil surface. In this study one of the two lysimeters (Lysimeters 56 and 57) received two applications.

The application was performed using [phenyl-U-^{14}C]-triticonazole as seed dressing formulation (EXP 80472B) to winter wheat seeds. The actual rate was 12.4 g ai/ha for each lysimeter. The seeding rate of the crop was equivalent to 250 kg/ha. The second sowing, of winter barley seeds, should have been with untreated seeds for one lysimeter and with treated seeds for the other. Untreated winter barley seeds were sown by error onto the lysimeter which was intended to be a treated plot. The small plants which emerged from these seeds were removed end of October 2001 as soon as the error was discovered and treated seeds were sown on the same day. The total radioactivity recovered in the plants was determined to be 0.10 % of the radioactivity applied in 2000,

i.e. no significant portion of radioactivity was removed from the lysimeter and it is considered that there will be no significant impact on the outcome of the study. On the treated plot the achieved application rate was equivalent to 13.1 g ai/ha. Additional chemicals added to the system were a fertiliser, fenprophimorph (both during the first vegetation period) and oxydemeton-methyl and fluoxypyr (both during the second vegetation period).

Following the first application in November 2000 the leachate was monitored for radioactivity in bi-weekly intervals until end November 2002. During the first year after application a total of 80 mm of irrigation were added in May, June and July in order to compensate for the low natural precipitation in May. This resulted in a total of 855.5 mm of total precipitation and irrigation. During the second year only 5 mm of irrigation were added in June 2002 (total of 934.5 mm).

The leachate sample containing the highest level of triticonazole equivalents was analysed by high performance liquid chromatography. An aliquot was concentrated by vacuum-evaporation and the precipitating solids were separated out by centrifugation. These were extracted with acetonitrile/water (1:1, v/v) and acetonitrile. The liquid fractions were combined and reduced in volume by evaporation.

The total radioactive residues (TRRs) were determined in the crops grown on the lysimeters. This was achieved by homogenising each plant part and radio-assaying sub-samples by combustion followed by the LSC of trapped combustion gases.

Lysimeter soil samples were analysed at study termination, two years after the application of triticonazole, in 10 cm segments up to a depth of 110 cm. The upper 30 cm of the soil monoliths were completely disassembled into 10 cm layers. For the depth of 30 cm to ca. 110 cm, eight soil cores per lysimeter were taken. Cores were separated into 10 cm depth segments and combined prior to analysis. Extraction was carried out three times with acetonitrile/water (1/1; v:v). Soil extracts were subjected to HPLC analysis.

Air temperature, air humidity, wind speed, solar radiation and precipitation were recorded at half-hour intervals. Precipitation was additionally recorded on a working-day basis using a volumetric device. Soil temperature and humidity were also recorded.

Table B. 8.1.4.1.2-1: Soil Characteristics

Lysimeter Soil	Depth (cm)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)
Gleyic Cambisol, silty sand	0 - 30	76.4	20.3	3.65	1.32	5.60
	30 - 85	84.7	13.9	0.95	0.20	5.85
	85 - 130	85.1	13.9	1.10	0.05	5.80

Table B. 8.1.4.1.2-2: Overview: Cultivation of crops

1st monitoring year: 16.11.2000 - 27.11.2001	16.11.2000	Winter wheat seeding (treated)
	27.07.2001	Harvest
	09.11.2001	Winter barley seeding
2nd monitoring year: 04.12.2001 - 18.11.2002	28.07.2002	Harvest
	18.09.2002	*Phacelia* seeding
	21.11.2002	Harvest

Findings:

Soil

The majority of radioactivity at termination of the study was located within the upper two soil layers, 28.6 % AR and 44.4 % AR in the 0 - 10 cm layer and 19.6 and 17.1 % AR in the 10 - 20 cm layer for lysimeter 56 and 57, respectively. The higher value for the one lysimeter is obviously a result of the application of the different radiolabel performed by error in autumn 2001. In the 20 - 30 cm layer 5.4 % and 3.3 % AR were detected. No radioactivity was found below 30 cm of depth in both lysimeters.

The absolute radioactivity in the soil extracts was too low for HPLC chromatography and the extracts were pooled before analysed in order to increase the chance to obtain chromatographic information at all. In the semi-quantitative HPLC analysis the majority of the radioactivity represented the unmodified parent compound triticonazole.

Leachate

No radioactivity was detected at any event during the entire first monitoring year in the leachate of any lysimeter at or above the limit of detection for the LSC counting of leachate samples of ca. 0.012 µg/L ai equivalent. Very low amounts of radioactivity never exceeding 0.10 µg/L ai equivalent were found in the second monitoring year. The maximum concentration was found with 0.073 µg/L in July 2002 for lysimeter 56 and 0.051 µg/L in April 2002 for lysimeter 57. The annual average concentration of ai equivalent in the second monitoring year was 0.022 and 0.026 µg/L.

The one selected sample semi-quantitative analysed by radio-HPLC (0.073 µg/L collected in July 2002 from lysimeter 56) demonstrated that triticonazole was obviously not present in this leachate sample. It was also shown that the majority of the radioactivity present in the leachate did not match with the reference metabolites RPA 404766 (Cis-diol), RPA 406341 (Trans-diol). The radioactivity detected was slightly more polar than the most polar reference metabolite RPA 404766 (Cis-diol).

Table B. 8.1.4.1.2-3: Overall balance of radioactivity after the first and second monitoring year

	Lysimeter 56	Lysimeter 57
1st monitoring year		
Precipitation + irrigation (mm)	907.4 (827.4 + 80.0)	
Amount of leachate collected in 1st year (l)	413.1	356.3
Mean conc. of equivalents in leachate of 1st year (µg/L)	**nd**	**nd**
Max. conc. of equivalents in leachate of 1st year (µg/L)	nd	nd
Total amount of radioactivity in leachate of the 1st year (% AR)	< LOD	< LOD
Amount of radioactivity in the first crop (% AR)	0.89	0.85
Total radioactivity recovered in the 1st year	**0.89**	**0.85**
2nd monitoring year		
Precipitation + irrigation (mm)	929.0 (924.0 + 5.0)	
Amount of leachate collected in 2nd year (l)	554.0	505.1
Mean conc. of equivalents in leachate of 2nd year (µg/L)	**0.022**	**0.026**
Max. conc. of equivalents in leachate of 2nd year (µg/L)	0.073	0.051
Total amount of radioactivity in leachate of the 2nd year (% AR)	0.93	0.99
Amount of radioactivity in the second and third crop (% AR)	0.06	0.49
Amount of radioactivity in the soil (% AR)	53.62	64.75
Total radioactivity recovered in the 2nd year	**54.61**	**66.23**
Total material balance (% AR)	**55.50**	**67.08**

n.d. = not detectable (LOD = approx. 0.012 µg/L)

Crops

The TRRs in winter wheat harvested on 27th of July 2001 were 21.37 µg/kg and 20.62 µg/kg (dry mass) in the straw and 0.60 µg/kg and < LOD in the grain for lysimeter 56 and 57, respectively. The total amount of radioactivity in this crop was 0.89 % and 0.85 % of the total applied radioactivity. In the second vegetation period winter barley was harvested on 8th of July 2002, and the TRRs in winter barley straw were 2.42 and 7.14 µg/kg for lysimeter 56 and 57, respectively. In the winter barley grain, the TTRs were 0.23 and 8.51 µg/kg for lysimeter 56 and 57, respectively. Phacelia was grown for the rest of the 2002 vegetation period and harvested at the end of the study on 21th of November 2002. The TTRs were 0.53 and 3.19 µg/kg for lysimeter 56 and 57, respectively.

Soil

In the soil samples investigated at the end of the monitoring period radioactivity was only found in the upper three 10-cm-soil-layers of both lysimeters. The majority was located in the upper 10-cm-soil-layer with 3.23 µg/kg and 4.68 µg ai equivalent/kg (dry mass) in lysimeter 56 and 57 (28.55 % and 44.38 % AR), respectively. The total amount of radioactivity recovered in the soil was 53.62 % AR (lys. 56) and 64.75 % AR (lys. 57).

Table B. 8.1.4.1.2-4: Radioactivity in the soil layers of lysimeter 56 and 57 at study termination

Soil layer	% AR		Equivalent concentrations (µg/kg dry mass)	
	Lysimeter 56	Lysimeter 57	Lysimeter 56	Lysimeter 57
0 - 10 cm	28.55	44.38	3.23	4.68
10 - 20 cm	19.63	17.09	2.13	1.80
20 - 30 cm	5.44	3.27	0.44	0.29

30 - 40 cm	< LOD	< LOD	< LOD	< LOD
40 - 50 cm	< LOD	< LOD	< LOD	< LOD
50 - 60 cm	< LOD	< LOD	< LOD	< LOD
60 - 70 cm	< LOD	< LOD	< LOD	< LOD
70 - 80 cm	< LOD	< LOD	< LOD	< LOD
80 - 90 cm	< LOD	< LOD	< LOD	< LOD
90 - 100 cm	< LOD	< LOD	< LOD	< LOD
> 100 cm	< LOD	< LOD	< LOD	< LOD
Sum	**53.62**	**64.75**	**-**	**-**

LOD of the combustion analysis approx. 0.22 µg/kg

A sample of the upper 10 cm layer of lysimeter 54 was investigated but only qualitative/semi-quantitative information was obtained due to the very low amount of radioactivity in the soil extract. About half of the radioactive residues in soil remained non-extractable. Traces of triticonazole, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) as well as polar material were observed in the soil extracts in the order of 1 µg/kg.

Conclusions:

From the lysimeter study conducted in Münster (northern Germany) with formulated ^{14}C-triticonazole uniformly labelled in the benzene ring (formulation: EXP 80472B) it can be concluded that concentrations in groundwater of triticonazole and the two major soil metabolites RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) can be expected to be well below the trigger value of 0.1 µg/L if applied under the proposed conditions of use and under Good Agricultural Practice.

Comments (RMS AT):

- The study follows the BBA guideline IV, 4-3, 1990, and is still considered reliable.
- The RMS AT notes that with a soil *p*H of 5.6 - 5.9 the lysimeter study is considered not necessarily worst case for a leaching assessment of triticonazole, as sorption of triticonazole was shown to be lower in more alkaline soils. Nevertheless, the study gives indication that leaching of triticonazole and its two major soil metabolites RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) above the parametric threshold of 0.1 µg/L is unlikely to occur if applied as a seed treatment at the intended use rate of 12.5 g a.i./ha.
- No unidentified radioactivity above 0.1 µg/L has been detected in this study with [phenyl-U-^{14}C]-triticonazole applied.

Reference:	**Triticonazole[triazole-3,5-^{14}C]: Outdoor lysimeter study (final report)**
Author(s), year:	Schnoeder, F., 2004 (amended 2004)
Report/Doc. Number:	2004/5000399 & amendments 2004/5000555 & 2004/5000556
Guideline(s):	BBA IV, 4-3, 1990
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

A lysimeter study with the test item triticonazole was conducted at Covance Laboratories GmbH near Münster, Germany. Two square lysimeters are involved in this study with columns of 110 cm undisturbed soil in depth and 1 m^2 soil-surface (identified as lysimeters 54 and 55). The application was performed using [triazole-3(5)-^{14}C]-triticonazole as a seed treatment formulation (EXP 80472B). The proposed rate of application was 12.5 g ai/ha. The compound was applied on 17th of November 2000 to the winter wheat seeds and the seeds sown in the

lysimeter on the same day at actual rates of 12.4 g ai/ha for lysimeter 54 and 55. In the second vegetation period, winter barley seeds treated with [triazole-3(5)-^{14}C]-triticonazole were sown on 26th of October 2001 in lysimeter 54 only at an actual rate of 13.1 g ai/ha, while untreated winter barley seeds were applied to lysimeter 55.

Following the first application of triticonazole, in November 2000, the leachate was monitored for radioactivity in bi-weekly intervals until end of November 2003. During the first year after application a total of 80 mm of irrigation were added in May, June and July in order to compensate for the low natural precipitation in May. This resulted in a total of 855.5 mm of total precipitation and irrigation. During the second year only 5 mm of irrigation were added in June 2002 (total of 934.5 mm). A total of 150 mm of irrigation was performed in the third year, resulting in 820 mm of total precipitation plus irrigation for the year (up to November 2003). The leachate sample containing the highest level of triticonazole equivalents was analysed by high performance liquid chromatography. An aliquot was concentrated by vacuum-evaporation and the precipitating solids were separated out by centrifugation. These were extracted with acetonitrile/water (1:1, v/v) and acetonitrile. The liquid fractions were combined and reduced in volume by evaporation.

The total radioactive residues (TRRs) were determined in the crops grown on the lysimeters. This was achieved by homogenising each plant part and radio-assaying sub-samples by combustion followed by the LSC of trapped combustion gases.

Lysimeter soil samples were analysed at study termination, two years after the application of triticonazole, in 10 cm segments up to a depth of 110 cm. The upper 30 cm of the soil monoliths were completely disassembled into 10 cm layers. For the depth of 30 cm to ca. 110 cm, eight soil cores per lysimeter were taken. Cores were separated into 10 cm depth segments and combined prior to analysis. Extraction was carried out three times with acetonitrile/water (1:1; v/v). Soil extracts were subjected to HPLC analysis.

Air temperature, air humidity, wind speed, solar radiation and precipitation were recorded at half-hour intervals. Precipitation was additionally recorded on a working-day basis using a volumetric device. Soil temperature and humidity were also recorded.

Table B. 8.1.4.1.2-5: Soil Characteristics

Lysimeter Soil	Depth (cm)	Sand (%)	Silt (%)	Clay (%)	OC (%)	*p*H ($CaCl_2$)
Gleyic Cambisol, silty sand	0 - 30	76.4	20.3	3.65	1.32	5.60
	30 - 85	84.7	13.9	0.95	0.20	5.85
	85 - 130	85.1	13.9	1.10	0.05	5.80

Table B. 8.1.4.1.2-6: Overview: Cultivation of crops

1st monitoring year: 17.11.2000 - 27.11.2001	17.11.2000	Winter wheat seeding (treated)
	27.07.2001	Harvest
	25.09.2001	Winter barley seeding (lysimeter 55)
	26.10.2001	Winter barley seeding (treated), lysimeter 54 only
2nd monitoring year: 28.11.2001 - 27.11.2002	08.07.2002	Harvest
	22.10.2002	Winter wheat seeding
3rd monitoring year 28.11.2002 - 25.11.2003	21.07.2003	Harvest
	25.08.2003	Oil seed rape seeding
	27.11.2003	Harvest (BBCH 15)

Findings:

Leachates

Table B. 8.1.4.1.2-7: Overview balance of radioactivity after the first, second and third monitoring year

	Lysimeter 54 (2 treatments)	Lysimeter 55 (1 treatment)
1st monitoring year (17. Nov. 2000 – 27. Nov. 2001)		
Precipitation + irrigation (mm)	905.4 (825.4 + 80.0)	
Amount of leachate collected in 1st year (l)	403.3	420.6
Mean conc. of equivalents in leachate of 1st year (µg/L)	**0.002**	**nd**

Max. conc. of equivalents in leachate of 1st year (µg/L)	**0.016**	**nd**
Total amount of radioactivity in leachate of the 1st year (% AR)	0.02(a)	< LOD
Amount of radioactivity in the crops of 1st monitoring year (% AR)	1.25	2.21
Total radioactivity recovered in the 1st year	**1.27**	**2.21**
2nd monitoring year (28. Nov. 2001 – 27. Nov. 2002)		
Precipitation + irrigation (mm)	934.5 (929.5 + 5.0)	
Amount of leachate collected in 2nd year (l)	582.9	589.6
Mean conc. of equivalents in leachate of 2nd year (µg/L)	**0.089**	**0.042**
Max. conc. of equivalents in leachate of 2nd year (µg/L)	**0.159**	**0.077**
Total amount of radioactivity in leachate of the 2nd year (% AR)	1.89(a)	1.99(a)
Amount of radioactivity in the second crop (% AR)	1.32	0.85
Total radioactivity recovered in the 2nd year	**3.21**	**2.84**
3rd monitoring year (28. Nov. 2002 – 25. Nov. 2003)		
Precipitation + irrigation (mm)	820.0 (670.0 + 150.0)	
Amount of leachate collected in 3rd year (l)	303.3	294.6
Mean conc. of equivalents in leachate of 3rd year (µg/L)	**0.180**	**0.084**
Max. conc. of equivalents in leachate of 3rd year (µg/L)	**0.231**	**0.098**
Total amount of radioactivity in leachate of the 3rd year (% AR)	2.15(a)	1.99(a)
Amount of radioactivity in the crops of the 3rd year (% AR)	1.06(a)	0.77(a)
Amount of radioactivity in the soil at the end of the 3rd year (% AR)	52.69(a)	51.32(a)
Total radioactivity recovered in the 3rd year	**55.90(a)**	**54.08(a)**
Overall mass balance	**60.38(a)**	**59.13(a)**

nd = not detectable (LOD approx. 0.014 µg/L)
(a) Referring to the total applied radioactivity in 2000 and 2001

No radioactivity was detected in lysimeter 55 during the 1st monitoring year, while in lysimeter 54 a concentration of 0.012 µg/L a.i. equivalent on 16 Oct. 2001 and 0.016 µg/L on 27 Nov. 2001 was detected, corresponding to a total of 0.04 % AR for this 1st monitoring year.

Low amounts of radioactivity not exceeding 0.1 µg/L ai equivalent were found in lysimeter 55 during the 2nd monitoring year, with a maximum of 0.077 µg/L in November 2002. In lysimeter 54 the equivalent concentrations exceeded 0.1 µg/L in several samples from March 2002 onwards. The maximum concentration was found at 0.159 µg/L in November 2002. The annual average concentrations of ai equivalent in the 2nd monitoring year were 0.089 µg/L for lysimeter 54 and 0.042 µg/L for lysimeter 55.

During the 3rd monitoring year the concentrations of ai equivalent in lysimeter 55 always remained slightly below 0.1 µg/L with a maximum of 0.098 µg/L in Jan 2003, decreasing to 0.070 µg/L at the end of the monitoring period. The concentrations in lysimeter 54 increased in the 3rd monitoring year to a peak of 0.231 µg/L ai equivalent in Feb 2003. Thereafter the concentrations continuously decreased during the further course of the study down to 0.071 µg/L at the end of the study. The annual average concentrations for the 3rd year were 0.180 µg/L and 0.084 µg/L for lysimeter 54 and 55, respectively.

Because the annual average concentration did not exceed 0.1 µg/L ai equivalent in the two lysimeters over the first two years of the study, HPLC analysis was only performed on selected samples from lysimeter 54 and few from lysimeter 55 collected during the second monitoring year. For the third monitoring year samples approaching or exceeding 0.1 µg/L ai equivalents in lysimeter 54 were analysed as well as selected samples from lysimeter 55. These investigations demonstrated that neither triticonazole, nor the soil metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) were detectable in any of the leachates water samples (LOD 0.008 - 0.01 µg/L).

Based on the HPLC results from the analyses performed, the a.i. equivalents in the leachate were considered to be unidentified radioactivity. The vast majority was very polar material eluting within the first five minutes of the HPLC runs accounting for 0.198 µg/L ai equivalents at the concentration peak in February 2003, and then decreasing to 0.065 µg/L at the end of the study resulting in an annual average of 0.150 µg/L in lysimeter 54 during the third monitoring year. In lysimeter 55 the annual average concentration of this most polar fraction was calculated to be 0.024 µg/L. There was indication from the routine HPLC method that this polar material consisted of several peaks (integrated separately in several samples as 'polar1' to 'polar3'). Therefore selected samples were analysed using different HPLC methods. One of the methods which performed best in the separation of these polar compounds was applied for a series of samples from lysimeter 54 collected during the third year. Results of this analysis indicated that there were at least 3 - 5 peaks separated with the most polar one ('polar1') representing the majority of the polar material. Further efforts to separate the polar material using different reversed phase and normal phase HPLC conditions were not successful to refine quantification of the

polar material. The approach selected also considered a wide *p*H range in order to evaluate effects of de-/protonation of possible organic ions present in the polar fraction. For the normal phase chromatography an aliquot of the selected sample was evaporated to dryness and re-dissolved in tetrahydrofuran.

Crops
The TRRs in winter wheat harvested on 21. July 2003 were 20.77 µg/kg and 7.83 µg/kg (dry mass) in the straw and 50.43 µg/kg and 15.48 µg/kg (dry mass) in the grain for lysimeter 54 and 55, respectively. The total amount of radioactivity in this crop was 0.97 % and 0.69 % of the total applied radioactivity. Immature oil seed rape investigated at the end of the monitoring period (27th of Nov. 2003) contained 57.58 µg/kg (lys. 54) and 23.97 µg/kg dry mass (lys. 55) corresponding to less than 0.1 % of the total applied radioactivity.

Soil
In the soil samples investigated at the end of the monitoring period radioactivity was only found in the upper three 10-cm-soil-layers of both lysimeters. The majority was located in the upper 10-cm-soil-layer with 5.87 µg/kg and 2.60 µg ai equivalent/kg (dry mass) in lysimeter 54 and 55 (26.96 % and 26.28 % AR), respectively. The total amount of radioactivity recovered in the soil was 52.69 % AR (lys. 54) and 51.32 % AR (lys. 55).

Table B. 8.1.4.1.2-8: Radioactivity in the soil layers of lysimeter 54 and 55 at study termination

Soil layer	% AR		Equivalent concentrations (µg/kg dry mass)	
	Lysimeter 54	Lysimeter 55	Lysimeter 54	Lysimeter 55
0 - 10 cm	26.96	26.28	5.87	2.60
10 - 20 cm	19.08	17.48	3.69	1.79
20 - 30 cm	6.65	7.56	1.07	0.60
30 - 40 cm	< LOD	< LOD	< LOD	< LOD
40 - 50 cm	< LOD	< LOD	< LOD	< LOD
50 - 60 cm	< LOD	< LOD	< LOD	< LOD
60 - 70 cm	< LOD	< LOD	< LOD	< LOD
70 - 80 cm	< LOD	< LOD	< LOD	< LOD
80 - 90 cm	< LOD	< LOD	< LOD	< LOD
90 - 100 cm	< LOD	< LOD	< LOD	< LOD
> 100 cm	< LOD	< LOD	< LOD	< LOD
Sum	**52.69**	**51.32**	**-**	**-**

LOD of the combustion analysis approx. 0.28 µg/kg

A sample of the upper 10 cm layer of lysimeter 54 was investigated but only qualitative/semi-quantitative information was obtained due to the very low amount of radioactivity in the soil extract. About half of the radioactive residues in soil remained non-extractable. Traces of triticonazole, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) as well as polar material were observed in the soil extracts in the order of 1 µg/kg.

Conclusions:

Results of a lysimeter study conducted in German indicate that triticonazole and its main metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) do not pose an unacceptable risk to groundwater if triticonazole is applied according to the intended use and Good Agricultural Practice.

In the leachates of the lysimeters triticonazole and its two metabolites have not been detected at any time point during the course of the study (LOD 0.008 - 0.01 µg/L).

Annual average concentrations in the leachates expressed as ai equivalents exceeded 0.1 µg/L in the third monitoring year and were close to 0.1 µg/L in the second monitoring year. HPLC analysis of the leachate water samples revealed that the radioactivity consists of polar material. Different HPLC methods were used to further characterize this fraction, showing that it very likely consists of several components. Reasonable further efforts to separate the polar material using different reversed phase and normal phase HPLC conditions were unsuccessful and no refined quantification of the polar material was possible.

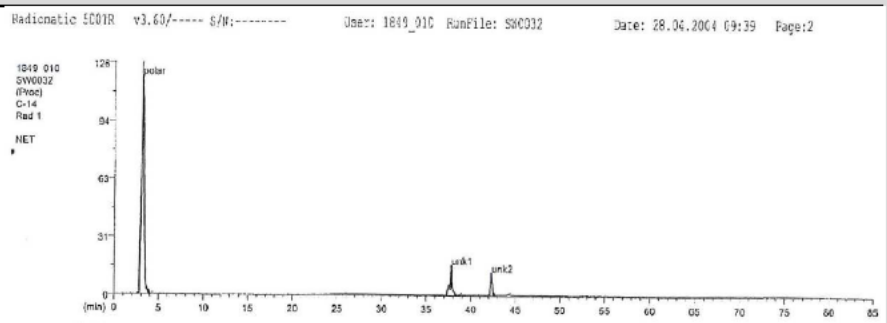
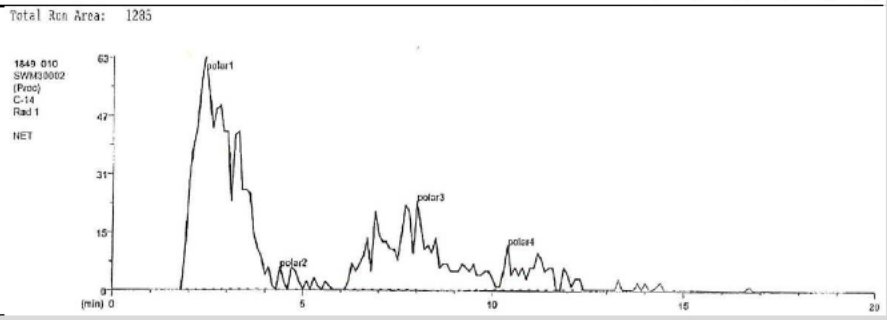
The polar material was not retained and eluted in or right after the void volume of the columns. Based on these results it is expected that the polar fraction consists of one or several highly polar components of low molecular weight. Considering that the highest annual concentration associated to the very polar material was 0.15 µg/L a.i. equivalent in year 3 of lysimeter 54 and the probable low molecular weight of the material, it is expected that the actual concentration of any single component in the polar fraction would be significantly lower than 0.1 µg/L.

Comments (RMS AT):

- The study follows the BBA guideline IV, 4-3, 1990, and is still considered reliable. Results may be handled as supportive information.

- The RMS AT notes that with a soil *p*H of 5.6 - 5.9 the lysimeter study is considered not necessarily worst case for a leaching assessment of triticonazole, as sorption of triticonazole was shown to be lower in more alkaline soils. Nevertheless, the study gives indication that leaching of triticonazole and its two major soil metabolites RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol) above the parametric threshold of 0.1 µg/L is unlikely to occur if applied as a seed treatment at the intended use rate of 12.5 g a.i./ha.

- Unidentified radioactivity at mean annual concentrations of 0.180 µg/L parent equivalents (3rd year, lysimeter 54) has been detected in this study with [triazole-3(5)-^{14}C]-triticonazole applied. The vast majority (0.150 µg/L mean annual concentration) was very polar material eluting within the first five minutes of the HPLC runs. There was indication from the routine HPLC method that this polar material consisted of several compounds. In view of additional data provided (HPLC chromatograms applying different HPLC methods, see figures below) the RMS AT considers it unlikely that unknown polar compounds exceeded 0.1 µg/L on individual basis in this study. However, as the peak concentration was observed in the last year, the study does not allow concluding on residues in the leachates in subsequent years.

Example chromatogram of a leachate sample (Lys 54, 26th Nov. 2002) - 'routine' HPLC (total amount of polars: 0.133 µg/L equivalents)	
Example chromatogram of a leachate sample (Lys 54, 4th Feb. 2003) - additional HPLC method (total amount of polars: 0.198 µg/L equivalent)	

B.8.1.4.3. Field leaching studies

Field leaching studies for the active substance triticonazole have not been performed since it is not required under Commission Regulation (EU) No 283/2013 in accordance with Regulation (EC) No 1107/2009.

B.8.1.4.4. Summary on adsorption and mobility in soil

Soil adsorption of triticonazole, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) in soil has been assessed in OECD guideline 106 batch studies and is summarised in the tables below. The RMS AT notes that the dossier on triticonazole accounts for several studies on sorption of triticonazole and the metabolites which may not be considered fully reliable owing to missing pre-equilibration phases in these experiments. However, as results obtained in studies without pre-equilibration phase are close to results with adequate pre-equilibration phase, results from these studies are considered equally reliable. It is noted that these studies have been repeated some few years later using the same soils (albeit different batches). Unfortunately, there is no guidance on when to consider a soil being 'identical' to another soil. On overall, the soils are considered fairly similar with respect to soil properties. However, in some cases there are quite some differences with respect to soil *p*H or organic matter as well as with respect to the sorption results obtained.

Table B.8.1.4.4-1: Summary on soil adsorption of triticonazole

Soil name	Soil type (USDA)	OC (%)	*p*H ($CaCl_2$)	K_d (mL/g)	K_{oc} (mL/g)	K_f (mL/g)	K_{foc} (mL/g)	1/*n* (-)	Ref.
Wildacker	Silt loam	1.85	5.7	na	na	11.8	636	0.92	Vasques (2015a)
LUFA 2.3	Sandy loam	0.99	6.7	na	na	3.67	370	0.89	
LUFA 2.1	Sand	0.60	5.6	na	na	5.23	871	0.93	
Li 10	Loamy sand	0.95	6.2	na	na	4.79	504	0.91	
La Gironda	Sandy clay loam	1.22	7.4	na	na	3.97	325	0.94	
Wildacker	Silt loam	2.01	5.8	na	na	13.4	665	0.893	Simmonds (2017a)
LUFA 2.3	Sandy loam	0.66	5.3	na	na	4.52	685	0.898	
LUFA 2.1	Sand	0.72	5.6	na	na	5.60	778	0.889	
Li 10	Loamy sand	0.89	6.1	na	na	5.11	574	0.888	
La Gironda	Silty clay loam	1.92	7.1	na	na	5.56	290	0.848	
	Arithmetic mean (n = 10)			**-**	**-**	**-**	**-**	**0.90**	
	Geometric mean (n = 10)			**-**	**-**	**5.78**	**537**	**-**	
	Minimum[(b)]					**-**	**307**	**-**	
	Maximum[(c)]					**-**	**823**	**-**	
	pH-dependency: y/n			y[(a)]					

(a) Refer to text below
(b) Geometric mean of the two similar La Gironda soils (both sandy clay loam soils, *p*H 7.1 - 7.4).
(c) Geometric mean of the two similar LUFA 2.1 soils (both sand soils, *p*H 5.6)

Table B.8.1.4.4-2: Summary on soil adsorption of RPA 406341 (Trans-diol)

Soil name	Soil type (USDA)	OC (%)	*p*H ($CaCl_2$)	K_d (mL/g)	K_{oc} (mL/g)	K_f (mL/g)	K_{foc} (mL/g)	1/*n* (-)	Ref.
Wildacker	Clay silt	1.97	5.8	na	na	2.59	132	0.95	Vasques (2015b)
LUFA 2.3	Loamy sand	0.7	7.1	na	na	0.80	114	0.96	
LUFA 2.1	Sand	0.6	6.0	na	na	0.68	114	0.98	
Li 10	Silty sand	0.6	5.5	na	na	1.94	324	1.00	
La Gironda	Sandy clay loam	1.3	7.7	na	na	1.38	106	0.94	
Wildacker	Silt loam	2.01	5.8	na	na	3.72	185	0.919	Kingman (2017)
LUFA 2.3	Sandy loam	0.66	5.3	na	na	1.02	154	0.945	
LUFA 2.1	Sand	0.72	5.6	na	na	1.35	188	0.937	
Li 10	Loamy sand	0.89	6.1	na	na	1.31	148	0.932	
La Gironda[(a)]	Silty clay loam	1.92	7.1	na	na	1.57	81.6	0.839	
	Arithmetic mean (all soil, n = 10)			**-**	**-**	**-**	**-**	**0.94**	
	Geometric mean (all soil, n = 10)			**-**	**-**	**1.45**	**144**	**-**	
	pH-dependency: y/n			n					

(a) Sorption coefficients have been reassessed by the RMS AT excluding NER in the calculation (refer to Kingman, 2017)

Table B.8.1.4.4-3: Summary on soil adsorption of RPA 404766 (Cis-diol)

Soil name	Soil type (USDA)	OC (%)	*p*H ($CaCl_2$)	K_d (mL/g)	K_{oc} (mL/g)	K_f (mL/g)	K_{foc} (mL/g)	1/*n* (-)	Ref.
Wildacker	Clay silt	1.97	5.8	na	na	0.68	161	0.95	Vasques (2015b)
LUFA 2.3	Loamy sand	0.7	7.1	na	na	0.83	49.0	0.90	
LUFA 2.1	Sand	0.6	6.0	na	na	0.28	46.1	0.97	
Li 10	Silty sand	0.6	5.5	na	na	0.34	139	0.98	

La Gironda	Sandy clay loam	1.3	7.7	na	na	3.17	52.6	0.99	
Wildacker[(a)]	Silt loam	2.01	5.8	na	na	1.71	85.3	0.889	O'Brien (2017)
LUFA 2.3	Sandy loam	0.66	5.3	na	na	0.48	72.6	0.920	
LUFA 2.1	Sand	0.72	5.6	na	na	0.68	94.0	0.946	
Li 10	Loamy sand	0.89	6.1	na	na	0.67	74.8	0.922	
La Gironda[(a)]	Silty clay loam	1.92	7.1	na	na	1.03	53.6	0.868	
	Arithmetic mean (all soil, n = 10)			**-**	**-**	**-**	**-**	**0.93**	
	Geometric mean (all soil, n = 10)			**-**	**-**	**0.76**	**75.7**	**-**	
	pH-dependency: y/n			n					

(a) Sorption coefficients have been reassessed by the RMS AT excluding NER in the calculation (refer to O'Brian, 2017)

The RMS AT investigated a possible relationship between sorption coefficient (K_{foc}) and soil *p*H for triticonazole, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) more in detail (Figure B.8.1.4.4-1). It may be noted that there are neither strong structural reasons nor evidence from phys-chem data to expect a strong *p*H effect (no dissociation, no *p*H effect on Log P_{ow} or solubility). The same is probably true for the metabolites RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol), both structurally similar to the parent. Nevertheless, there appears to be a fairly strong *p*H dependent sorption in case of the parent triticonazole with lower sorption in more alkaline soils with $p = 0.001$ applying Kendall's Tau-b test (two-tailed) on basis of the combined dataset. No such relationship could be found for the $1/n$ value. There is also some indication of *p*H dependent sorption for the two metabolites. However, the relationship is less obvious in these cases (although still significant ($p = 0.01$) in case of RPA 406341 (Trans-diol) applying Kendall's Tau-b test; no significant correlation is given in case of RPA 404766 (Cis-diol)). In order to adequately address these findings in the exposure assessment, the RMS AT recommends accounting for *p*H dependent sorption in case of triticonazole but not necessarily in case of the metabolites as *p*H dependency is much less pronounced for these substances. In case of triticonazole, the RMS AT recommends using the minimum/maximum K_{foc} (307 and 823 mL/g, respectively, both calculated on basis of two similar soils) in combination with the arithmetic mean $1/n$ of 0.90 derived on basis of the entire dataset for the groundwater and surface water exposure assessment.

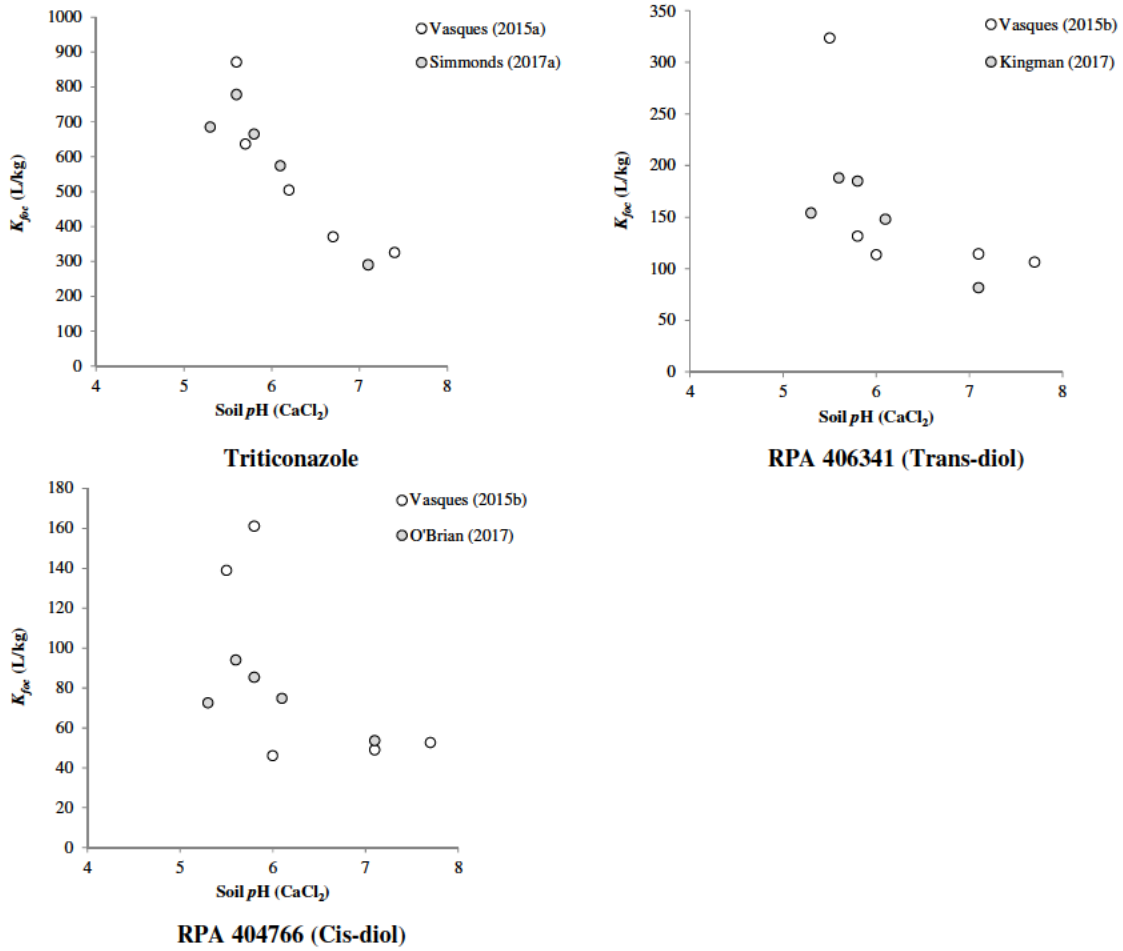


Figure B.8.1.4.4-1: Soil sorption (K_{foc}) of triticonazole and its metabolites *vs.* soil *p*H (in $CaCl_2$)

On basis of their relative HPLC retention time (rRT) observed in Ayliffe & Austin (1993), set into context with measured mean adsorption properties and retention times of triticonazole, RPA 406341 (Trans-diol) and RPA 404766 (Cis-diol) observed in this study, K_{foc} values of the two metabolite fractions **'Met 6 (MWT 333)'** (rRT = 0.63) and **'Met 7 (MWT 315)'** (rRT = 0.70) are estimated to be approx. 278 mL/g and 327 mL/g, respectively (on basis of the regression K_{foc} (mL/g) = 697 × rRT - 161, r^2 = 0.999).

Results of a **non-aged and aged column study** show that the mobility of triticonazole was dependent on the soil type, having a medium to low mobility in all but a sand soil where up to 71 % AR (non-aged experiment) was found in the leachate. In the experiment on aged residues (with still 95 % of triticonazole present after 30 days) amounts of triticonazole in the leachate of the sand soil have been reduced to 27.1 % AR indicating that triticonazole is prone to aged sorption in soil. This is also evident from the OECD guideline 106 batch experiments with sorption coefficients consistently increasing with the number of desorption cycles. In view of the RMS AT aged sorption of triticonazole in soil is also most probably responsible for the bi-phasic decline behaviour observed in many laboratory degradation experiments.

Two **lysimeter studies** have been conducted on a silty sand (1.32 % OC) with either [phenyl-U-^{14}C] or [triazole-3(5)-^{14}C] labelled triticonazole. Triticonazole was applied as a seed treatment in winter cereals with an intended application rate of 12.5 g ai/ha. Application took place in the first year only or in the first and second year with study durations of two years in case of the phenyl label and three years in case of the triazole label. Annual amounts of leachates collected were in the range from 295 - 590 L/m^2. Neither triticonazole nor RPA 406341 (Trans-diol) or RPA 404766 (Cis-diol) have been detected in the leachate samples (LOD = 0.008 - 0.01 µg/L). Unknown radioactivity did not exceed annual mean concentrations of 0.026 µg/L a.i. equivalents for the phenyl label. In case of the triazole label unidentified radioactivity at annual mean concentrations of 0.180 µg/L a.i. equivalents has been detected. The vast majority (0.150 µg/L mean annual concentration) was very polar material considered not to exceed 0.1 µg/L on individual basis. However, as the peak concentration was observed in the last year, the study does not allow concluding on residues in the leachates in subsequent years.

B.8.2. FATE AND BEHAVIOUR IN WATER AND SEDIMENT

B.8.2.1. Route and rate of degradation in aquatic systems (chemical and photochemical degradation)

B.8.2.1.1. Hydrolytic degradation

Studies submitted for first Annex I inclusion:

- **Corgier & Robin (1991)**), investigating triazolyl labelled triticonazole

New studies submitted:

- **Hassink (2013)**, investigating triazolyl labelled triticonazole

Reference:	**^{14}C-RPA 400727: Hydrolysis at 25 °C**
Author(s), year:	Corgier, M. M. C., Robin, J. M., 1991
Report/Doc. Number:	R013023/426940
Guideline(s):	US-EPA N, 161-1
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

[Triazole-3(5)-^{14}C]-triticonazole (called RPA 400727 in the report, radiochemical purity > 98.9 %) was applied to *p*H 5, 7 and 9 buffer solutions at an initial concentration of 3.87 mg/l. The test vessels were incubated under sterile conditions in the dark at 25 °C for 30 days. On days 0, 7, 12, 19, 26 and 30 two samples were taken and analysed by TLC and HPLC. The *p*H of buffers was determined at each sampling interval.

Findings:

Temperature was kept in the range of 24.75 - 25.25 °C and the *p*H differed less than 0.2 units during the course of the hydrolysis study. The mean measured radioactivity in the samples was between 97.3 and 101.8 % of applied radioactivity, indicating that no volatile compound had evolved. No degradation of the test substance was observed.

Conclusion:

Triticonazole is hydrolytically stable at *p*H 5 to *p*H 9 and an environmentally relevant temperature of 25 °C.

Comments RMS AT:

- The study broadly follows OECD guideline 111 and is still considered reliable.

Reference:	**Triticonazole: Aqueous hydrolysis at four different *p*H values**
Author(s), year:	Hassink, J., 2013
Report/Doc. Number:	2012/1300793
Guideline(s):	EEC 94/37, EEC 95/36, EEC 91/414, SETAC Procedures for assessing the environmental fate and ecotoxicity for pesticides (March 1995), JMAFF 2-6-1, OECD 111, EPA 835.2120
GLP:	Yes

Validity:	Yes
Status:	**New submission**

Material and methods:

Radiolabelled test material	[Triazole-3(5)-^{14}C]-triticonazole
Reg. No.:	4378513
Batch No.:	867-1201
Specific Activity:	5.07 MBq/mg
Radiochemical purity:	> 99 %
Reference items	Triticonazole (unlabelled)
Reg. No.:	4378513
Batch No.:	L76-154
Purity	99.8 %
	Z-isomer (RPA 406203)
Reg. No.:	Reg. No. 5079359
Batch No.:	BESS0578
Purity	99.9 %
	S-Triticonazole
Reg. No.:	5079361
Batch No.:	L76-160
Purity	99.0 %
	R-Triticonazole
Reg. No.:	5079385
Batch No.:	HUT918
Purity	99.9 %

Test solutions
The buffer solutions were prepared from Titrisol-solutions (Merck) by 10-fold dilution with bi-distillated water:

- *p*H 4: Titrisol 1.09884 (citrate-HCI)
- *p*H 5: Titrisol 1.09885 (citrate-NaOH)
- *p*H 7: Titrisol 1.09887 (phosphate)
- *p*H 9: Titrisol 1.09889 (boric acid/KCI-NaOH)

Test solutions were prepared by evaporating a volume of 3.2 mL of stock solution (1.27 mg/mL, purity 97.5 %) to dryness and reconstituting the residue with 5 mL acetonitrile and bringing up to 1000 mL with the respective diluted buffer. The sterile samples (100 mL subsets) were stored in a climatic chamber at 25 ± 1°C for up to 30 days in the dark. The sampling times were 0 d, 2 d, 5 d, 8 d, 12 d, 15 d and 30 d after treatment. At each sampling time, samples were checked for pH and sterility. All samples of the test solutions were analysed directly without work-up. They were analysed by LSC for radioactivity determination and by HPLC to determine the residue pattern. Furthermore, all samples were analysed using a chiral HPLC column to obtain a separation of S- and R-triticonazole.

Findings:

Results from the hydrolysis test, including the material balances and the results obtained with both HPLC methods are presented in the tables below.

Table B. 8.1.4.1.2-1: Hydrolysis of triticonazole at *pH* 4, 25 °C

DAT	Material Balance	HPLC – non-chiral column (% AR)			HPLC – chiral column (% AR)		
		Triticonazole (sum of *R* and *S* isomers)	RPA 406203 (Z-isomer)	Sum[(a)]	S-isomer	R-isomer	RPA 406203 (Z-isomer)

0	100.0	95.4	2.0	97.4	50.9	47.9	1.1
2	99.0	95.6	1.6	97.2	50.7	48.3	n.d.
5	99.5	95.4	1.4	96.8	49.3	50.1	n.d.
8	99.5	95.1	2.5	97.6	49.6	49.0	0.9
12	99.4	94.5	1.8	96.3	49.8	48.5	1.0
15	98.6	94.5	2.1	96.6	49.3	49.3	n.d.
30	97.5	92.6	2.1	94.7	49.7	47.8	n.d.

(a) Some minor peaks ≤ 2 % AR not included

Table B. 8.1.4.1.2-2: Hydrolysis of triticonazole at *pH* 5, 25 °C

DAT	HPLC – non-chiral column (% AR)				HPLC – chiral column (% AR)		
	Material Balance	Triticonazole (sum of *R* and *S* isomers)	RPA 406203 (Z-isomer)	Sum[(a)]	S-isomer	R-isomer	RPA 406203 (Z-isomer)
0	100.0	96.8	1.3	98.1	50.0	48.8	1.3
2	101.3	97.0	1.8	98.8	49.6	51.6	n.d.
5	102.7	99.7	1.7	101.4	52.0	50.7	n.d.
8	100.9	96.5	2.3	98.8	50.8	50.1	n.d.
12	99.7	96.0	2.1	98.1	50.2	48.6	0.9
15	100.8	95.6	2.1	97.7	51.2	49.6	n.d.
30	97.4	92.1	1.6	93.7	48.8	48.6	n.d.

(a) Some minor peaks ≤ 2 % AR not included

Table B. 8.1.4.1.2-3: Hydrolysis of triticonazole at *pH* 7, 25 °C

DAT	HPLC – non-chiral column (% AR)				HPLC – chiral column (% AR)		
	Material Balance	Triticonazole (sum of *R* and *S* isomers)	RPA 406203 (Z-isomer)	Sum[(a)]	S-isomer	R-isomer	RPA 406203 (Z-isomer)
0	100.0	95.9	2.3	98.2	49.7	50.3	n.d.
2	90.7	86.4	1.3	97.7	46.1	43.4	1.2
5	99.8	95.4	1.7	97.1	49.5	49.4	0.8
8	97.1	94.1	2.0	96.1	48.4	47.6	1.1
12	100.5	97.3	1.8	99.1	51.3	49.3	n.d.
15	99.5	95.7	2.2	97.9	50.2	48.3	0.9
30	100.4	95.6	1.7	97.3	50.4	49.9	n.d.

(a) Some minor peaks ≤ 2 % AR not included

Table B. 8.1.4.1.2-4: Hydrolysis of triticonazole at *pH* 9, 25 °C

DAT	HPLC – non-chiral column (% AR)				HPLC – chiral column (% AR)		
	Material Balance	Triticonazole (sum of *R* and *S* isomers)	RPA 406203 (Z-isomer)	Sum[(a)]	S-isomer	R-isomer	RPA 406203 (Z-isomer)
0	100.0	94.7	2.3	97.0	49.2	49.8	1.1
2	98.3	94.9	1.7	96.6	49.2	47.8	1.3
5	98.4	93.5	1.9	95.4	49.9	48.4	n.d.
8	98.5	93.3	2.2	95.5	50.4	48.1	n.d.
12	98.9	95.1	2.6	97.7	49.2	49.6	n.d.
15	97.7	92.4	1.9	94.3	50.2	46.5	1.0
30	96.0	91.5	1.8	93.3	47.7	48.3	n.d.

(a) Some minor peaks ≤ 2 % AR not included

Conclusion:

Triticonazole is stable in aqueous solution at *p*H 4, 5, 7 and 9 (25 °C). There are no indications that a change to the Z-isomer or a change in the ratio of *S*- and *R*-enantiomers of triticonazole will occur in aqueous solutions in the range of *p*H 4 to *p*H 9 and at 25 °C.

Comments (RMS AT):

- The study follows OECD guideline 111 and is considered reliable.

B.8.2.1.2. Direct photochemical degradation

Studies submitted for first Annex I inclusion:

- **Corgier & Robin (1992)**), investigating triazolyl labelled triticonazole at *p*H 5
- **Corgier & Turier (1995)**, investigating the quantum yield and environmental half-life of triticonazole

New studies submitted:

- **Sing (2007a)**, investigating triazolyl and phenyl labelled triticonazole at *p*H 5

Reference:	**^{14}C-RPA 400727: Aqueous photolysis**
Author(s), year:	Corgier, M. M. C, Robin, J. M., 1992
Report/Doc. Number:	R013068, 429307, 91-50, AG/CRLD/AN/9216236
Guideline(s):	US-EPA N, 161-2
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The test substance [triazole-3(5)-^{14}C]-triticonazole was added to a buffer solution (*p*H 5) and incubated at 25 ± 1 °C under sterile conditions and continuous irradiation (using a Xenon lamp) at an initial concentration of 3.9 mg/l. Radiation below 290 nm was removed by a filter. Acetone was added to one test set as a photosensitizer at a concentration of 2 %. Volatiles were trapped in an aqueous solution of ethylenglycol monomethylether and NaOH. Duplicate samples were taken after 0, 2, 4, 8, 24, 72 and 144 h for the experiment without acetone and after 0, 2, 4, 8, 24 and 48 h for the experiment with acetone. At each sampling time the *p*H was measured and the radioactivity in samples and traps was counted. Analysis was conducted by means of TLC. HPLC was used for confirmation of the identity of the main compounds.

Findings:

The radioactivity balance of the samples ranged from 97 to 104.5 % of the initial radioactivity. Practically no volatile compounds were formed. Triticonazole was transformed to its Z-isomer RPA 406203. Polar products reached 12.4 % AR by study end (6 days) with maximum 4.2 % on individual basis. No other metabolites exceeded 10 % AR at any time. The half-lives, with and without acetone, of triticonazole were determined graphically. The *DT50* was reached 9.4 times faster in the presence of acetone than without. With acetone an equilibrium of triticonazole with its Z-isomer RPA 406203 was established. Without acetone triticonazole decreased fast in a first phase and slower in a second phase. The results achieved with the xenon lamp were extrapolated to natural summer days in Florida.

Table B. 8.1.4.1.2-1: Phototransformation of triticonazole in aqueous solution (% AR, numbers shaded in grey exceed 10 % AR)

Sensitizer	Incubation time (hrs)	Triticonazole	RPA 406203 (Z-isomer)
None	**0**	99.2	0.0
	2	88.7	10.3
	4	78.3	20.9
	8	65.8	33.2
	24	59.7	39.1
	72	51.0	42.3
	144	35.9	42.0

Acetone (2 %)	**0**	96.2	2.3
	2	71.4	26.8
	4	62.1	36.8
	8	49.8	47.9
	24	44.1	51.3
	48	41.6	48.0

Conclusion:

Without acetone the *DT50* were 75.9 hrs (xenon lamp) and 2.97 hrs (summer day Florida); *DT50* with acetone were 8.08 hrs (xenon lamp) and 0.32 hrs (summer day Florida).

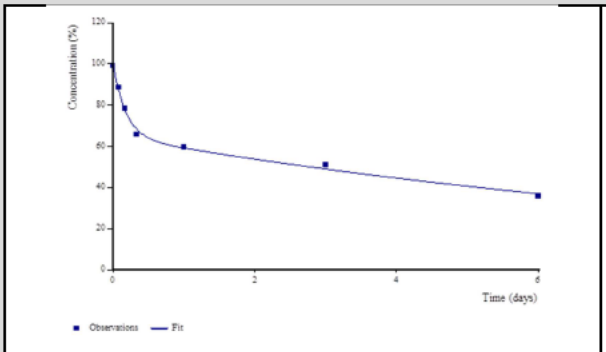
Comments (RMS AT):

- The study broadly follows OECD guideline 316 is still considered reliable. Notice that only triazole labelled triticonazole was investigated in this study. Both, phenyl and triazole labelled triticonazole was investigated in Singh (2007).
- The RMS AT notes, that transformation of RPA 406203 (Z-isomer) from triticonazole is considered to be reversible as long as irradiation is present, approaching equilibrium by approx. 1 day in this experiment (see figure below). In addition, one has to assume further that degradation of both, triticonazole and RPA 406203 (Z-isomer), taking place at probably different rates, accompanied by steady equilibration between the two compounds. In principal, such a complex system may be modelled by a multi-compartment pathway fit considering reversible transformation from triticonazole to RPA 406203 (Z-isomer). However, from a regulatory point of view (trigger assessment) the RMS AT recommends to stay with dissipation rates only (see results below). Considering that triticonazole is virtually stable under conditions of hydrolysis, the slow-phase *DT50* of approx. 10 days obtained (without and with sensitizer), representing dissipation of triticonazole after equilibrium has been reached, indicates quite a substantial impact of photolysis on the overall dissipation of triticonazole in irradiated aquatic environments.

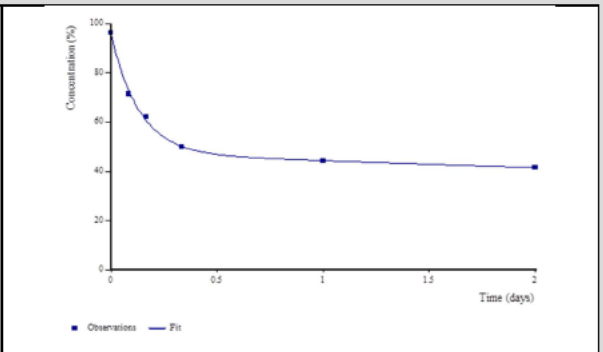
Table B. 8.1.4.1.2-2: Dissipation rates of triticonazole under conditions of aquatic photolysis - RMS AT assessment

Test system	Model	Para-meter	Value	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*Total DT50* (d)	*Total DT90* (d)	*Slow phase DT50 (d)*
Without sensitizer	DFOP	k1	5.57	2.11	9.03	0.01				
		k2	0.09	0.05	0.14	< 0.01	2.2	2.8	20.0	7.4
		g	0.35	0.25	0.45	na				
With sensitizer (acetone)	DFOP	k1	7.57	3.25	11.90	0.01				
		k2	0.07	-0.12	0.25	0.13	1.5	0.4	24.4	10.6
		g	0.51	0.38	0.64	na				

Table B. 8.1.4.1.2-3: Dissipation rates of triticonazole under conditions of aquatic photolysis (fits) - RMS AT assessment



Without sensitizer



With sensitizer (acetone)

Reference:	**Triticonazole - Quantum yield and environmental half-life in water**
Author(s), year:	Corgier, M. M. C., Turier, G. P., 1995
Report/Doc. Number:	R012072, 439237, 95-90, R&D/CRLD/AN/9516639, 8533
Guideline(s):	BBA Part IV, 6-1, UBA Phototransformation of Chemicals, Part A
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The quantum yield of direct phototransformation of triticonazole in water and its theoretical half-life in the top layers of aqueous media was determined by actinometry. For actinometry the same test conditions were applied as in the photolysis study (Corgier & Robin, 1992). The light intensity was 198.3 Wm^{-2}. Quantum yield was calculated with the use of the computer program QUANTUS. Solar light intensity data for Central Europe and the adjacent North Sea (R. Frank, Kloepffer, Chemosphere, 1988, 17, 985-94) were used for calculation of environmental half-lives.

Findings and conclusion:

The quantum yield was calculated as 0.05. The environmental half-live ranged between 344 h (~14 d) in July to about 4000 h (~167 d) in December, at a latitude of 52 °N.

Comments (RMS AT):

- The study is still considered reliable.

Reference:	**Aqueous photolysis of ^{14}C-BAS 595 F (Triticonazole)**
Author(s), year:	Singh, M., 2007
Report/Doc. Number:	2007/7001058
Guideline(s):	US-EPA N, 161-2
GLP:	Yes
Validity:	Yes
Status:	**New Submission**

Material and methods:

Test material

^{14}C-triazole-triticonazole (BAS 595 F)

Reg. No.:	4378513
Molecular Weight:	317.82 g/mol (unlabelled)
Site of radiocarbon labeling:	triazole-4(5)-^{14}C
Batch No.:	867-1103
Specific Activity:	391780.8 dpm/µg
Radiochemical purity:	> 99.3 %

^{14}C-phenyl-triticonazole (BAS 595 F)

Reg. No.:	4378513
Molecular Weight:	317.82 g/mol (unlabelled)
Site of radiocarbon labeling:	phenyl-U-^{14}C
Batch No.:	866-1103

Specific Activity: 400915 dpm/µg
Radiochemical purity: > 99.4 %

Test System
The *p*H 5 buffer solutions were prepared by dissolving sodium acetate (1.36 g) in HPLC grade water (1000 mL), and then adding 235 µL of acetic acid to obtain a 0.01 M *p*H 5 buffer solution. The buffer solution was filtered using a sterilized filtration unit (pore size 0.2 µm) prior to the treatment to make it sterile.

Experimental conditions
The photolysis setup consisted of a rectangular metallic hollow block equipped with coolant inlet and outlet. The thermostated block was provided with 6 wells to house 6 photolysis glass vessels with a quartz glass disc at the top. Each test vessel was filled with 200 mL of a treated buffer solution which was prepared by adding appropriated amounts of ^{14}C-labelled triticonazole stock solution to sterile *p*H 5 buffer. Initial concentrations of ^{14}C-labeled triticonazole in the test solutions (irradiated samples and dark controls) were 3.6 and 5.5 mg/L for the triazole and phenyl label, respectively.

Samples were continuously exposed to a Xenon arc lamp in an Atlas Suntest CPS Plus apparatus. Wavelengths < 290 nm were filtered out. The measured intensity and spectrum of the irradiation was comparable to natural sunlight at 40° N latitude.

The irradiation temperature was maintained at 22 ± 1 °C. The test vessels were continuously flushed with sterile moistened CO_2-free air, and volatiles were collected in a series of trapping solutions (ethylene glycol and NaOH). Possible losses of water during irradiation were fixed by weighing the irradiated test vessel and adding appropriate amounts of untreated sterile buffer solutions

In addition, aliquots (~1 mL each) of the treated solution were transferred to a number of HPLC vials. Vials were capped and stored in the dark inside an incubator maintained at 22 ± 1 °C. These samples were used as dark controls.

Sampling
The sampling intervals for the triazole label experiment were 0, 19, 24, 48, 72, 168, 240, 336 and 408 hours. The sampling intervals for the phenyl label experiment were 0, 8, 24, 48, 72, 168, 240, 360 and 408 hours. Irradiated samples and dark controls were removed at the same time. Volatile trapping solutions were removed at every sampling interval.

Description of analytical procedures
Volatile trapping solutions from irradiated samples were analysed by LSC to quantify the amount of volatile radioactivity. For a selected time interval, the trapped carbon dioxide was characterized by reacting a measured aliquot of the trapping solution with sulfuric acid, trapping the carbon dioxide generated into Harvey cocktail, and finally counting the Harvey sample by LSC.

To determine the material balances in irradiated and dark samples, aliquots of the solutions were analysed by LSC. HPLC was used to obtain the quantitative distribution profile of radioactive residues in the sample.

At the end of the study, the remaining buffer solutions in the irradiated triazole-labelled samples were pooled and partitioned with ethyl acetate. The resultant fractions were assayed by LSC, concentrated to dryness, reconstituted with an acetonitrile water mixture and fractionated using a HPLC method. Each relevant fraction was assayed by LSC to generate a histogram. Fractions of relevance were pooled assayed by LSC and HPLC. Then, they were concentrated further and analysed by HPLC co-chromatography with reference standard (if available) and mass spectrometry.

A similar procedure was used for the irradiated phenyl-labelled samples, but lyophilisation was applied in the first step instead of partitioning and NMR was used as an additional identification method.

Determination of degradation kinetics
Estimation of the half-life of triticonazole was done only for the irradiated samples. The half-life estimation was not done for the dark control samples because triticonazole was stable under this condition for at least 17 days after the treatment. The guidance of FOCUS (2006) was used as the basis for conducting the kinetic analysis, statistical assessment, and selection of the best fit kinetic model. Optimization of model parameters, including

estimation of parameter standard errors, was performed using the software ModelMaker 4.0. Decline of ^{14}C-triticonazole and rise and decline of the Z-isomer photoproduct were evaluated using a single first-order (SFO) reversible model and three biphasic models (first-order multi compartment or FOMC, double first-order in series or DFOS, and double first-order in parallel or DFOP).

Findings:

Mass balance

During the course of the study the mean material balance for the irradiated samples ranged between 100.1 - 102.5 % of the total applied radioactivity (AR) (triazole label) and 94.3 - 103.6 % AR (phenyl label). The mean material balance for the dark control samples ranged between 100.2 -106.5 % AR (triazole label) and 99.8 - 104.4 % AR (phenyl label). Less than 1 % AR was found as volatile radioactivity for both labels, all of which was identified as $^{14}CO_2$.

Findings

Triticonazole degraded photolytically with the major photo-degradation pathway involving isomerization of triticonazole to its Z-isomer (RPA 406203). The minor degradation pathway involved hydroxylation at various positions of triticonazole (parent) and the Z-isomer and further oxidation of these hydroxylated derivatives to corresponding carbonyl compounds.

The distribution of radioactivity in the test solutions is summarized in the tables below. In the irradiation experiment using both labels, a large number of radioactive residues was observed but triticonazole and the Z-isomer were the only components > 5 % AR. The test item triticonazole decreased with time while the Z-isomer (RPA 406203) first increased and started declining after about 48 hours of irradiation. All other degradation products were minor (none > 5 % TAR).

Table B. 8.1.4.1.2-4: Distribution of radioactivity in irradiated and dark samples of ^{14}C-phenyl-labelled-triticonazole in aqueous *p*H 5 buffer solution; mean of two replicates (% AR, numbers shaded in grey exceed 10 % AR)

Peak name	Sampling time (hrs)								
T_R (min)	0	8	24	48	72	168	240	360	408
Phenyl label – irradiated samples									
Peak 1	n.d.	n.d.	n.d.	n.d.	n.d.	0.7	0.9	1.9	1.7
Peak 2	n.d.	n.d.	n.d.	n.d.	n.d.	1.4	2.0	2.9	2.9
Peak 3	n.d.	n.d.	n.d.	n.d.	n.d.	1.0	1.4	2.1	2.2
Peak 4	n.d.	n.d.	n.d.	n.d.	n.d.	0.7	1.0	2.7	2.7
Peak 5	n.d.	n.d.	n.d.	n.d.	n.d.	1.1	1.1	1.5	1.5
Triticonazole	100.0	70.7	62.9	61.2	61.0	56.0	54.7	51.1	47.0
RPA 406203 (Z-isomer)	1.1	30.5	40.7	40.2	40.1	36.2	34.2	30.9	27.8
Others[(a)]	n.d.	n.d.	n.d.	0.9	n.d.	3.7	3.8	8.1	8.6
Phenyl label – dark samples									
Triticonazole	100.0	102.8	101.0	100.2	101.3	98.2	98.9	98.4	96.0
RPA 406203 (Z-isomer)	1.1	1.6	1.2	0.8	1.5	1.6	1.4	1.5	1.7
Others	n.d.	n.d.	n.d.	n.d.	n.d.	0.8	n.d.	n.d.	2.1

n.d. = not detected

(a) Sum of multiple components, none of them more than 2 % AR

Table B. 8.1.4.1.2-5: Distribution of radioactivity in irradiated and dark samples of ^{14}C-triazole labelled-triticonazole in aqueous *p*H 5 buffer solution; mean of two replicates (% AR, numbers shaded in grey exceed 10 % AR)

Peak name	Sampling time (hrs)								
T_R (min)	0	19	24	48	72	168	240	336	408
Triazole label - irradiated samples									
Peak 1[(a)]	n.d.	n.d.	n.d.	n.d.	1.9	5.0	7.9	11.9	16.3
Peak 2	n.d.	n.d.	n.d.	n.d.	n.d.	1.3	2.2	3.6	4.3
Peak 3	n.d.	n.d.	n.d.	n.d.	n.d.	0.8	1.5	2.1	2.5
Peak 4	n.d.	n.d.	n.d.	n.d.	n.d.	1.5	2.1	2.6	3.4
Peak 5	n.d.	n.d.	n.d.	n.d.	n.d.	0.8	0.6	1.9	1.9
Triticonazole	99.2	61.1	60.9	61.2	60.0	53.7	49.6	43.9	41.2
RPA 406203 (Z-isomer)	1.0	39.0	39.5	40.0	38.9	33.9	32.1	27.6	26.4

Others[(b)]	n.d.	n.d.	n.d.	n.d.	0.8	4.2	4.7	7.1	6.7
Triazole label – dark samples									
Triticonazole	99.2	105.4	100.0	101.0	100.9	100.5	100.7	99.8	100.1
RPA 406203 (Z-isomer)	1.0	1.1	1.2	1.1	1.2	1.3	1.2	1.3	1.2

n.d. = not detected
(a) Peak 1 is a mixture of several products (n > 6, no individual compound > 5 %)
(b) Sum of multiple components, none of them more than 2 % AR

Considering that photolytic conversion of ^{14}C-triticonazole (E-isomer) to the Z-isomer is reversible and that pseudo equilibrium is established, the aqueous photolysis of ^{14}C-triticonazole was well described by a SFO kinetic model (using the software ModelMaker 4.0). The photochemical degradation trigger endpoints in aqueous *p*H 5 buffer solution are presented in the table below.

Table B. 8.1.4.1.2-6: Triticonazole photochemical degradation trigger endpoints in aqueous *p*H 5 buffer solution

Substance	Parameter estimates ± standard error[(a)]	χ^2 error (%)	r^2	t-test	*DT50* (hrs)	*DT90* (hrs)
Triticonazole	$M_0 = 102.23 \pm 0.54751$ $k = 0.074232 \pm 0.004914$	2.80	0.973	$p < 0.001$	9.34	31.0
RPA 406203 (Z-isomer)	$C_1 = 0.98197 \pm 0.0012318$ $k = 0.11662 \pm 0.008152$	3.47	0.981	$p < 0.001$	5.94	19.7

(a) Units: M_0 (% AR); k (d^{-1})

Given the reversible process, ^{14}C-triticonazole is being reformed concurrently with its loss.

Conclusion:

The major photo-degradation pathway for triticonazole in irradiated aqueous buffer solutions involved reversible isomerization of the E-isomer (parent triticonazole) to its Z-isomer (RPA 406203). All other degradation products were minor (none > 5 % AR).

The *DT50* and *DT90* values for the degradation of triticonazole were 9.3 and 31.0 hours, respectively, considering that photolytic conversion is reversible. Therefore, the *DT50* value is short compared to the graphical time at which 50 % of the initial amount remains (about 250 hours). The *DT50* and *DT90* values for the degradation of the Z-isomer (RPA 406203) were 5.9 and 19.7 hours, respectively.

Comments (RMS AT):

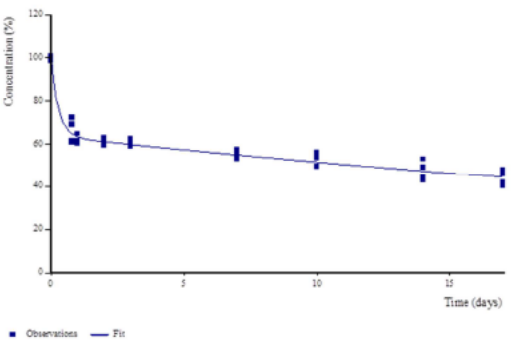
- The study broadly follows OECD guideline 316 and is considered reliable. However, with an incubation temperature of 22 ± 2 °C the study was somewhat cooler than recommended by OECD guideline 316 (25 ± 2 °C).
- Similar to Corgier & Robin (1992), the RMS AT considers the multi-compartment pathway fit with a reversible transformation from triticonazole to RPA 406203 (Z-isomer) overly complex. This is particularly true as this approach leads to fairly short degradation rates when compared to overall dissipation of both substances. From a regulatory point of view (trigger evaluation) the RMS AT recommends to stay with dissipation rates only, for both, triticonazole and RPA 406203 (Z-isomer) (see results below). Once equilibrium is reached (by 1 to 2 days in this experiment), triticonazole dissipated with a *DT50* of 32.7 days (i.e. DFOP slow phase), whereas RPA 406203 (Z-isomer) appeared to dissipate slightly faster (*DT50* of 27.6 days), which in principal should not be the case considering steady equilibrium between these two compounds.

Table B. 8.1.4.1.2-7: Dissipation rates of triticonazole and RPA 406203 (Z-isomer) under conditions of aquatic photolysis - RMS AT assessment

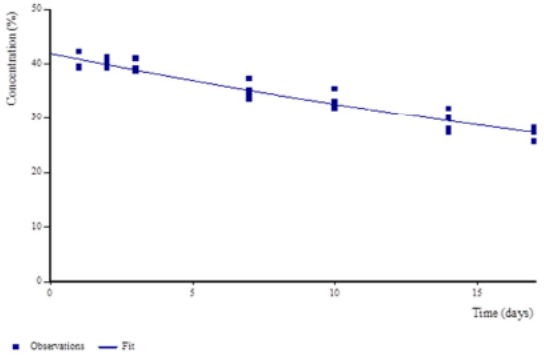
Substance	Model	Para-meter	Value	Confidence interval (95 %) Lower	Upper	p > t	χ^2 err. (%)	*Total DT50* (d)	*Total DT90* (d)	*Slow phase DT50 (d)*
Triticonazole	DFOP	k1	3.52	1.42	5.62	< 0.01	1.1	11.7	87.6	32.7

		k2	0.02	0.02	0.03	< 0.01				
		g	0.36	0.33	0.39	na				
RPA 406203 (Z-isomer)	SFO (Decline fit)	k	0.025	0.022	0.028	< 0.01	1.1	27.6	91.5	na

Table B. 8.1.4.1.2-8: Dissipation rates of triticonazole and RPA 406203 (Z-isomer) under conditions of aquatic photolysis (fits) - RMS AT assessment



Triticonazole - DFOP model



RPA 406203 (Z-isomer) - decline fit (SFO model)

B.8.2.1.3. Indirect photochemical degradation

The indirect photochemical degradation of triticonazole was not investigated. Under irradiated conditions, triticonazole is converted to RPA 406203 (Z-isomer) and furthermore to numerous minor metabolites (all < 10 % AR), including carbon dioxide. The photolytic conversion to RPA 406203 (Z-isomer) is considered to be reversible since equilibrium with the parent compound triticonazole was established within 1 to 2 days under laboratory conditions. Under laboratory conditions the *DT50* values for the dissipation of triticonazole obtained in two independent studies were 7.4 and 32.7 days, respectively, once equilibrium has been reached. The *DT50* value for the dissipation of the Z-isomer (RPA 406203) was 27.6 days.

B.8.2.2. Route and rate of biological degradation in aquatic systems

B.8.2.2.1. 'Ready biodegradability'

Studies submitted for first Annex I inclusion:

- **Handley & Horton (1992)**, investigating technical triticonazole

No new study was submitted.

Reference:	**Assessment of the ready biodegradability (modified Sturm Test) of RPA 400727**
Author(s), year:	Handley, J. W., Horton, M. R., 1992
Report/Doc. Number:	R013073, 430264, 282/321
Guideline(s):	OECD 301B (1981)
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

Triticonazole (called RPA 400727 in the report) was applied at concentrations of 10 and 20 mg/l to test flasks containing activated sludge. The flasks were incubated in darkness at 21 ± 1 °C for 28 days. CO_2 was trapped with NaOH. One control consisted of culture medium and inoculum. Sodium benzoate (20 mg/l) was added to the second control as a standard. Samples were taken on days 0, 1, 2, 3, 6, 8, 10, 14, 16, 21, 23, 27 and 28 and analysed by means of a carbon analyser 'Ionics 555 TOC analyser'.

Findings:

The *p*H values of the test material, standard material and control cultures on day 27 were 5.6 (10 mg/l), 5.7 (20 mg/l), 5.4 (standard) and 5.3 (control). Sodium benzoate attained 86 % degradation after 28 d thereby confirming the suitability of the inoculum and test medium. Triticonazole was not degraded until the end of test.

Conclusion:

Triticonazole is not ready biodegradable.

Comments (RMS AT):

- The study follows OECD guideline 301B and is still considered reliable.

B.8.2.2.2. Aerobic mineralisation in surface water

This type of study is a new data requirement according to Commission Regulation (EU) No. 283/2013 and was, therefore, not addressed within the former Annex I inclusion dossier. A new study (**Adam, 2014a**) was performed which is summarized below.

Reference:	**^{14}C-Triticonazole (BAS 595 F): Aerobic mineralisation in surface water - Simulation biodegradation test**
Author(s), year:	Adam, D., 2014
Report/Doc. Number:	2014/1083345
Guideline(s):	OECD 309 (April 2004), SANCO 11802/2010/ rev.7 amending EC 1107/2009

GLP:	Yes
Validity:	Yes
Status:	**New submission**

Material and methods:

Test material

[Phenyl-U-^{14}C]-triticonazole (BAS 595 F)

Reg. No.:	4378513
Lot/Batch number:	866-1501
Molecular Weight:	317.82 g/mol (non-labelled)
Site of radiocarbon labelling:	Phenyl-U-^{14}C
Radiochemical purity:	99.4 % (96.6 % determined before use)
Specific activity of ai:	5.86 MBq/mg

[Triazole-3(5)-^{14}C]-triticonazole (BAS 595 F)

Reg. No.:	4378513
Lot/Batch number:	867-1401
Molecular Weight:	317.82 g/mol (non-labelled)
Site of radiocarbon labelling:	triazole-3(5)-^{14}C
Radiochemical purity:	98.8 % (97.5 % determined before use)
Specific activity of ai:	6.44 MBq/mg

Reference material

[Phenyl-U-^{14}C]-benzoic acid

Lot/Batch number:	121214
Molecular Weight:	122.12 g/mol
Site of radiocarbon labelling:	phenyl-U-^{14}C
Radiochemical purity:	> 99 %
Specific activity of ai:	37.87 MBq/mg

Water

Water was freshly sampled from a pond in Rheinfelden, Switzerland. The sampling location was in an area not subject to effluent discharges and removed from human activity. The water was sampled from the surface and filtered with a 0.1 mm sieve and then transported to IES Ltd in sealed containers. The water was stored at about 4 °C in an open container under aerated conditions in the dark for one day until use. Physicochemical characteristics of the test water are presented in the tables below.

Table B. 8.1.4.1.2-1: Pond water characteristics

Origin		**Fröschweiher, Rheinfelden, Switzerland N47°543495 / E07°817899**
Sampling date		22 May 2014
Water parameters measured at field sampling		
Temperature	[°C]	19.2
*p*H		8.02
Oxygen concentration	[mg/L]	8.83
Redox potential (E_h)	[mV]	236
Sampling depth	[cm]	On the surface (5 – 10 cm)
Water parameters measured post-handling		
DOC	[mg/L]	8.18
Nitrate	[mg/L]	1.57
Nitrite	[mg/L]	< 0.82
Ammonium	[mg/L]	0.45
N total	[mg/L]	2.65
P total	[mg/L]	0.39

Test system

Each test system consisted of an open gas-flow-system with 350 mL Erlenmeyer glass flasks, containing 100 mL of natural pond water. For the high dose experiment, concentrations of 0.093 and 0.084 mg/L were assayed in

[phenyl-U-^{14}C]- and [triazole-3(5)-^{14}C]-triticonazole treated systems, respectively. Additionally, single test systems of the high dose experiments of the phenyl label were incubated under sterile conditions to get information about abiotic degradability of the test item. For the low dose experiment, concentrations of 0.008 and 0.009 mg/L were assayed in [phenyl-U-^{14}C]- and [triazole-3(5)-^{14}C]-triticonazole treated systems, respectively.

Treated and untreated test systems (two non-sterile and one sterile) were incubated in the dark for up to 59 days at 21.2 ± 0.2 °C. The test systems were continuously flushed with moistened CO_2-free air, and volatiles were collected in a series of trapping solutions (ethylene glycol and NaOH). The samples were continuously and gently stirred to maintain particles and microorganisms in suspension.

The microbial activity of the test system was assessed by using the same experimental set-up and monitoring the degradation of [^{14}C-U]-benzoic acid in duplicate samples.

Sampling
Duplicate water samples per label and test concentration were taken for analysis 0, 1, 3, 8, 14, 31 and 59 days after treatment (DAT). Radioactivity in the trapping solutions was also monitored by LSC and solutions were exchanged after 36 days. Single samples were taken for the sterile experiment of [phenyl-U-^{14}C]-triticonazole at DAT 0, 1, 3, 8, 14, 31, 59. Duplicate water samples of [^{14}C-U]-benzoic acid were sampled at 0, 7 and 14 DAT.

Analytical procedures
At each sampling time, *p*H and oxygen concentration were measured, the water phase volume recorded and the radioactivity present analysed by LSC. Subsequently, an aliquot of the water phase of each sample was concentrated by rotary evaporation, re-analysed by LSC and later on submitted to HPLC analysis. Selected samples were additionally analysed by TLC in order to confirm the HPLC results. Furthermore, the stability of the enantiomeric ratio of triticonazole was checked in selected samples collected at DAT 0 and 59 using a chiral HPLC method.

Radioactivity in the volatile trapping solutions was monitored by LSC, and solutions were exchanged after 36 days. Prior to measuring the radioactivity, the volume of liquid in each ethylene glycol and sodium hydroxide trap was recorded.

Aliquots (1 mL) of the samples treated with [phenyl-U-^{14}C]-benzoic acid were directly analysed by LSC and submitted for HPLC analysis in order to obtain the remaining concentration of benzoic acid in the test system. Additionally, to determine the associated amounts of dissolved radioactive carbon dioxide and volatile radioactivity, duplicate aliquots were removed from the trapping solutions.

For the LSC analysis of the water samples, the limit of detection (LOD) was 0.093 and 1.063 % AR for the high and low dosed samples, respectively. The limit of quantification (LOQ) was 0.139 and 1.594 % TAR in the high and low dosed samples, respectively.

For the HPLC analysis of the water samples, LOD was 0.690 and 0.780 % TAR for the high and low dosed samples, respectively. LOQ was 1.380 and 1.560 % TAR in the high and low dosed samples, respectively.

Calculation of DT50 and DT90 values
As the test item was stable under all conditions in all test systems, the calculation of meaningful *DT50* and *DT90* values was not possible. Therefore, there was no kinetics component to this study.

Findings:

The degradation of the reference item [phenyl-U-^{14}C]-benzoic acid confirmed that the test systems are microbially active.

Mass balance
In the tested systems, the total mean recoveries ranged from 96.1 ± 2.3 to 102.4 ± 2.8 % AR. Volatiles represented less than 3.1 % AR in either of the treated systems, regardless of dosage level. The material balance and the distribution of radioactivity in the systems treated with [phenyl-U-^{14}C]-triticonazole and [triazole-3(5)-^{14}C]-triticonazole are presented in the tables below.

Table B. 8.1.4.1.2-2: Material balance and distribution of radioactivity after application of [phenyl-U-^{14}C]-triticonazole (% AR)

DAT	Aqueous phase (% AR)	Volatiles (% AR)		Recovery (% AR)
		$^{14}CO_2$	Other ^{14}C-volatiles	
Test systems – low dose (mean values)				
0	102.0	na	na	102.0
1	98.8	< 0.1	< LOQ	98.9
3	98.4	< 0.1	< LOQ	98.5
8	101.2	< 0.1	< LOQ	101.3
14	99.6	< 0.1	< LOQ	99.6
31	100.7	< 0.1	< LOQ	100.8
59	97.0	3.1	1.3	101.4
			Mean ± SD	**100.4 ± 1.8**
Test systems – high dose (mean values)				
0	102.0	na	na	102.0
1	99.5	< 0.1	< 0.1	99.5
3	101.0	< 0.1	< 0.1	101.1
8	102.1	< 0.1	< 0.1	102.2
14	101.8	0.3	< 0.1	102.2
31	100.7	0.1	< 0.1	100.9
59	96.0	1.0	< 0.1	97.0
			Mean ± SD	**100.7 ± 2.0**
Sterile samples – high dose (single values)				
0	108.2	na	na	108.2
1	99.5	< 0.1	< 0.1	99.5
3	100.8	< 0.1	< 0.1	100.9
8	102.9	< 0.1	< 0.1	102.9
14	101.0	< 0.1	0.2	101.3
31	101.0	< 0.1	0.2	101.3
59	102.5	< 0.1	< 0.1	102.6
			Mean ± SD	**102.4 ± 2.8**

na denoted not applicable
SD = Standard deviation
LOQ = Limit of quantification

Table B. 8.1.4.1.2-3: Material balance and distribution of radioactivity (LSC) after application of [triazole-3(5)-^{14}C]-triticonazole (% AR)

DAT	Aqueous phase (% AR)	Volatiles (% AR)		Recovery (% AR)
		$^{14}CO_2$	Other ^{14}C-volatiles	
Test systems – low dose (mean values)				
0	102.5	na	na	102.5
1	99.2	< 0.1	< 0.1	99.3
3	97.9	< 0.1	< 0.1	98.3
8	100.8	< 0.1	< 0.1	100.8
14	105.1	< 0.1	< 0.1	105.6
31	99.9	< 0.1	< 0.1	100.4
59	102.3	< 0.1	< 0.1	102.7
			Mean ± SD	**101.4 ± 3.7**
Test systems – high dose (mean values)				
0	99.1	na	na	99.1
1	98.5	< 0.1	< 0.1	98.5
3	93.6	< 0.1	< 0.1	93.6
8	96.6	< 0.1	< 0.1	96.6
14	95.6	< 0.1	< 0.1	95.7
31	95.4	0.2	< 0.1	95.6
59	93.5	0.3	< 0.1	93.8
			Mean ± SD	**96.1 ± 2.3**

na denoted not applicable
SD = Standard deviation

The amounts of triticonazole and its metabolites recovered at each sampling time in the viable test systems are presented in the tables below. Results showed that triticonazole remained stable throughout the study and that all

metabolites are classified as minor (each ≤ 4.3 % AR). In the high dose sterile system, the parent was also stable (102.5 % at DAT 59).

MI, M2 and M3 had the same elution time on HPLC as the standards RPA 406203 (Z-isomer), RPA 404766 (Cis-diol) and RPA 406341 (Trans-diol), respectively, while the others remained unknown. As all fractions were classified as minor metabolites, none of them were identified or characterised further. There were no metabolites detected in the high dose sterile system.

Table B. 8.1.4.1.2-4: Pattern of degradation and formation of metabolites after application of [phenyl-U-^{14}C]-triticonazole (% AR)

Compound	Incubation time (days)						
	0	1	3	8	14	31	59
Test systems – low dose							
Triticonazole	97.9	98.8	96.0	100.2	96.9	79.1	94.4
M1 (RPA 406203, Z-isomer)	4.1	n.d.	2.4	1.0	2.7	1.9	2.6
M2 (RPA 404766, Cis-diol))	n.d.	n.d.	n.d.	n.d.	n.d.	1.3	n.d.
M3 (RPA 406341, Trans-diol)	n.d.	n.d.	n.d.	n.d.	n.d.	1.8	n.d.
M4	n.d.	n.d.	n.d.	n.d.	n.d.	2.2	n.d.
M6	n.d.	n.d.	n.d.	n.d.	n.d.	1.1	n.d.
M7	n.d.	n.d.	n.d.	n.d.	n.d.	1.5	n.d.
M8	n.d.	n.d.	n.d.	n.d.	n.d.	1.6	n.d.
M9	n.d.	n.d.	n.d.	n.d.	n.d.	2.6	n.d.
M10	n.d.	n.d.	n.d.	n.d.	n.d.	3.9	n.d.
M11	n.d.	n.d.	n.d.	n.d.	n.d.	3.7	n.d.
Test systems – high dose							
Triticonazole	102.0	99.5	101.0	99.5	99.4	98.2	94.4
M1 (RPA 406203, Z-isomer)	n.d.	n.d.	n.d.	2.6	n.d.	n.d.	1.6
M4	n.d.	n.d.	n.d.	n.d.	2.3	1.1	n.d.
M5	n.d.	n.d.	n.d.	n.d.	n.d.	1.4	n.d.

n.d. not detected

Table B. 8.1.4.1.2-5: Pattern of degradation and formation of metabolites after application of [triazole-3(5)-^{14}C]-triticonazole (% AR)

Compound	Incubation time (days)						
	0	1	3	8	14	31	59
Test systems – low dose							
Triticonazole	98.2	98.3	96.1	100.8	103.0	95.3	99.9
M1 (RPA 406203, Z-isomer)	4.3	0.9	1.8	n.d.	2.1	n.d.	2.4
M4	n.d.	n.d.	n.d.	n.d.	n.d.	2.6	n.d.
M8	n.d.	n.d.	n.d.	n.d.	n.d.	2.0	n.d.
Test systems – high dose							
Triticonazole	99.1	98.5	93.6	95.5	95.6	92.8	92.4
M1 (RPA 406203, Z-isomer)	n.d.	n.d.	n.d.	1.1	n.d.	n.d.	1.1
M4	n.d.	n.d.	n.d.	n.d.	n.d.	2.5	n.d.

n.d. not detected

Isomerization

Results of chiral-HPLC analysis of treated systems taken at 0 DAT and 59 DAT showed that the ratio between the R and S enantiomers of [phenyl-U-^{14}C]-triticonazole remained stable at approximately 1:1 throughout the study.

Conclusion:

In conclusion, [^{14}C]-triticonazole, regardless of its concentration and ^{14}C-label position, remained stable and degraded in neither biotic nor abiotic surface water systems. Additionally, the enantiomeric ratio of [^{14}C]-triticonazole remained stable throughout the entire incubation period. The stable nature of the test item precluded the use of kinetics and thus the determination of meaningful *DT50* and *DT90* values was not possible.

Comments (RMS AT):

- The study follows OECD guideline 309 and is considered reliable.

B.8.2.2.3. Water/sediment studies

Studies submitted for first Annex I inclusion:

- **Wyss-Benz (1995)**, investigating phenyl labelled triticonazole in two water/sediment systems

New kinetic assessment study provided:

- **Jarvis & Montesano (2014)**, re-evaluating the degradation/dissipation kinetics of triticonazole in Wyss-Benz (1995)

Reference:	**^{14}C-RPA 400727: Degradation and metabolism in aerobic aquatic systems**
Author(s), year:	Wyss-Benz, M., 1995
Report/Doc. Number:	R012987
Guideline(s):	BBA Part IV, 5-1 (1990)
GLP:	Yes
Validity:	Yes
Status:	**Already submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The aerobic metabolism and degradation of [phenyl-U-^{14}C]-triticonazole (called RPA 400727 in the report) was studied in two different water sediment systems. The two sediments and the adjacent waters originated from the river Rhine and from a pond (Anwil). 260 g wet weight of river sediment, 200 g wet weight of pond sediment and 520 ml of river and pond water were filled into one litre test flasks. After 5 weeks of acclimatisation at 20 ± 2 °C in the dark, 0.0683 mg ^{14}C-triticonazole was added to the test vessels (corresponding to 205 g ai/ha).

The flasks were aerated with CO_2 free and moistened air and the water surface was gently stirred without disturbing the sediment. Duplicate flasks were removed for analysis on 0, 6, 24 and 48 hours, 7, 14, 28, 63 and 105 days of the incubation period. The water was partitioned twice with ethyl acetate prior to analysis by LSC, TLC and HPLC. The remaining sediment was extracted with acetonitrile and acetonitrile/water (8:2). Radioactivity of the extracts was measured by LSC and the compounds identified by TLC and HPLC. The distribution of sediment residues between humin, humic and fulvic acids were determined for the samples taken at day 105. Volatiles were trapped with NaOH and ethylene glycol. The NaOH traps and ethylene glycol traps were monitored for radioactivity by LSC at the respective sampling interval or every second week, whichever was shorter.

Table B. 8.1.4.1.2-1: Physical and chemical properties of the two test systems

Compartment	Parameter	Location	
		System 1: River, Rhine, Mumpf, AG, Switzerland	System 2: Pond, Anwil, BL, Switzerland
Water	Temperature[(a)]	10.1	12.4
	*p*H[(a)]	7.7	8.04
	O_2-concentration (mg/l)[(a)]	11.3	15.5
	Total hardness (°dH)[(a)]	18	22
	Total organic carbon (mg/l)	2.7	2.9
	Total nitrogen (mg/l)	2.3	3.8
	Total phosphorous (mg/l)	0.1	0.07
Sediment	*p*H (KCl)	6.89	6.85
	C_{org} [g C/100 g dry soil]	1.13	1.41

Total nitrogen (g/kg sediment)	0.332	0.099
Total phosphorus (g/kg sediment)	0.229	0.375
Redox potential [mV]	-200	-165
Cation exchange capacity [mVal/100 g dry soil]	8.3	23.4
Microbial biomass [mg C/100g]	127.12	128.35
Texture / particle size distribution:	Loamy sand	Clay loam
sand [%]	74.4	21.1
silt [%]	20	50.4
clay [%]	5.6	28.5

(a) Parameters determined at sampling site, 5 cm above sediment surface

Findings:

Table B. 8.1.4.1.2-2: Radioactivity distribution, partitioning and balance (% AR, mean values) during the degradation in water- and sediment phase within the 'River Rhine' and 'Pond Anwil' system

DAT	Water	Sediment extract	NER	CO_2	Total	Triticonazole water	Triticonazole sed.	W1-W3	S1-S3
					'River Rhine'				
0	95.1	3.2	0.5	np	98.8	94.4	3.2	nd	nd
6 hrs	95.4	3.4	0.5	< 0.1	99.3	94.6	3.4	nd	nd
1	86.3	12.0	3.1	< 0.1	101.3	86.1	11.9	nd	< 0.1
2	60.2	36.9	2.8	< 0.1	99.9	60.0	34.4	nd	2.5
7	46.7	50.2	3.3	0.1	100.3	46.1	50.2	nd	nd
14	32.0	60.4	4.8	0.2	97.4	31.6	59.4	nd	1.0
28	20.4	73.3	7.3	0.4	101.3	19.4	71.9	0.3	1.3
63	14.5	77.4	9.7	0.7	102.3	12.8	76.0	0.7	1.4
105	10.7	73.1	14.5	1.7	99.9	8.9	70.9	0.6	2.1
					'Pond Anwil'				
0	99.3	1.3	0.2	np	108.8	98.8	1.3	nd	nd
6 hrs	96.6	2.3	0.3	< 0.1	99.1	95.9	2.3	nd	nd
1	90.4	8.5	1.2	< 0.1	100.1	90.2	8.3	nd	0.2
2	75.5	22.3	1.9	< 0.1	99.6	75.2	22.3	nd	nd
7	56.7	39.2	4.0	< 0.1	99.8	56.4	38.9	nd	0.2
14	44.4	52.9	6.9	0.1	104.2	44.1	51.8	nd	1.0
28	27.3	62.0	12.9	0.1	102.2	25.7	60.0	1.1	1.9
63	17.7	68.1	17.2	0.4	103.2	16.0	66.6	1.1	1.5
105	12.4	63.4	25.0	1.3	102.1	10.2	61.2	1.4	2.2

np denotes not performed
nd denotes not detected
W1-W3: Sum of three unknown radioactive fractions in the water phase
S1-S3: Sum of three unknown radioactive fractions in the sediment phase

The active substance behaved similar in both systems. It can be concluded that triticonazole was removed from the water phase and shifted towards the sediment phase.

Mineralization and degradation of triticonazole was very slow. Only 1.7 and 1.3 % CO_2 evolved after 105 days of incubation. Three unknown radioactive fractions were found in the water and the sediment phase. On individual basis these components did not exceed levels of 2.5 % AR ('Rhine River') and 1.8 % AR ('Pond Anwil') of applied radioactivity at any time of the test. The proportion of radioactivity bound to humin, humic and fulvic acid were 2.6, 0.9 and 2.1 for 'Rhine River' and 6.3, 1.2 and 3.7 for 'Pond Anwil'.

Conclusion:

Three unknown radioactive components were detected in both the water phases and the sediments. Any single component accounted for no more than 2.5 % AR for the river system and for no more than 1.8 % AR for the pond system (total system).

Comments RMS AT:

- The study broadly follows OECD guideline 308 with some limitations:

- The two water/sediment systems are very close with respect to organic carbon as well as water and sediment *p*H. However, as degradation of triticonazole in (dark) aquatic systems is anyhow limited, the impact of more acidic *p*H values or higher organic carbon is not considered to lead to significantly different results.
- The study was conducted of with the phenyl label only. In light of the limited degradation of triticonazole observed in these systems, no further information can be gained applying a different label.
- With an application rate of 205 g ai/ha the study is clearly overdosed (intended use rate is 12.5 g/ha)

On overall the study is still considered reliable.

- The study was kinetically re-assessed by Jarvis & Montesano (2014d).

Reference:	**Recalculation of Triticonazole water sediment study kinetics according to FOCUS (2006) Guidance**
Author(s), year:	Jarvis, T. J., Montesano, V., 2014b
Report/Doc. Number:	2014/1083346BBA
Guideline(s):	FOCUS Kinetics (2006)
GLP:	Not applicable (modelling study)
Validity:	Yes
Status:	**New submission**

Material and methods:

One water/sediment study with two systems (river and pond) was considered in which the parent triticonazole was applied (Wyss-Benz, 1995). Residues of triticonazole in water and sediment (in percentage of applied) were obtained from the water/sediment study and used as input for the kinetic evaluation. Analytical data used for the kinetic evaluation are presented in the table below.

Table B. 8.1.4.1.2-3: Analytical results for triticonazole degradation (percentage of applied) in water sediment systems (Wyss-Benz, 1995)

DAT	River system			Pond system		
	Water phase	Sediment phase	Whole system	Water phase	Sediment phase	Whole system
0	95.0	2.0	97.0	97.1	1.4	98.5
0	93.8	4.3	98.1	100.4	1.1	101.5
0.25	92.9	4.7	97.6	95.4	1.8	97.2
0.25	96.2	2.1	98.3	96.3	2.7	99.0
1	85.4	12.2	97.6	90.2	7.4	97.6
1	86.8	11.6	98.4	90.2	9.3	99.5
2	58.9	34.6	93.5	75.6	22.0	97.6
2	61.0	34.1	95.1	74.8	22.5	97.3
7	48.4	47.7	96.1	57.0	37.8	94.8
7	43.7	52.7	96.4	55.8	40.0	95.8
14	35.6	55.7	91.3	42.7	52.5	95.2
14	27.5	63.1	90.6	45.5	51.2	96.7
28	24.8	69.1	93.9	24.0	62.1	86.2
28	14.1	74.8	88.9	27.3	58.0	85.3
63	14.0	73.2	87.3	15.8	65.2	81.0
63	11.6	78.7	90.3	16.1	68.0	84.1
105	9.1	70.2	79.3	10.0	62.4	72.4
105	8.7	71.7	80.3	10.4	59.9	70.3

The simulation modelling was performed using KinGui Version 2. Dissipation and degradation rates of triticonazole at level P-I were derived. P-II approaches were not considered. Comparing the rapid dissipation rate

of triticonazole from the water phase to its slower degradation in the whole system it can be expected that the P-II level fit would not result in significant degradation rates.

Findings:

The evaluation of the water/sediment study showed that the FOMC model provided the best fit for dissipation in the water phase while SFO was chosen for degradation in the whole system. No endpoints could be derived for the sediment phase. Results are valid as persistence and modelling endpoints and are presented in the table below:

Table 7.2.2.3-2: Degradation and Dissipation of Triticonazole in Water and Sediment

Study	System	Water phase			Total system		
		Kinetic model	*DissT50* (d)	*DissT90* (d)	Kinetic model	*DegT50* (d)	*DegT90* (d)
Wyss-Benz, 1995	River	FOMC	5.3	97.8	SFO	399	1325
	Pond	FOMC	9.5	125	SFO	225	748

Conclusion:

Degradation and dissipation of triticonazole in water and sediment was re-evaluated according to FOCUS (2006). Modelling endpoints for the parent were derived and can be used in environmental fate modelling. The same endpoints are also valid for use as persistence endpoints.

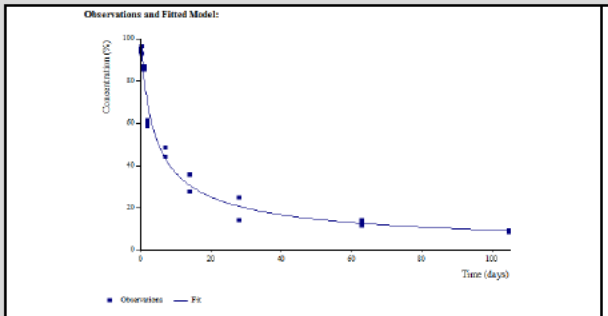
Comments (RMS AT):

- The RMS AT notes that in the Pond system residues observed at study end (water phase only) were slightly above 10 % AR, thus triggering the DFOP or HS model according to FOCUS degradation kinetics 2006 (EC, 2014). However, FOMC is considered indeed the best fit model for the water phase. Thus, FOMC is accepted for the pond system as well. Details on the applicant fits (accepted by the RMS AT) are given in the tables below.

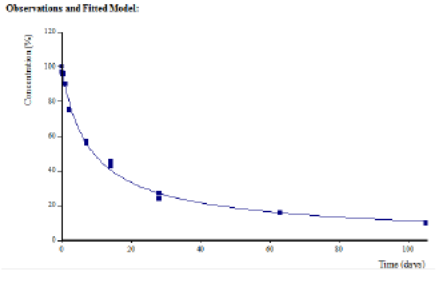
Table 7.2.2.3-2: Degradation and dissipation of triticonazole in water and sediment - applicant assessment (accepted by the RMS AT)

System	Compartment	Kinetic model	Parameter	*DT50* (d)	*DT90* (d)	χ^2 error (%)	p. > t
River	Water phase	FOMC	α = 0.637 β = 2.703	5.3	97.8	6.6	na
	Whole system	SFO	k = 0.00174	399	1325	1.5	< 0.001
Pond	Water phase	FOMC	α = 0.759 β = 6.353	9.5	125	3.3	na
	Whole system	SFO	k = 0.00308	225	748	1.6	< 0.001

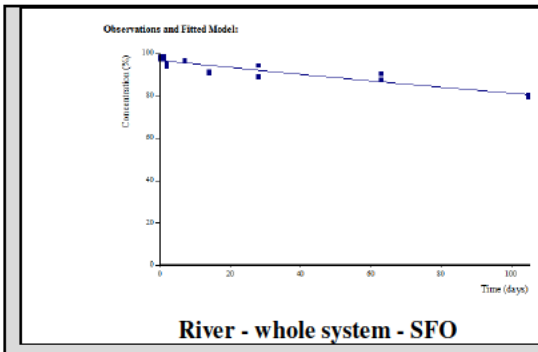
Table 7.2.2.3-2: Degradation and dissipation of triticonazole in water and sediment (fits) - applicant assessment (accepted by the RMS AT)



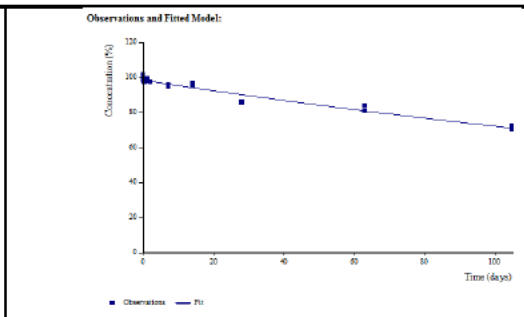
River - water phase - FOMC



Pond - water phase - FOMC



River - whole system - SFO



Pond - whole system - SFO

B.8.2.2.4. Irradiated water/sediment study

This type of study was not performed as it is not needed as a higher tier option.

B.8.2.3. Degradation in the saturated zone

As neither triticonazole, nor any of its soil metabolites are expected to constitute a leaching risk, no investigations on the fate of these compounds in the saturated zone are required.

B.8.2.4. Potential effects of water treatment processes

[The following statement was provided by the applicant]

Currently there is neither a guideline for testing the effect of water treatment on pesticides (or other chemicals) nor is there a risk assessment procedure. Since conditions of water treatment are extremely variable across Europe (different treatment methods and intensities used in different sequences on different types of raw waters) it is currently not possible to comprehensively assess the potential formation of harmful by-products during drinking water production. An experimental guideline is essential because the effect of ozonation or chlorination strongly depends on treatment conditions (e.g. duration, applied concentration, properties of the raw water) which should be representative for real water treatment plants.

In the absence of such guidance documents an evaluation was made based on knowledge on the chemistry of triticonazole and its degradation products and applying chemical principles.

Experimental data on the aerobic degradation of triticonazole in soil demonstrate that the main degradation pathway is hydroxylation to form the three major transformation products RPA 406341 (Trans diol), RPA 404766 (Cis-diol) and RPA 407922 as well as some minor hydroxylated metabolites. Subsequent degradation processes are a further hydroxylation to minor dihydroxylated metabolites, ring cleavage as well as the formation of bound residues and carbon dioxide. Triticonazole is hydrolytically stable at environmentally relevant *p*H values (*p*H 4 - 9) at 25 °C.

Neither triticonazole nor its metabolites contain any comparable aliphatic side chains as present in the chemical structure of tolylfluanid, which caused the problem of nitrosamine formation during water treatment for drinking water production. No N-nitrosamine formation is expected for triticonazole and its metabolites, since no secondary amine function is present. The only nitrogen-containing moiety is the electron-deficient heteroaromatic triazine ring, which is little prone to electrophilic attack of either ozone or NO+.

With chlorine-based treatments, chlorination or hydroxylation and the possible loss of substituted chlorinated and hydroxylated structures is conceivable. However, when chlorine enters water it reacts chemically with any organic matter found in the water. There is always some organic matter in natural waters and by-products of this reaction include e.g. trihalomethanes. Any potential harmful degradation products resulting from any organic matter in the water treatment process will be eliminated in subsequent clean-up steps by using e.g. activated carbon filtration or sand filter beds.

It is therefore highly unlikely that water treatment processes such as ozonation or chlorination will result in the formation of by-products that would require a detailed health risk assessment. Consequently, further information on the effect of water treatment processes on the nature of residues present in surface water and groundwater is not considered necessary.

Comments (RMS AT):

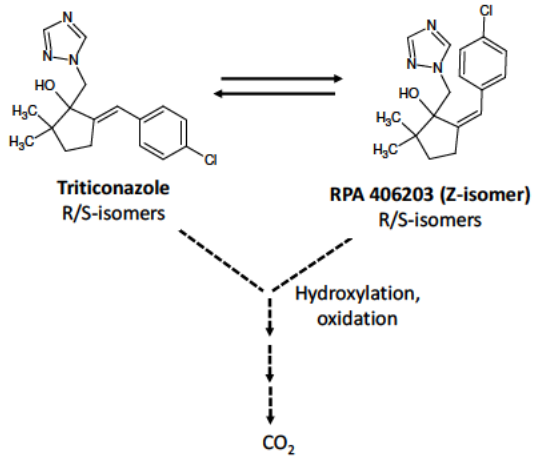
- The RMS AT largely agrees on the applicant's statement.

B.8.2.4.1. Summary on fate and behaviour in water and sediment (compiled by the RMS AT)

Triticonazole (phenyl and triazole label) is considered stable under conditions of **aquatic hydrolysis**. No isomeric conversation (from the *R* to the *S* enantiomer) could be observed.

Under conditions of **direct photochemical degradation** conducted in sterile buffer solutions at *p*H 5 triticonazole (phenyl and triazole label) is converted into its Z-isomer RPA 406203 (maximum 42.3 % AR after 3 days, without sensitizer). The photolytic conversion from triticonazole (E-isomer) to RPA 406203 (Z-isomer) is considered to be reversible since equilibrium with the parent compound triticonazole was established within 1 to 2 days. No other metabolites were observed > 5 % AR. Under laboratory conditions the *DT50* values for the dissipation of triticonazole obtained in two independent studies were 7.4 and 32.7 days, respectively, once equilibrium has been reached. The *DT50* value for the dissipation of RPA 406203 (Z-isomer) was 27.6 days.

Figure B.8.2.4.1-1: Proposed route of degradation of triticonazole under conditions of direct photochemical degradation



Triticonazole is considered **not ready biodegradable** under conditions of a CO_2 evolution (Modified Sturm) test.

Triticonazole (phenyl and triazole label) is considered stable under conditions of **aerobic mineralisation studies in surface water** (studied at low and high dose level). No metabolite fraction above 5 % AR was observed. Formation of CO_2 was limited with maximum 3.1 % AR at study end (59 days).

The fate and behaviour of phenyl labelled triticonazole in **aerobic water/sediment** was investigated in two water/sediment systems. The RMS AT notes that these two water/sediment systems are very close with respect to organic carbon as well as water and sediment *p*H. However, as degradation of triticonazole in (dark) aquatic systems is anyhow limited, the impact of more acidic *p*H values or higher organic carbon is not considered to significantly alter the study results. Degradation of triticonazole in the entire system was indeed limited with transfer to the sediment being representing the mayor dissipation process in the water phase. No individual metabolite fraction exceeded 5 % AR in the total system. Formation of CO_2 was limited with maximum 1.7 % AR at study end (105 days), NER accounted for maximum 25 % AR at study end. The RMS AT notes that water/sediment studies were conducted with phenyl labelled parent only. However, as degradation of triticonazole was limited in the water/sediments systems metabolites from the triazole label are not considered to occur at significant amounts.

Table B.8.2.4.1-1: Summary on maximum occurrence (% AR) of identified and non-identified (unknown) metabolites in aquatic laboratory studies conducted with triticonazole (metabolites shaded in grey require an exposure assessment in surface water)

Compound	Aquatic hydrolysis (25 °C)	Direct photolytic degradation	Aerobic mineralisation in surface water (low dose)	Water/sediment		
				Water phase	Sediment phase	Entire system
Triticonazole	na	na	na	na	76.0	na
RPA 404766 (Cis-diol)	ni	ns	1.3	ni	ni	ni
RPA 406341 (Trans-diol)	ni	ni	1.8	ni	ni	ni
RPA 406203 (Z-isomer)	2.6	42.3[(a)]	4.2[(b)]	ni	ni	ni
Unknowns	≤ 2	4.3	3.9	0.7	2.5	2.5

na denotes not applicable
ni denotes not investigated
ns denotes not stated
(a) Without sensitizer
(b) Arithmetic mean of phenyl and triazole label

The rate of degradation/dissipation of triticonazole in water/sediment systems is summarized below.

Table B.8.2.4.1-2: Summary on degradation and dissipation of triticonazole in the total water/sediment system as well as in the water and sediment phase (20 °C) - trigger & modelling endpoints

Water / sediment system	*p*H water / sed.[(a)]	Label	*DegT50* system (d)	*DegT90* system (d)	Kinetic model	*DissT50* water (d)	Kinetic model	*DissT50* sed. (d)	Kinetic model	Reference
Rhine River	7.7 / 6.9	Ph	399	1325	SFO	5.3	FOMC	-	-	Wyss-Benz, 1995
Anwil Pond	8.0 / 6.9	Ph	225	748	SFO	9.5	FOMC	-	-	
Geometric mean (n = 2)			**300**	**996**	SFO	**-**		**-**		

(a) Measured in KCl (sediment phase)

B.8.3. FATE AND BEHAVIOUR IN AIR

B.8.3.1. Route and rate of degradation in air

Studies submitted for first Annex I inclusion:

- **Voelkel (1999)** investigating triticonazole

No new studies submitted.

Reference:	**Estimation of the degradation of triticonazole by photo-oxidation in air**
Author(s), year:	Voelkel, W., 1999
Report/Doc. Number:	R012052 / 202492 / 751983
Guideline(s):	94/37/EC (of 22 July 1994) Point 2.10
GLP:	Yes
Validity:	Yes
Status:	**Previously submitted**

[The following study report is a copy/paste of the original text in the DAR for Annex I inclusion slightly modified in order to meet editorial settings and to improve readability]

Material and methods:

The rate constant for the atmospheric reaction between photo-chemically produced hydroxyl radicals and triticonazole was estimated with the computer program AOPWIN. The estimated rate constants enabled the calculation of the atmospheric half-life of triticonazole based upon average atmospheric concentrations of hydroxyl radicals. An OH-concentration of 1.5×10^5 per cm^3 is used. Furthermore, the reaction rate for the reaction between ozone and the ethylene group of triticonazole was calculated. The program estimated an overall OH-radical reaction rate constant by summing individual OH-radical reaction pathways, which could be regarded to operate independently. The rate constants are estimated at 25°C.

Findings:

The rate constant for the H-atom abstraction was $k_{hydr} = 5.933 \times 10^{-12}$ cm^3 molecule-1 sec^{-1}. The most important individual rate constant was that of the hydrogen abstraction at the methylene group between cyclopentane and triazole ring. The rate constant for OH-radical addition to the ethylene group is $86\ 900 \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1}. This reaction rate constant is the most important of all individual reactions. The rate constant for the addition of OH-radicals to the aromatic ring was estimated to be 0.140×10^{-12} cm^3 $molecule^{-1}$ sec^{-1}. The rate constant for the reaction of OH radicals with the hydroxy group was estimated to be $k_{OH} = 0.140 \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1}.

The overall OH-radical reaction rate constant was the sum of the individual OH-radical reaction rate constants. For triticonazole, the overall rate constant resulted in $k_{OH} = 94.3628 \times 10^{-12}$ cm^3 $molecule^{-1}$ sec^{-1}. The overall reaction rate constant of triticonazole with ozone was estimated to be 13.650×10^{-17} cm^3 $molecule^{-1}$ sec^{-1}. The half-life of triticonazole was calculated as 0.084 days when the ozone concentration is considered as 7×10^{11} $molecules/cm^3$.

Conclusion:

The half-life of triticonazole was calculated as 0.113 days when a 12-hour day is considered and 0.057 days when a 24-hour day is considered.

Comments (RMS AT):

- Re-calculation with AOPWIN version 1.92 gave an atmospheric *DT50* of 0.114 days (12-hrs day, 1.5e6 OH/cm^3).

B.8.3.2. Transport via air

The transport of triticonazole via air was not studied since its vapour pressure is below the trigger values of 10^{-5} Pa (plants) and 10^{-4} Pa (soil).

B.8.3.3. Local and global effects

As triticonazole is not applied in high volumes, local and global effects are not expected. The long range transport of triticonazole can be disclosed due to the short atmospheric half-life of the substance.

B.8.4. DEFINITION OF THE RESIDUES

B.8.4.1. Definition of the residue for risk assessment

The residue definitions relevant for risk assessment for each compartment are the following:

Compartment	Residue Definition
Soil	Triticonazole, RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406203 (Z-isomer)[(a)], 'Met 6 (MWT 333)'[(b)], 'Met 7 (MWT 315)'[(b)]
Groundwater	Triticonazole, RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406203 (Z-isomer)[(a)], 'Met 6 (MWT 333)'[(b)], 'Met 7 (MWT 315)'[(b)]
Surface Water	Triticonazole, RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406203 (Z-isomer)[(c)], 'Met 6 (MWT 333)'[(b)], 'Met 7 (MWT 315)'[(b)]
Sediment	Triticonazole, RPA 406341 (Trans-diol), RPA 404766 (Cis-diol), RPA 406203 (Z-isomer)[(c)], 'Met 6 (MWT 333)'[(b)], 'Met 7 (MWT 315)'[(b)]
Air	Triticonazole

(a) RPA 406203 (Z-isomer) has to be included in the exposure assessment in case of spray applications only (exposure to irradiation at the soil surface)
(b) Metabolite fraction observed > 5 % AR at two consecutive sampling points in a legacy soil degradation study (Ayliffe & Austin, 1993)
(c) Above 10 % AR in aquatic photolysis

B.8.4.2. Definition of the residue for monitoring

Refer to the section on ecotoxicology.

B.8.5. MONITORING DATA CONCERNING FATE AND BEHAVIOUR OF THE ACTIVE SUBSTANCE, METABOLITES, DEGRADATION AND REACTION PRODUCTS

Publically available ground and surface water monitoring data as well as peer reviewed scientific literature were checked for analyses and findings of triticonazole. No data were found for the metabolites in either ground or surface water. Additional monitoring studies were not conducted.

Publically available groundwater monitoring data for triticonazole shows that, following application according to the label, the leaching of unacceptable amounts of triticonazole is highly unlikely. Additionally entry of unacceptable amounts of triticonazole into surface water is highly unlikely.

1. Publically available ground and surface water monitoring data

Data for triticonazole in ground water were found for France. Data for triticonazole in surface water were found for France, for the Czech Republic and for Italy. These data are summarized in Table 7.5-1 to Table 7.5-3 for groundwater and in Table 7.5-4 for surface water.

All detections in groundwater were below 0.1 µg/L. Thus, the leaching of unacceptable amounts of triticonazole is highly unlikely.

Out of several thousand samples, concentration in surface water exceeded on two times 0.1 µg/L. Due to the low number of findings a risk to aquatic organisms is not expected.

Table B.8.5-1: Monitoring data for triticonazole in ground water available for France

Country Data Source Data for years			FR ADES Database 2007 - 2011		
Year	Number of wells sampled	Number of analyses	Number of detections > LOQ	Number of detections > 0.1 µg/L	Number of wells with detections > 0.1 µg/L
2007	52	75	0	0	0
2008	284	1001	0	0	0
2009	1301	2186	0	0	0
2010	1503	4116	2	0	0
2011	1655	4448	0	0	0

Table B.8.5-2: Monitoring data for triticonazole in ground water available for Czech Republic

Country Data Source Data for years			CZ CHMI 2009 - 2012		
Year	Number of wells sampled	Number of analyses	Number of detections > LOQ	Number of detections > 0.1 µg/L	Number of wells with detections > 0.1 µg/L
2009	652	1265	1	0	0
2010	653	1264	1	0	0
2011	653	653	5	0	0
2012	651	1260	0	0	0

Table B.8.5-3: Monitoring data for triticonazole in ground water available for Italy

Country Data Source Data for years			IT ISPRA 2009 - 2010		
Year	Number of wells sampled	Number of analyses	Number of detections > LOQ	Number of detections > 0.1 µg/L	Number of wells with detections > 0.1 µg/L
2009	12	25	0	0	0
2010	1	2	0	0	0

Table B.8.5-4: Monitoring data for triticonazole in surface water available for France

Country Data Source Data for years			FR IFEN Database 2008 - 2012		
Year	Number of sites sampled	Number of analyses	Number of detections > LOQ	Number of detections > 0.1 µg/L	Number of wells with detections > 0.1 µg/L
2008	311	1567	23	0	0
2009	578	5446	52	1	1
2010	1091	6898	27	0	0
2011	1136	8428	23	2	2
2012	1471	9815	15	1	1

2. Peer reviewed scientific literature

Additionally, some information on its occurrence in the environment is available in parts of the study of Reilly et al. (2012) who investigated the occurrence of fungicides in surface water, groundwater, bed sediments and suspended solids. Triticonazole was detected in one surface water sample out of a total of 60 samples with a concentration of 66.8 ng/L. The study of Reilly et al. (2012) can be regarded as supplemental information but does not affect the risk assessment. It is summarized below.

Reference:	**Occurrence of boscalid and other selected fungicides in surface water and groundwater in three targeted use areas in the United States, Chemosphere 89 (2012) 228–234**
Author(s), year:	Reilly, T.J., Smalling, K.L., Orlando, J.L., Kuivila, K.M., 2012
Report/Doc. Number:	-
Guideline(s):	Not applicable
GLP:	Not applicable
Validity:	Yes
Status:	**Peer review public literature**

To provide an assessment of the occurrence of fungicides in water resources, the US Geological Survey used a newly developed analytical method to measure 33 fungicides and an additional 57 current-use pesticides in water samples from streams, ponds, and shallow groundwater in areas of intense fungicide use within three geographic areas across the United States. Sampling sites were selected near or within farms using prophylactic fungicides at rates and types typical of their geographic location. Triticonazole was detected in 2 of 72 surface water samples with a maximum concentration of 66.8 ng/L.

Conclusions:

Publically available groundwater monitoring data for triticonazole shows that, following application according to the label, the leaching of unacceptable amounts of triticonazole is highly unlikely. Entry of unacceptable amounts of triticonazole into surface water is highly unlikely.

Comments (RMS AT):

- The public monitoring reports are not available to the RMS AT.
- Data may be handled as supplemental information.

B.8.6. REFERENCES RELIED ON

Literature research

Reference:	**Literature search report final - Triticonazole - BASF confidential**
Author(s), year:	Zander-El-Metwally, M., Esswein U., 2015
Report/Doc. Number:	2015/1216973
Guideline(s):	EFSA (2011)
GLP:	Not applicable
Validity:	Yes
Status:	**Peer review public literature**

Search profiles for literature searches needed for (re)registration of crop protection agents were developed and optimized during the last ten years. Current requirements for the present literature search for triticonazole were defined in close cooperation between triticonazole AIR3 Scientific Expert Team and Agro Information Professionals. Main searches for the section on E-Fate were done on 25th of September 2014. Last update search for E-Fate was done on 16th of June 2015. Duplicates of search results from different databases in a respective section were removed in STN databases by the "duplicate remove" command. The search process is documented in all details with search profiles, search histories and summary tables according the EFSA (2011)[6].

The process of selection of relevant scientific peer-reviewed open literature was done in two steps:

The first selection step for relevance based on summary records (e.g. titles, abstracts, index terms, keywords) was done by the Agro Information Professionals.

- Obviously irrelevant records were tagged as 'Ballast'. This ballast was controlled by scientific experts in the corresponding subject areas but was not further processed.
- Summary records which appear to be relevant and those of unclear relevance were tagged as 'Hit' and went to the next level of evaluation.

The second detailed assessment was done by the scientific experts in the corresponding areas. Records tagged as 'Hit' were further evaluated in depth.

To facilitate a comprehensible listing of the 'Hits' an Excel file was generated for each section with 3 typical registers, namely:

- 'no relevant endpoint'
- 'evaluated - not-relevant'
- 'used for dossier'

In a first step (rapid assessment) the 'Hits' were reviewed based on the information given in the title and the abstract with regard to relevance for the regulatory endpoints in the respective regulatory area. Those records which were clearly judged as not assignable to any regulatory endpoint were shifted into the register 'no relevant endpoint' with an explaining reasoning. In a second step (detailed assessment), all remaining records were assessed in detail based on the complete report by the respective expert(s) and separated into relevant reports for further discussion and those clearly not relevant.

Criteria to assign a record to the register 'evaluated - not-relevant' were:

- Those records which provided information supporting the existing regulatory data package without any new relevant data or information were classified as "confirmatory data"
- Those records which were not assignable to the substance of interest (for example mixtures, not about test substance or other relevant substance)
- Secondary literature linking to primary literature already discussed under relevant records
- Records with limited reliability of grade 3 or 4 based on the 'Klimisch' scoring system (see below).
- and those which were judged as not relevant due to other reasons with a respective justification.

[6] EFSA (2011) Submission of scientific peer-reviewed open literature for the approval of pesticide active substances under Regulation (EC) No 1107/2009, EFSA Journal 2011;9(2):2092.

Criteria to assign a record to the register 'used for dossier' were:

- Records providing information about additional/new/unknown/potentially contradictory effects or data which might impact the hazard assessment endpoints or the risk assessments parameters and which in addition have a high grade of reliability of grade 1 or 2 based on the 'Klimisch' scoring system (see below).

Those records assigned to the category 'used for dossier' were provided with a Doc ID and discussed in detail in the respective dossier chapter.

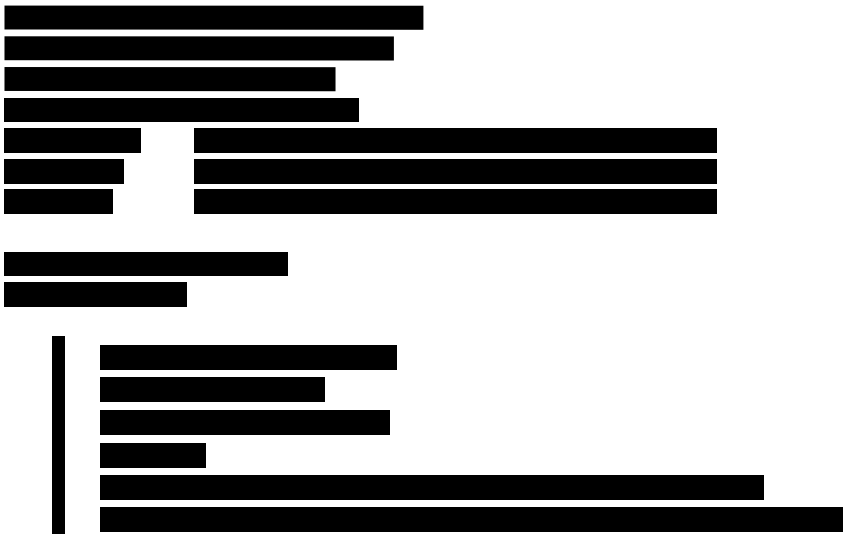
Reliability scoring system based on Klimisch et al., 1997[7]:

Reliability 1: reliable without restrictions
Studies or data generated according to generally valid and/or internationally accepted testing guidelines (preferably performed according to GLP) or in which the test parameters documented are based on a specific (national) testing guideline or in which all parameters described are closely related/comparable to a guideline method. (e.g. literature about toxicity / ecotoxicity study consistent with requests of international testing guidelines and performed under GLP conditions with experienced and trained personal)

Reliability 2: reliable with restrictions
Studies or data (mostly not performed according to GLP), in which the test parameters documented do not totally comply with the specific testing guideline, but are sufficient to accept the data or in which investigations are described which cannot be subsumed under a testing guideline, but which are nevertheless well documented and scientifically acceptable (appropriately documented studies which meets basic scientific principles, mechanistic studies)

Reliability 3: not reliable
Studies or data in which there were interferences between the measuring system and the test substance or in which organisms/test systems were used which are not relevant in relation to the exposure (e.g. unphysiologic pathways of application) or which were carried out or generated according to a method which is not acceptable, the documentation of which is not sufficient for assessment and which is not convincing for an expert judgement (e.g. literature studies with insufficient information or according to unvalidated method)

Reliability 4: not assignable
Studies or data which do not give sufficient experimental details and which are only listed in short abstracts or secondary literature



[7] Klimisch HJ, Andreae M, Tillmann U. (1997) A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. Regul Toxicol Pharmacol; 25(1):1-5.

[redacted]

[redacted]

Results:

Database:	**Total**	**CAPLUS Chemical Abstracts Plus**	**BIOSIS**	**CAB Abstracts**
Provider:		STN International	STN International	STN International
Justification for choosing the source: **- for STN databases referring to STN database summary sheets**		The Chemical Abstracts (CA) database covers all areas of Biochemistry, Chemistry and Chemical engineering, and related sciences. Sources include over 8,000 journals, patents from 38 national patent offices and two international patent organizations, technical reports, books, conference proceedings, and dissertations. Electronic only journals and Web preprints are also covered. Bibliographic terms, indexing terms, roles, CAS Registry Numbers, International Patent Classification, and abstracts are searchable.	BIOSIS Previews® is the largest and most comprehensive life science database in the world. Amongst others subject coverage includes Agriculture, Biochemistry, Biophysics, Botany, Environmental Biology, Physiology, Toxicology. Sources include periodicals, journals, conference proceedings, reviews, reports, patents, and short communications. Nearly 6,000 life source journals, 1,500 international meetings as well as review articles, books, and monographs are reviewed for inclusion. Bibliographic information, indexing terms, abstracts, and CAS Registry Numbers are all searchable.	The CAB Abstracts database covers worldwide literature from all areas of agriculture and related sciences including Agriculture, Agricultural chemicals, Animal sciences and production, Crop protection, Crop sciences and production, Environment, Soils and fertilizers. Sources for CABA include journals, books, reports, published theses, conference proceedings, and patents. Bibliographic information, indexing terms, abstracts, and CAS Registry Numbers are searchable.
Date span of the source:		1907 – to present	1926 – to present	1973 – to present
Date of main search:		2014-09-25	2014-09-25	2014-09-25
Date span of the search:		2005 - 2014	2005 - 2014	2005 – 2014
Date of the latest database update included in the search:		2014-09-24/UP	2014-09-24/UP	2014-09-24/UP
Search strategies used for this data requirement (including any limits):		see above	see above	see above
Total number of summary records for triticonazole and metabolites retrieved:		84	11	18
Total number of summary records after removing duplicates:	**97**	84	5	8
Total number of summary records retrieved after first selection step:				
Category: E-Fate	**12**			
Category: E-Fate Ballast	**85**			

No	Title	Company Institute	Author Inventor	Source	Publ. Year	E-Fate Ballast First screening	Comment for relevance assessment	Relevant yes / no
1	Impact of selected seed dressings on soil microbiological activity in spring barley cultivation	Department of General and Environmental Microbiology, University of Life Sciences in Poznan, Poznan, 60-656, Pol.	Niewiadomska, Alicja Sawinska, Zuzanna Wolna-Maruwka, Agnieszka	Fresenius Environmental Bulletin (2011), 20(5a), 1252-1261 CODEN: FENBEL; ISSN: 1018-4619	2011	no	Relevance of effect on soil enzyme activity to be discussed.	yes
2	Determination of 22 triazole compounds including parent fungicides and metabolites in apples, peaches, flour, and water by liquid chromatography/tandem mass spectrometry	Office of Pesticide Programs, Biological and Economic Analysis Division, Analytical Chemistry Branch, U.S. Environmental Protection Agency, Fort George G. Meade, MD, 20755-5350, USA	Schermerhorn, Patricia G. Golden, Paul E. Krynitsky, Alexander J. Leimkuehler, William M.	Journal of AOAC International (2005), 88(5), 1491-1502 CODEN: JAINEE; ISSN: 1060-3271	2005	no	Focus on method development for triazole derivated metabolites. No concentrations for parent compounds reported. 1,2,4-triazole is not a major metabolite of triticonazole in soil and water.	no
3	High-Throughput Models for Exposure-Based Chemical Prioritization in the ExpoCast Project	National Center for Computational Toxicology, Office of Research and Development, United States Environmental Protection Agency, NC, 27711, USA	Wambaugh, John F. Setzer, R. Woodrow Reif, David M. Gangwal, Sumit Mitchell-Blackwood, Jade Arnot, Jon A. Joliet, Olivier Frame, Alicia Rabinowitz, James Knudsen, Thomas B. Judson, Richard S. Egeghy, Peter Vallero, Daniel Cohen Hubal, Elaine A.	Environmental Science + Technology (2013), 47(15), 8479-8488 CODEN: ESTHAG; ISSN: 0013-936X	2013	no	Human exposure models --> not relevant for E-Fate	no
4	Occurrence and persistence of fungicides in bed sediments and suspended solids from three targeted use areas in the United States	U.S. Geological Survey, Sacramento, CA, 95819, USA	Smalling, Kelly L. Reilly, Timothy J. Sandstrom, Mark W. Kuivila, Kathryn M.	Science of the Total Environment (2013), 447, 179-185 CODEN: STENDL; ISSN: 0048-9697	2013	no	Study of paper showed that no data was analysed for triticonazole.	no
5	Experimental assessment of the environmental fate and effects of triazoles and benzotriazole	Public Health Institute Maribor, Maribor, Slovenia	Durjava, Mojca Kos Kolar, Boris Arnus, Lovro Papa, Ester Kovarich, Simona Sahlin, Ullrika Peijnenburg, Willie	ATLA, Alternatives to Laboratory Animals (2013), 41(1), 65-75 CODEN: AALADQ; ISSN: 0261-1929	2013	no	Only ready biodegradability tested as only fate aspect, however not for triticonazole.	no
6	Pesticide nonextractable residue formation in soil: Insights from inverse modelling of degradation time series	Eawag, Swiss Federal Institute of Aquatic Science and Technology, Dubendorf, 8600, Switz.	Loos, Martin Krauss, Martin Fenner, Kathrin	Environmental Science + Technology (2012), 46(18), 9830-9837 CODEN: ESTHAG; ISSN: 0013-936X	2012	no	Full paper to be checked to see relevance for triticonazole.	??? (refer to comment section)

No	Title	Company Institute	Author Inventor	Source	Publ. Year	E-Fate Ballast First screening	Comment for relevance assessment	Relevant yes / no
7	Determination of azole fungicides in atmospheric samples collected in the Canadian prairies by LC/MS/MS	Department of Chemistry and Biochemistry, and Trace Analysis Facility, University of Regina, Regina, SK, S4S 0A2, Can.	Raina, Renata Smith, Erika	Journal of AOAC International (2012), 95(5), 1350-1356 CODEN: JAINEE; ISSN: 1060-3271	2012	no	Only method development presented for triticonazole, results not. Propiconazole, and desthio-prothioconazole dominated the samples.	no
8	Occurrence of boscalid and other selected fungicides in surface water and groundwater in three targeted use areas in the United States	US Geological Survey, West Trenton, NJ, 08628, USA	Reilly, Timothy J. Smalling, Kelly L. Orlando, James L. Kuivila, Kathryn M.	Chemosphere (2012), 89(3), 228-234 CODEN: CMSHAF; ISSN: 0045-6535	2012	no	Discussion of monitoring results necessary	yes
9	Modelling physico-chemical properties of (benzo)triazoles, and screening for environmental partitioning	QSAR Research Unit in Environmental Chemistry and Ecotoxicology, Department of Structural and Functional Biology (DBSF), University of Insubria, Varese, 21100, Italy	Bhhatarai, B. Gramatica, P.	Water Research (2011), 45(3), 1463-1471 CODEN: WATRAG; ISSN: 0043-1354	2011	no	QSAR Modelling - Not relevant as guideline conform experimental data is available	no
10	Comparison of a score-based approach with risk-based ranking of in-use agricultural pesticides in Canada to aquatic receptors	Science and Technology Branch, National Wildlife Research Centre, Environment Canada, Ottawa, ON, K1A 0H3, Can.	Whiteside, Melanie Mineau, Pierre Morrison, Clare Knopper, Loren D.	Integrated Environmental Assessment and Management (2008), 4(2), 215-236 CODEN: IEAMCK; ISSN: 1551-3777	2008	no	US EPA Exposure model used not relevant for EU registrations.	no
11	A new approach for calculating the relative risk level of pesticides	Faculty of Civil Engineering, Dept. of Environment Engineering, Istanbul Technical University, Istanbul, 34469, Turk.	Yazgan, Mustafa Sait Tanik, Aysegul	Environment International (2005), 31(5), 687-692 CODEN: ENVIDV; ISSN: 0160-4120	2005	no	Presented data not relevant for environmental exposure assessment.	no
12	Efficiency and persistence of fungicides in the control of powdery mildew of wheat through seed treatment. Original Title: Eficiencia a persistencia de fungicidas no controle do oidio do trigo via tratamento de sementes.	Univ Passo Fundo, Fac Agron and Med Vet, Cx 631, BR-99001970 Passo Fundo, RS, Brazil erleireis@tpo.com.br; a2rtc@cav.udesc.br	Reis, Erlei Melo [Reprint Author] Moreira, Eder Novaes Casa, Ricardo Trezzi Casa Blum, Marta Maria	Summa Phytopathologica, (OCT-DEC 2008) Vol. 34, No. 4, pp. 371-374. CODEN: SUPHDV. ISSN: 0100-5405.	2008	no	Persistence is used by the terms of duration of efficacy.	no

Comments (RMS AT):

On overall the RMS AT agrees on the literature research provided by the applicant.

- Paper Nr. 1 (Niewiadomska et al., 2011, Impact of selected seed dressings on soil microbiological activity in spring barley cultivation,) is more related to ecotoxicology and is therefore handled within this section (refer to Vol. 3CA, B-9, ecotoxicology).

- The applicant claims that paper Nr. 6 (Loos et al, 2012, Pesticide nonextractable residue formation in soil: Insights from inverse modelling of degradation time series) should be checked on its relevance for triticonazole. This was not done so far.

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evalu-ation
KCA 7.1.1.1 7.1.2.1.1 7.1.2.1.2	Ayliffe J.M., Austin D.J.	1993	Fungicides: RPA 400727-^{14}C: Aerobic soil metabolism in three soils C017917 Rhone-Poulenc Agriculture Ltd., Ongar, GBR Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.1.1 7.1.2.1.1 7.1.2.1.2	Ayliffe J.M., McMillan-Staff S.L.	1994	Addendum Report: Fungicides: RPA400727-^{14}C: Aerobic soil metabolism in three soils. R012981 Rhone-Poulenc Agriculture Limited, Ongar, England; Analytical Chemistry Department Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.1.1 7.1.2.1.1 7.1.2.1.2	Ayliffe J.M., Godward P.J.	1993	Fungicides: RPA400727-^{14}C: Rate of degradation in four soils. R012979 Rhone-Poulenc Agriculture Limited, Ongar, England; Analytical Chemistry Department Rhone-Poulenc Secteur Agro Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.1.1 7.1.2.1.1 7.1.2.1.2	Doble M.L., Ferreira E.M., Hardy I.A.J.	1996	[^{14}C]-triazole labelled triticonazole: Rate of degradation in clay soil under aerobic conditions. R012994 Rhone-Poulenc Agriculture Limited, Ongar, UK Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.1.1 7.1.2.1.1 7.1.2.1.2	Simmonds M B., Hardy I.J., Ferreira E.M.	1996	Triticonazole: Rate of degradation in one soil type under aerobic conditions with regard to varying temperature, soil moisture, treatment rate and soil viability. R012995 Rhone-Poulenc Agriculture Limited, Ongar, England; Rhone-Poulenc Agro Norden, Soberg, Denmark Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.1.1	Simmonds M., Lowden P.	2002	[^{14}C]-Triticonazole: Generation and Identification of Metabolites C021044 Battelle AgriFood Ltd, Ongar, UK Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.1.1	Ta C., Strobush A.	2012	Aerobic Soil Metabolism of ^{14}C-BAS 595 F 2012/7004893 BASF Crop Protection, Research Triangle Park NC, United States of America Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evalu-ation
KCA 7.1.1.1 7.1.2.1.1 7.1.2.1.2	Ta C., Strobush A.	2015	Aerobic soil metabolism of ^{14}C-BAS 595 F 2014/7000472 BASF Crop Protection, Research Triangle Park NC, United States of America Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.1.1 7.1.2.1.2 7.1.3.1.2	Szegedi K.	2018	Statement. Exposure assessment for “Met 6” and “Met 7”, potential degradation products of BAS 595F triticonazole 2018/1091281 BASF SE, Limburgerhof, Germany Fed.Rep. no Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.1.2 7.1.2.1.3 7.1.2.1.4	Goodyear A.	1994	[^{14}C]-RPA400727: Anaerobic soil metabolism R012982 Hazleton Europe, Harrogate, England; Environmental Fate Section Rhone-Poulenc Agriculture, Ongar, England Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.1.2 7.1.2.1.3 7.1.2.1.4	Goodyear A.	1998	[^{14}C]-RPA400727: Anaerobic soil metabolism - Addendum report R012983 Covance, Harrogate, England; Rhone-Poulenc Agriculture, Ongar, UK; Yes unpublished	No	No	-	BASF	Yes
KCA 7.1.1.3	Ayliffe J.M., Jones M.K.	1998	Fungicides: Triticonazole: Soil Photolysis P95/065, C017700, 201021 Rhone-Poulenc Agriculture, Ongar, UK; Yes unpublished	No	No	-	BASF	Yes
KCA 7.1.2.1.1	Grella B., Ta C., Strobush A.	2014	Rate of degradation of BAS 595 F in soils 2014/7000471 BASF Crop Protection, Research Triangle Park NC, United States of America Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.2.1.1 7.1.2.1.2	Szegedi K.	2016	Kinetic evaluation of laboratory soil degradation of triticonazole (BAS 595 F) and its metabolites RPA 406341 and RPA 404766 in a single soil for derivation of trigger and modelling endpoints according to FOCUS 2016/1171410 BASF SE, Limburgerhof Germany Fed.Rep. No Unpublished	No	Yes	New data for AIR3	BASF	Yes

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evalu-ation
KCA 7.1.2.1.2	McGhee I.	2000	[^{14}C]-RPA406341: Rate of degradation in three soils at 20 degrees Celsius C010570 Aventis CropScience UK Limited, GBR Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.2.1.2	Crowe A.	2002	[^{14}C]-RPA404766: Aerobic soil rate of degradation C021045 Covance, Yorks, UK Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.2.2.1	Wicks R.J.	1996	Triticonazole: Terrestrial field soil dissipation study in Europe (Final Report). R012996 Rhone-Poulenc Agrochimie, Lyon, France; Rhone-Poulenc Agriculture Ltd., Ongar, UK; Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.2.2.1	Doble M., Parsons R.G.	1994	Triticonazole (^{14}C-Phenyl): Soil persistence study using lysimeter tubes R012980 Rhône-Poulenc Agriculture Limited, Ongar, Essex, England, UK Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.2.2.1	Duncan P., Doran A., Old J.	2003	Triticonazole: Field Soil Dissipation Study in Europe – final report C032147 Inveresk Research Yes Unpublished	No	No	-	BASF	Yes

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evalu-ation
KCA 7.1.2.2.1	Richter T.	2009	Field soil dissipation study of RPA406341 (metabolite of BAS 595 F - Triticonazole) in the formulation EXP 5059144 F on bare soil at four different locations in Europe, 2007-2008 2009/1049703 BASF SE, Limburgerhof, Germany Fed.Rep. Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.2.2.1	Huber, S.	2007	Determination of trigger endpoints for triticonazole (BAS 595 F) from field dissipation studies 2007/1058036 BASF SE, Limburgerhof Germany Fed.Rep.No Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.2.2.1	Schwarz N., Jarvis T.	2014a	Determination of normalised rates of decline for Triticonazole from two field dissipation studies 2014/1083344 Exponent International Ltd., Harrogate North Yorkshire HG2 8RE, United Kingdom No Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.2.2.1	Huber S.	2008	Best-fit analysis and normalization of the field dissipation of the Triticonazole (BAS 595 F) metabolite RPA 406341 2008/1089810 BASF SE, Limburgerhof, Germany Fed.Rep. No Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.2.2.1	Schwarz N., Jarvis T.	2014b	Determination of normalised rates of decline for Triticonazole metabolite RPA406341 from a field dissipation study 2014/1083343 Exponent International Ltd., Harrogate North Yorkshire HG2 8RE, United Kingdom No Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.2.2.2	Davis H.	2004	Triticonazole - Long term soil dissipation study with repeated applications – final report 1849/034-D2149 Bayer CropScience GmbH, DEU; Environmental Chemistry, Frankfurt Covance Laboratories Ltd., Harrogate, GBR Yes Unpublished	No	No	-	BASF	Yes

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evalu-ation
KCA 7.1.3.1.1	Vasques A.C.	2015a	Adsorption / desorption behavior of ^{14}C-BAS 595 F on different European soils 2014/3001242 BASF SA, Guaratingueta, Brazil Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.3.1.1	Simmonds R.	2017a	[^{14}C]-BAS 595F: Adsorption to and Desorption from Five Soils 2017/1142046 Battelle UK Ltd., Springfield, Chelmsford, Essex, UK Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.3.1.2	Vasques A.C.	2015b	Adsorption / desorption behaviour of ^{14}C-RPA404766 / M595F001 (Reg. 5079295), ^{14}C-RPA406341 / M595F002 (Reg. 5059144) and ^{14}C-RPA407922 (Reg. 5079288) (metabolites of ^{14}C-BAS 595 F) on different European soils 2015/3000503 BASF SA, Guaratingueta, Brazil Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.3.1.2	O'Brien L.B.S.	2017	[^{14}C]-M595F001 (RPA 404766, Metabolite of BAS 595 F): Adsorption on Five European Soils 2017/7013112 BioChem, Machern, Germany Fed.Rep.Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.3.1.2	Kingman A.M.S.	2017	[^{14}C]-M595F002 (RPA 406341, Metabolite of BAS 595 F): Adsorption on Five European Soils 2017/7013113 BioChem, Machern, Germany Fed.Rep.Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.1.4.1.1	John A.E., Lowden P., Austin D.J.	1993	Fungicides: RPA400727-^{14}C (phenyl label): Fresh and aged leaching study with five soils (final report). R012972 Rhone-Poulenc Agriculture Limited, Ongar, England; Rhone-Poulenc Secteur Agro; Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.4.1.1	John A.E., Lowden P., Austin D.J.	1998	Amendment: Fungicides: RPA400727-14C (phenyl label): Fresh & aged leaching study with five soils (final report). R012973 Rhone-Poulenc Agriculture Limited, Ongar, England; Yes Unpublished	No	No	-	BASF	Yes

Data point	Author(s)	Year	Title Company Report No. Source (where different from company) GLP or GEP status Published or not	Vertebrate study Y/N	Data protection claimed Y/N	Justification if data protection is claimed	Owner	Previous evalu-ation
KCA 7.1.4.2	Schnoeder F.	2003	Triticonazole [benzene ring-U-^{14}C]: Outdoor Lysimeter Study - final report C032148 Covance, Munster, Germany Yes Unpublished	No	No	-	BASF	Yes
KCA 7.1.4.2	Schnoeder F.	2004	Triticonazole [triazole-3,5-^{14}C]: Outdoor Lysimeter Study - final report 1757-1849-010 Covance, Munster, Germany Yes Unpublished	No	No	-	BASF	Yes
KCA 7.2.1.1	Corgier M M.C., Robin J.M.	1991	^{14}C-RPA 400727 Hydrolysis at 25 °C R013023 Rhône-Poulenc Secteur Agro, Lyon France Yes Unpublished	No	No	-	BASF	Yes
KCA 7.2.1.1	Hassink J.	2013	Triticonazole: Aqueous hydrolysis at four different pH values 2012/1300793 BASF SE, Limburgerhof, Germany Fed.Rep. Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.2.1.2	Corgier M M.C, Robin J.M.	1992	^{14}C-RPA 400727: Aqueous Photolysis R013068 Rhône-Poulenc Secteur Agro, Lyon France Yes Unpublished	No	No	-	BASF	Yes
KCA 7.2.1.2	Corgier M M.C, Turier G.P.	1995	Triticonazole – Quantum Yield and Environmental Half Live in Water R012072 Rhône-Poulenc Secteur Agro, Lyon France; Yes Unpublished	No	No	-	BASF	Yes
KCA 7.2.1.2	Singh M.	2007	Aqueous photolysis of ^{14}C-BAS 595 F (Triticonazole) 2007/7001058 BASF Agro Research RTP, Research Triangle Park NC, United States of America Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.2.2.1	Handley J.W., Horton M.R.	1992	Assessment of the Ready Biodegradability (modified Sturm Test) of RPA 400727 R013073 Safepharm Laboratories Limited, Derby, England; Rhône-Poulenc Agrochimie, Lyon, France; Yes Unpublished	No	No	-	BASF	Yes

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KCA 7.2.2.2	Adam D.	2014	^{14}C-Triticonazole (BAS 595 F): Aerobic mineralisation in surface water - Simulation biodegradation test 2014/1083345 IES - Innovative Environmental Services Ltd., Witterswil, Switzerland Yes Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
Annex IIA 7.2.1	Wyss-Benz M.	1995	^{14}C-RPA 400727: Degradation and metabolism in aerobic aquatic systems. R012987 RCC Umweltchemie AG, Itingen, Switzerland; Rhône-Poulenc Agriculture Limited, Ongar, England Yes Unpublished	No	No	-	BASF	Yes
KCA 7.2.2.3	Jarvis T.J., Montesano V.	2014b	Recalculation of Triticonazole water sediment study kinetics according to FOCUS (2006) Guidance 2014/1083346 Exponent International Ltd., Harrogate North Yorkshire HG2 8RE, United Kingdom No Unpublished	No	Yes	New data for AIR3 renewal	BASF	No
KCA 7.3.1	Voelkel W.	1999	Estimation of the degradation of Triticonazole by photo-oxidation in air R012052 Rhone-Poulenc; RCC Ltd., Itingen, Switzerland; Pharmanalytics Division No Unpublished	No	No	-	BASF	Yes