RESPONDENT'S EXHIBIT 18

Aerobic degradation of TPA, a transformation product of DCPA in three soils

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Report:	MRID 49307516. Wales, S. 2014. (14C)-TPA, A Metabolite of DCPA: Degradation in Three Soils (Revised per PRN 11-03 and 86-5). Unpublished study performed by Covance Laboratories Ltd., North Yorkshire, England; sponsored and submitted by the AMVAC Chemical Company, Newport Beach, California. AMVAC ID.: 100-MET-011a. Covance No. 1708/016. Experiment started April 8, 2003, and completed September 19, 2003 (p. 15). Final report issued January 29, 2014.
Document No.:	MRID 49307516
Guideline:	OCSPP 835.4100
Statements:	The study was conducted according to UK GLP standards (p. 5). Signed and dated Data Confidentiality, GLP, Certification of Authenticity and Quality Assurance statements were provided (pp. 2, 5-7).
Classification:	This study is supplemental. The study author failed to use solvents with a range of dielectric constants (including a nonpolar solvent) to maximize extraction of the residues in the sandy clay loam soil and silt loam soil. The study was conducted using a transformation product. No US soils were used. Single samples were analyzed.
PC Code:	078701 (for DCPA)
Reviewer:	
	James Lin, Environmental Engineer U.S. EPA
	Signature: Date: January 13, 2017

EXECUTIVE SUMMARY

The aerobic transformation of [benzene-U-^{14}C]tetrachloroterephthalic acid (TPA), a transformation product of DCPA, was studied in three soils: a sandy loam soil (PT103, pH 3.9 in $CaCl_2$), a sandy clay loam soil (SK920191, pH 7.3 in $CaCl_2$), and a silt loam soil (SK15556090, pH 6.2 in $CaCl_2$). All three soils were obtained from commercial sources in the UK. The experiment was conducted for 120 days in darkness at 20°C and a soil moisture content of 45% of MWHC. The soils were treated at 8.24 mg a.i./kg, equivalent to a field application rate of 9 kg a.i./ha of DCPA. Single samples (duplicate flasks) were collected at each sampling interval. It was not confirmed that aerobic conditions were maintained in the soils throughout the study. The soils were viable at study initiation and at termination.

Overall mass balances averaged 98.3 ± 1.8% of the applied (range 94.1-100.2%) in the sandy loam soil, 98.9 ± 3.2% (range 96.5-106.0%) in the sandy clay loam soil, and 98.4 ± 1.3% (range 96.6-100.2%) in the silt loam soil. Recoveries were within guidelines (90-110%).

Observed DT_{50} values, calculated half-lives, and information on transformation products are listed in **Table 1**. TPA dissipated with SFO DT50 values of 1603 days in the sandy loam soil, 101 days in the sandy clay loam soil, and 208 days in the silt loam soil. No transformation products were conclusively identified.

In the sandy loam soil, total extractable radioactivity declined from 99.2% of the applied at time 0 to 90.8% at 120 days posttreatment. Unextracted radioactivity increased to a maximum of 6.5% at 120 days. In the 120-day sample, 5.3% of the applied was characterized as fulvic acids, 0.8% as humic acids, and 0.9% as humin. At study termination, CO_2 totaled a maximum of 1.4% of the applied; organic volatiles were 0.0% throughout the experiment.

In the sandy clay loam soil, total extractable radioactivity declined from 98.8% of the applied at time 0 to 40.2% at 120 days posttreatment. Unextracted radioactivity increased to a maximum of 21.5% at 120 days. In the 120-day sample, 6.0% of the applied was characterized as fulvic acids, 2.8% as humic acids, and 13% as humin. At study termination, CO_2 totaled a maximum of 34.8%; organic volatiles were 0.0% throughout the experiment.

In the silt loam soil, total extractable radioactivity declined from 96.9% of the applied at time 0 to 62.3% at 120 days posttreatment. Unextracted radioactivity increased to a maximum of 14.3% at 120 days. In the 120-day sample, 3.5% of the applied was characterized as fulvic acids, 4.6% as humic acids, and 5.4% as humin. At study termination, CO_2 totaled a maximum of 20.3%; organic volatiles were 0.0% throughout the experiment.

Table 1. Results Synopsis: Aerobic Soil Metabolism of TPA.

Soil Location and Texture (Temperature, pH)	Observed DT_{50} (days)	Calculated Half-life[1] (days)	Model Parameters and Statistics	Transformation Products (maximum % AR, associated interval)[2]	
				Major	Minor[3]
UK Sandy loam soil (20°C, pH 3.9)	>120	1603 SFO	C_0 = 93 k = 0.000433 S_C = 49.3 S_{SFO} = 32	None	Unextracted residues (6.5%, 120 days) CO_2 (1.4%, 120 days)
UK Sandy clay loam soil (20°C, pH 7.3)	*ca.* 90	101 SFO	C_0 = 98 k = 0.00689 S_C = 86.2 S_{SFO} = 102	Unextracted residues (21.5%, 120 days) CO_2 (34.8%, 120 days)	None
UK Silt loam soil (20°C, pH 6.2)	>120	208 SFO	C_0 = 94.2 k = 0.00333 S_C = 40.4 S_{SFO} = 23.9	Unextracted residues (14.3%, 120 days) CO_2 (20.3%, 120 days)	None

1 Calculated half-lives, model parameters, and kinetics models in accordance with the NAFTA kinetics guidance (USEPA, 2012); Single First-Order (SFO).
2 AR means “applied radioactivity”.

I. Materials And Methods

A. Materials:

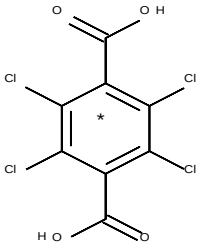
1. Test Material [Benzene-U-^{14}C]TPA (Chlorthal, p. 16; Appendix 2, p. 58)

Specific activity: 1.2 MBq/mg

Radiochemical purity: >98% by HPLC

Chemical purity: Not reported

Lot No.: 03BLY009



Solubility in water: Not reported

2. Reference Compounds: The following standards were used in the analysis (**Table 2**).

Table 2. Reference Compounds

Applicant's Code Name	Chemical Name	Purity (%)	Lot No.
TPA	Tetrachloroterephthalic acid	99.94	021101

Data obtained from pp. 16-17 and Appendix 2, p. 59, of the study report.

3. Soil: Soil collection and characterization are summarized in **Table 3** and **Table 4**, respectively.

Table 3. Description of Soil Collection and Storage

Description	PT103	SK920191	SK15556090
Geographic location	Baylham, Ipswich, UK.	South Witham Quarry, South Witham, Lincolnshire, UK.	Hartington Upper Quarter, Derbyshire, UK
Site Description	Grassland.	Edge of Quarry.	Grassland for cattle.
Soil series	Not reported.		
Pesticide use history at the collection site	None last 5 years.		
Collection date	February 25, 2003	February 25, 2003	February 25, 2003
Collection procedures	In accordance with ISO 10381-6.		
Sampling depth	14-17 cm	5-20 cm	10-20 cm
Storage conditions	Stored in the dark at 4 ± 2°C in loosely tied plastic bags.		
Storage length	<3 months.		
Soil preparation	Sieved (2.0-mm screen)		

Data obtained from pp. 14-15, 19 and Appendix 4, pp. 62-64, of the study report.

Table 4. Properties of the Soil

Property		PT103	SK920191	SK15556090
Soil Texture (USDA)		Sandy loam	Sandy clay loam	Silt loam
% Sand (2000-53 µm)		73	47	20
% Silt (53-2 µm)		15	23	61
% Clay (<2 µm)		12	30	19
pH	1:1 in water	5.3	8.0	7.0
	1M KCl	3.9	7.4	6.1
	0.01M $CaCl_2$	3.9	7.3	6.2
Organic carbon (%)		1.2	2.1	4.2
Organic matter (%) (Method not reported.)		2.1	3.6	7.2
Cation Exchange Capacity (meq/100 g) (method not reported)		8.7	14.6	20.2
Ca Base Saturation (%)		Not reported.		
Soil Moisture Content (g/100 g soil)				
pF 0 (0.01 bar)		49.9	58.7	93.5
pF 2.0 (0.1 bar)		9.9	22.8	32.8
pF 2.5 (0.33 bar)		9.8	21.8	32.9
Bulk density (disturbed, g/cm^3)		0.92	0.90	0.71
Microbial Biomass (µg C/g dry soil)				
Initiation		68.12	582.94	205.05
Termination		173.41	336.38	306.92
Soil taxonomic classification		Not reported		

Data obtained from pp. 13, 25; Appendix 4, pp. 62-64 of the study report. The soil texture was confirmed using USDA-NRCS technical support tools.

B. STUDY DESIGN

1. Experimental Conditions: (Summarized in **Table 5**).

Table 5. Experimental Design

Property	Details
Duration of the test (days)	120 days.
Soil condition (Air dried/fresh)	Soil was acclimated to study conditions for five days prior to treatment.
Soil (g/replicate)	*ca.* 50 g (dry wt).
Application rates	
Nominal	8.24 mg a.i./kg; equivalent to a field rate of 9 kg a.i./ha of DCPA[1]
Actual	8.22 mg a.i./kg, 411 µg/40 g.
Control conditions (if used)	Sterile controls were not used.
Number of Replicates	
Controls (if used)	Sterile controls were not used.
Treatment	Single flasks of each soil were collected at each sampling interval.

Property	Details
Test apparatus	
Type/material/volume	The test system consisted of glass bottles (size not reported) containing moist treated soil (50 g dry wt) that were attached to a continuous flow-through volatile trapping systems and incubated in the dark. The test system is illustrated on p. 20.
Details of traps for CO_2 and other volatiles (if any)	Humidified CO_2-free air was continually passed (flow rate not reported) through a sample flask, then through one bottle of ethanediol, 1 bottle of paraffin in xylene and two bottles of 2M NaOH. The volatile trapping system is illustrated on p. 20.
If no traps were used, is the system closed/open?	Volatile traps were used.
Identity and concentration of co-solvent	None, water.
Test Material:	
Volume of the test solution used/treatment	140 µL/50 g p. 21
Application method	The test solution was applied in drops to the soil surface and thoroughly mixed.
Is the co-solvent evaporated?	Yes
Any indication of the test material adsorbing to the walls of the test apparatus?	None
Experimental conditions:	
Temperature (°C)	20 ± 2°C (range not reported)
Continuous darkness	Yes
Moisture content	45% of MWHC
Moisture maintenance method	Samples were weighed every 2-8 days and remoistened with reverse-osmosis water if necessary.
Other details (if any)	Aged sorption coefficients were determined using the 61 day samples.

Data obtained from pp. 19-21, 23, of the study report.
1 Application rate assumes an even distribution of the test material in the top 10 cm of soil and a soil bulk density of 1.0 g/cm^3 (p. 20).

2. Sampling During Study Period: (Details summarized in **Table 6**).

Table 6. Sampling During Study Period

Criteria	Details
Sampling intervals (days)	0, 2, 7, 9, 14, 30, 61, 90 and 120 days
Sampling method	Single flasks of each soil were collected at each sampling interval.
Method of collection of CO_2 and organic volatile compounds	Volatile traps were collected at each sampling interval beginning at day 1.
Sampling intervals/times for:	
Sterility check (if used)	Sterile controls were not used.
Moisture content	Flasks were weighed every 2-8 days.
Redox potential, other	The redox potential was not measured
Sample storage before analysis	Not reported
Other observation (if any)	None.

Data obtained from p. 21 of the study report.

3. Analytical Procedures:

Extraction Methods: The soils were extracted three times with acetonitrile:water (1:1, v:v) by shaking (30 minutes/extraction) at room temperature (p. 22). After each extraction, the samples were centrifuged and the supernatant decanted; aliquots were analyzed using LSC.

All extracts from a sample were combined and concentrated by rotary evaporation (p. 22). Aliquots were analyzed using LSC and HPLC.

Determination of Unextracted Residues: Portions of the extracted soils were air-dried, ground, and analyzed for total remaining radioactivity using LSC following combustion (p. 22).

Additional samples of 120 day extracted soil were further extracted one time with 0.5M NaOH by shaking for 24 hours/extraction at room temperature (p. 22). The soil was washed with twice with 0.5M NaOH. The supernatants were combined and aliquots analyzed using LSC. The remaining supernatant was acidified to *ca.* pH 1 (5M HCl), and the resulting supernatant (fulvic acids) and precipitate (humic acids) were quantified using LSC. Portions of the extracted soil were air-dried and analyzed using LSC following combustion.

The flasks were rinsed with acetonitrile (p. 23). The rinseate was analyzed by LSC.

Determination of Volatile Compounds: Aliquots of the trapping solutions were analyzed by LSC (p. 23). The identification of residues as CO_2 in the trapping solutions was confirmed by precipitation with barium chloride.

Total radioactivity measurement: Total [^{14}C]residues were determined by summing the concentrations of residues in the soil extracts, extracted soil, and volatile traps (Tables 1-3, pp. 32-33).

Derivatization method A derivatization method was not employed.

Identification and quantification of Parent and Transformation Compounds: Aliquots of the concentrated extracts were analyzed by HPLC using a Waters µ Bondapak column eluted with a mobile gradient phase of (A) water with 0.2% TFA and (B) acetonitrile with 0.2% TFA (p. 24). The eluate was monitored using UV (220 nm) and radiomatic flow detection. Radioactive regions of interest were identified by comparison to the mobility of reference standards.

Identification of radiolabeled compounds in the routine sample extracts was confirmed using one dimensional TLC on silica gel plates developed in butan-1-ol:water:acetic acid (25:10:4, v:v:v).

Detection Limits (LOD, LOQ) for the Parent and Transformation Products: Limits of Detection were not reported. The Limit of Quantification was 1.5 times the background (p. 25).

II. Results and Discussion

A. Data

Study results including total mass balances and distribution of radioactivity are presented in **Tables 7a-7c**. No determinations were made to verify that aerobic conditions were maintained in the soils. Soils were viable at study termination (pp. 13, 15).

B. Mass Balance

Overall mass balances averaged 98.3 ± 1.8% of the applied (range 94.1-100.2%) in the sandy loam soil, 98.9 ± 3.2% (range 96.5-106.0%) in the sandy clay loam soil, and 98.4 ± 1.3% (range 96.6-100.2%) in the silt loam soil (Tables 1-3, pp. 32-33). Recoveries were within guidelines (90-110%).

C. Unextracted and Extractable Residues

In the sandy loam soil, total extractable radioactivity declined from 99.2% of the applied at time 0 to 90.8% at 120 days posttreatment (Table 1, p. 32). Unextracted radioactivity increased to a maximum of 6.5% at 120 days. In the 120-day sample, 5.3% of the applied was characterized as fulvic acids, 0.8% as humic acids, and 0.9% as humin (Table 7, p. 35).

In the sandy clay loam soil, total extractable radioactivity declined from 98.8% of the applied at time 0 to 40.2% at 120 days posttreatment (Table 2, p. 32). Unextracted radioactivity increased to a maximum of 21.5% at 120 days. In the 120-day sample, 6.0% of the applied was characterized as fulvic acids, 2.8% as humic acids, and 13% as humin (Table 7, p. 35).

In the silt loam soil, total extractable radioactivity declined from 96.9% of the applied at time 0 to 62.3% at 120 days posttreatment (Table 3, p. 33). Unextracted radioactivity increased to a maximum of 14.3% at 120 days. In the 120-day sample, 3.5% of the applied was characterized as fulvic acids, 4.6% as humic acids, and 5.4% as humin (Table 7, p. 35).

D. Volatilization

At study termination, CO_2 totaled maximums of 1.4% of the applied in the sandy loam soil, 34.8% in the sandy clay loam soil, and 20.3% in the silt loam soil (Tables 1-3, pp. 32-33). Organic volatiles were 0.0% of the applied in the soils throughout the experiments.

Table 7a. Transformation of TPA, expressed as a percentage of applied radioactivity, in sandy loam soil.

Sampling Interval (days)	0	2	7	14	30	61	90	120
Replicate	**A**	**A**	**A**	**A**	**A**	**A**	**A**	**A**
TPA	96.0	93.3	93.3	88.0	92.4	89.5	89.1	89.4
Largest Unknown	3.1	2.9	2.8	2.9	2.3	2.5	2.1	0.9
Other Unknowns	n.d.	n.d.	n.d.	0.0	n.d.	n.d.	0.4	n.d.
Unresolved background	0.1	0.6	0.4	0.5	0.4	0.5	0.3	0.5
Extracted residues	99.2	96.8	96.5	91.4	95.1	92.5	91.9	90.8
Unextracted residues	1.0	1.5	2.0	2.3	3.2	5.3	5.5	6.5
CO_2	n.a.	0.2	0.0	0.4	0.6	0.8	1.1	1.4
Organic Volatiles	n.a.	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass balance	100.2	98.5	98.5	94.1	98.9	98.6	98.5	98.7

Data obtained from Table 1, p. 32, and Table 4, p. 33, of the study report.
n.d. = not detected; n.a. = not analyzed.

Table 7b. Transformation of TPA, expressed as a percentage of applied radioactivity, in sandy clay loam soil.

Sampling Interval (days)	0	2	7	14	30	61	90	120
Replicate	**A**	**A**	**A**	**A**	**A**	**A**	**A**	**A**
TPA	95.3	94.4	92.5	89.4	88.5	64.0	52.3	39.5
Largest Unknown	3.0	3.2	2.5	1.6	1.2	0.2	0.6	0.6
Other Unknowns	n.d.	n.d.	n.d.	n.d.	n.d.	0.3	n.d.	n.d.
Unresolved background	0.5	0.1	0.5	0.1	0.4	0.5	0.0	0.2
Extracted residues	98.8	97.6	95.5	91.1	90.2	65.1	52.9	40.2
Unextracted residues	0.9	1.3	2.4	3.9	7.6	13.7	16.5	21.5
CO_2	n.a.	0.3	1.5	2.2	8.2	18.0	27.2	34.8
Organic Volatiles	n.a.	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass balance	99.7	99.2	99.4	97.2	106.0	96.8	96.6	96.5

Data obtained from Table 2, p. 32, and Table 5, p. 34, of the study report.
n.d. = not detected; n.a. = not analyzed.

Table 7c. Transformation of TPA, expressed as a percentage of applied radioactivity, in silt loam soil.

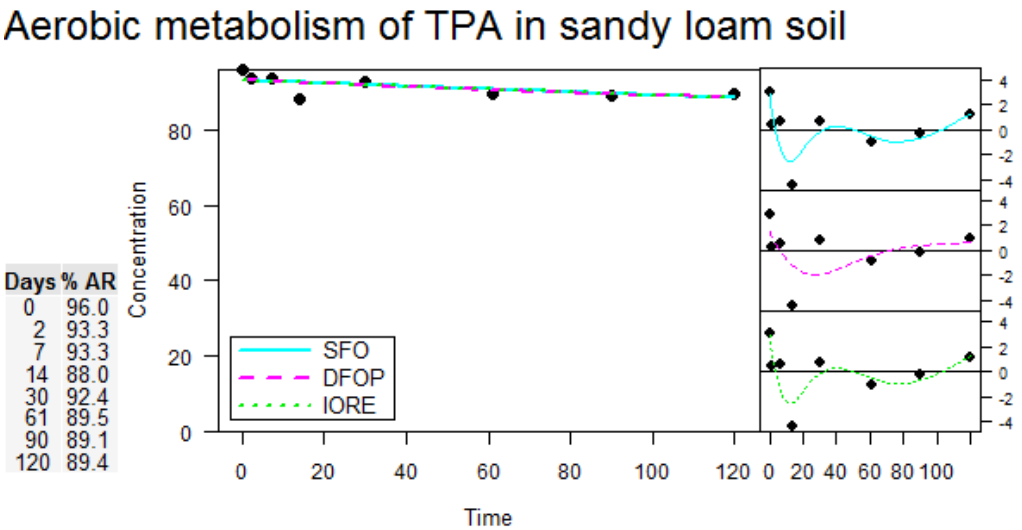
Sampling Interval (days)	0	2	7	14	30	61	90	120
Replicate	**A**	**A**	**A**	**A**	**A**	**A**	**A**	**A**
TPA	93.4	94.6	89.8	88.7	88.6	78.3	69.7	61.6
Largest Unknown	3.2	3.3	2.2	2.1	1.1	0.7	0.4	0.3
Other Unknowns	n.d.	n.d.	n.d.	n.d.	n.d.	0.5	0.6	n.d.
Unresolved background	0.3	0.3	0.6	0.4	0.3	0.5	0.1	0.4
Extracted residues	96.9	98.2	92.7	91.2	90.1	80.0	70.7	62.3
Unextracted residues	1.8	1.7	6.7	3.4	5.1	8.7	11.6	14.3
CO_2	n.a.	0.2	0.8	2.0	3.7	8.9	15.7	20.3
Organic Volatiles	n.a.	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Mass balance	98.7	100.1	100.2	96.6	98.9	97.6	98.0	96.9

Data obtained from Table 3, p. 33, and Table 6, p. 34, of the study report.
n.d. = not detected; n.a. = not analyzed.

E. Transformation of the Test Compound

Transformation kinetics of the parent compound in the total system are summarized in the following **Figures**, with transformation product information summarized in **Table 8**.

Using Excel with a Single First Order model, the study author determined SFO DT50 values of 1286 days for the sandy loam soil, 100 days in the sandy clay loam soil, and 208 days in the silt loam soil (pp. 26, 28).

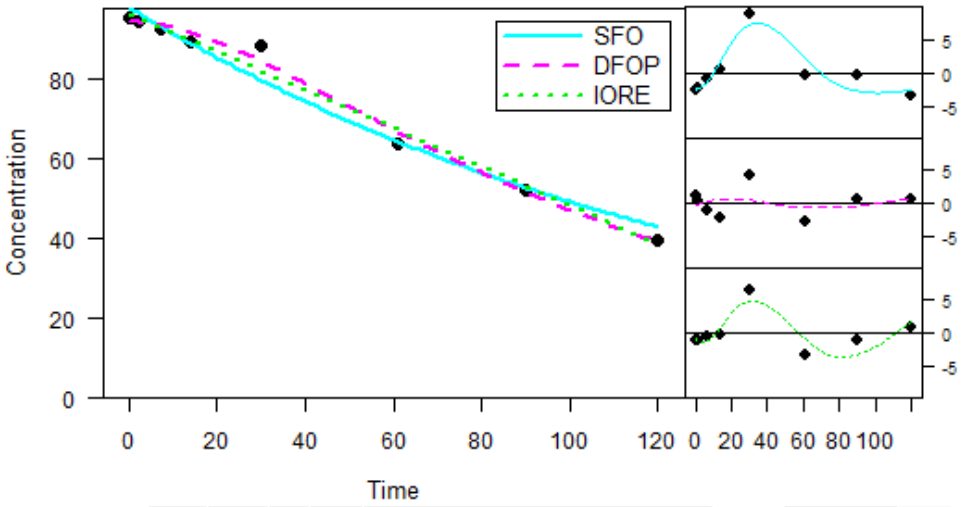


	DT_{50}	DT_{90}	χ^2	C_0	Parameters
SFO	1603	5324	1.7	93	k = 0.000433
DFOP	NA	NA	2	93	f = 0.155, k_0 = 0.00424, k_1 = -0.000112
IORE	2006	12270	1.9	93	N = 1.65, k = 2.26e-05

S_C	49.3
S_{SFO}	32
Slow $t_{1/2}$	-6.17e+03
$t_{R\ IORE}$	3.69e+03

Aerobic metabolism of TPA in sandy clay loam soil

Days	% AR
0	95.3
2	94.4
7	92.5
14	89.4
30	88.5
61	64.0
90	52.3
120	39.5

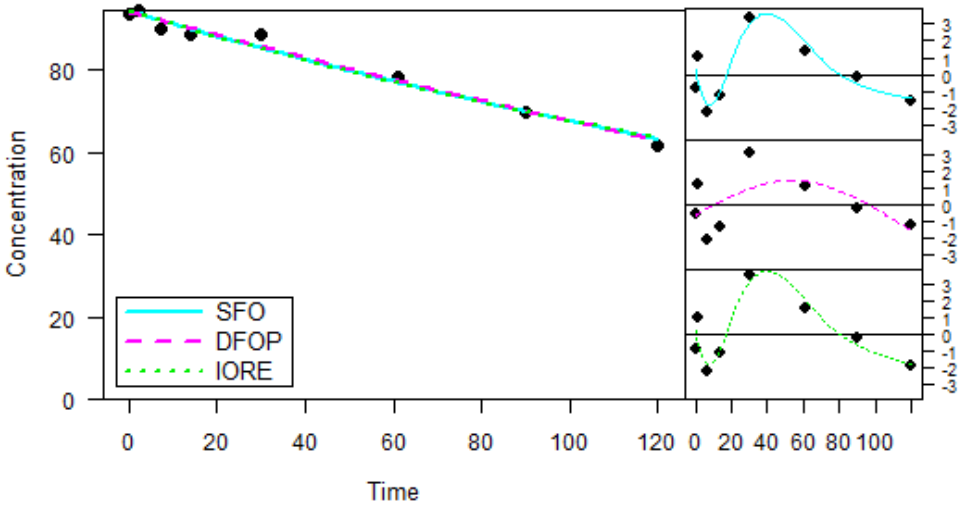


	DT_{50}	DT_{90}	χ^2	C_0	Parameters
SFO	101	334	3.7	98	k = 0.00689
DFOP	100	269	2.4	94.3	f = -0.321, k_0 = 0.0405, k_1 = 0.0096
IORE	100	177	2.9	96.4	N = -0.0469, k = 0.586

S_C	86.2
S_{SFO}	102
Slow $t_{1/2}$	72.2
$t_{R\ IORE}$	53.3

Aerobic metabolism of TPA in silt loam soil

Days	% AR
0	93.4
2	94.6
7	89.8
14	88.7
30	88.6
61	78.3
90	69.7
120	61.6



	DT_{50}	DT_{90}	χ^2	C_0	Parameters
SFO	208	692	1.7	94.2	k = 0.00333
DFOP	197	580	1.7	93.9	f = -0.622, k_0 = 0.00732, k_1 = 0.00466
IORE	218	881	1.8	94.3	N = 1.23, k = 0.00121

S_C	40.4
S_{SFO}	23.9
Slow $t_{1/2}$	149
$t_{R\ IORE}$	265

Kinetics models: Single First Order (SFO); Double First Order in Parallel (DFOP), and Indeterminate Order Rate Equation (IORE). Calculated half-lives and model parameters in accordance with the NAFTA kinetics guidance (USEPA, 2012).

Table 8. Transformation Products of TPA in Soil.

	Transformation Products	Maximum %AR Observed	Associated Interval (days)	Final %AR Observed	Final Interval (days)
UK Sandy loam soil (20°C, pH 3.9)	None	--	--	--	--
UK Sandy clay loam soil (20°C, pH 7.3)	None	--	--	--	--
UK Silt loam soil (20°C, pH 6.2)	None	--	--	--	--

Data obtained from Tables 4-6, pp. 33-34, in the study report.

An aerobic transformation pathway in soil was not provided by the study author.

III. STUDY DEFICIENCIES AND REVIEWER'S COMMENTS

1. During the study, unextracted residues comprised maximums of 21.5% in the sandy clay loam soil and 14.3% in the silt loam soil (Tables 2-3, pp. 32-33). The study author failed to use solvents with a range of dielectric constants (including a nonpolar solvent) to maximize extraction of the residues.

2. Single samples were collected and analyzed. It is preferred that duplicate samples be analyzed at each interval so that sample variability can be assessed.

3. No US soils were used (Appendix 4, pp. 62-64). The soils were from the UK and were not compared to US soils.

4. The incubation temperature was reported to be 20 ± 2°C; supporting documentation was not provided (p. 21).

5. The study was conducted with a transformation product of DCPA.

6. Aged sorption coefficients were determined by shaking day 61 soils with 0.01M $CaCl_2$ for *ca*. 24 hours (p. 23). The extracts were analyzed by LSC and HPLC. The soils were then extracted with acetonitrile:water (1:1, v:v) by shaking (30 minutes/extraction) at room temperature (p. 22). The extracts were analyzed by LSC and HPLC. The aged sorption coefficients are shown below (p. 29).

Unit	Organic Carbon	Organic Matter	K_d	K_{oc}[1]	K_{om}[2]
PT103	1.2	2.1	0.239	19.9	11.4
SK920191	2.1	3.6	0.304	14.5	8.44
SK15556090	4.2	7.2	0.500	11.9	6.94

[1] where: $K_{oc}\ (mL/g) = \frac{K_d \times 100}{Organic\ Carbon\%}$

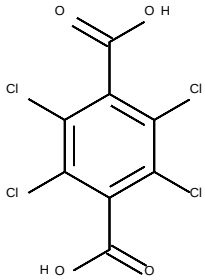
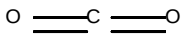
[2] where: $K_{om}\ (mL/g) = \frac{K_d \times 100}{Organic Matter\%}$

IV. REFERENCES

1. U.S. Environmental Protection Agency. 2008. Fate, Transport and Transformation Test Guidelines, OCSPP 835.4100, Aerobic Soil Metabolism. Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-08-016.

2. U.S. Environmental Protection Agency. 2012. NAFTA Guidance for Evaluating and Calculating Degradation Kinetics in Environmental Media.

DER ATTACHMENT 1. TPA and Its Environmental Transformation Products. [A]

Code Name/ Synonym	Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)		Final %AR (study length)
PARENT							
TPA (Chlorthal, Dacthal diacid, SDS-954)	**IUPAC:** 2,3,5,6-Tetrachloroterephthalic acid **CAS #:** 2136-79-0 **Formula:** $C_8H_2Cl_4O_4$ **MW:** 303.9 g/mol **SMILES:** c1(c(c(c(c(c1Cl)Cl)C(=O)O)Cl)Cl)C(=O)O		835.4100 Aerobic soil metabolism	49307516	PRT		PRT
MAJOR (>10%) TRANSFORMATION PRODUCTS							
Carbon dioxide	**IUPAC:** Carbon dioxide **Formula:** CO_2 **MW:** 44 g/mol **SMILES:** C(=O)=O		835.4100 Aerobic soil metabolism	49307516	Sandy loam	1.4% (120 d)	1.4% (120 d)
					Sandy clay loam	**34.8%** (120 d)	**34.8%** (120 d)
					Silt loam	**20.3%** (120 d)	**20.3%** (120 d)
Unextractable residues	NA	NA	835.4100 Aerobic soil metabolism	49307516	Sandy clay loam	**21.5%** (120 d)	**21.5%** (120 d)
					Silt loam	**14.3%** (120 d)	**14.3%** (120 d)
MINOR (<10%) TRANSFORMATION PRODUCTS							
No minor transformation products were identified.							
REFERENCE COMPOUNDS NOT IDENTIFIED							
All compounds used as reference compounds were identified.							

[A] AR means “applied radioactivity”. MW means “molecular weight”. PRT means "parent". NA means “not applicable”.

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Attachment 2: Statistics Spreadsheets and Graphs

DER Attachment 3: Calculations

Calculations were performed by the reviewer using PestDF, and the following equations.

Single First-Order (SFO) Model

$$C_t = C_0 e^{-kt} \quad \text{(eq. 1)}$$

where,

C_t = concentration at time t (%)
C_0 = initial concentration (%)
e = Euler's number (-)
k = SFO rate constant of decline (d^{-1})
t = time (d)

The SFO equation is solved with PestDF by adjusting C_0 and k to minimize the objective function (S_{SFO}) shown in equation 9.

DT_{50} = natural log (2)/k (eq. 2)

DT_{90} = ln (10)/k (eq. 3)

Indeterminate Order Rate Equation (IORE) Model

$$C_t = \left[C_0^{(1-N)} - (1-N)k_{IORE}t\right]^{\left(\frac{1}{1-N}\right)} \quad \text{(eq. 4)}$$

where,

N = order of decline rate (-)
k_{IORE} = IORE rate constant of decline (d^{-1})

This equation is solved with PestDF by adjusting C_0, k_{IORE}, and N to minimize the objective function for IORE (SIORE) (See equation 9). Half-lives for the IORE model are calculated using equation 5, which represents a first-order half-life that passes through the DT_{90} of the IORE model. (Traditional DT_{50} and DT_{90} values for the IORE model can be calculated using equations 6 and 7.)

$$t_{IORE} = \frac{\log(2)}{\log(10)} \frac{{C_0}^{1-N}\left(1-0.1^{(1-N)}\right)}{(1-N)k_{IORE}} \quad \text{(eq. 5)}$$

$$DT_{50} = \frac{(C_0/2)^{(1-N)} - C_0^{(1-N)}}{k(N-1)} \quad \text{(eq. 6)}$$

$$DT_{90} = \frac{(C_0/10)^{(1-N)} - C_0^{(1-N)}}{k(N-1)} \quad \text{(eq. 7)}$$

Double First-Order in Parallel (DFOP) Model

$$C_t = C_0 g^{-k_1 t} + C_0 (1-g)^{-k_1 t} \quad \text{(eq. 8)}$$

where,

g = the fraction of C_0 applied to compartment 1 (-)
k_1 = rate constant for compartment 1 (d^{-1})
k_2 = rate constant for compartment 2 (d^{-1})

If $C_0 \times g$ is set equal to a and $C_0(1-g)$ is set equal to c, then the equation can be solved with R kinetics software for a, c, k_1, and k_2 by minimizing the objective function (S_{DFOP}) as described in equation 9.

DT_{50} and DT_{90} values can be calculated using equations 2 and 3, with k_1 or k_2 in place of k.

Objective Function: SFO, IORE, and DFOP are solved by minimizing the objective function (S_{SFO}, S_{IORE}, or S_{DFOP}).

$$S_{SFO}, S_{IORE}, \text{ or } S_{DFOP} = \sum (C_{model,t} - C_{d,t})^2 \quad \text{(eq. 9)}$$

where,

S_{SFO} , S_{IORE}, or S_{DFOP} = objective function of kinetics model fit ($\%^2$)
n = number of data points (-)
$C_{model,t}$ = modeled value at time corresponding to $C_{d,t}$ (%)
$C_{d,t}$ = experimental concentration at time t (%)

Critical Value to Determine Whether SFO is an Adequate Kinetics Model

If S_{SFO} is less than S_C, the SFO model is adequate to describe kinetics. If not, the faster of t_{IORE} or the DFOP DT_{50} for compartment 2 should be used.

$$S_c = S_{IORE}\left(1 + \frac{p}{n-p} F(\alpha, p, n-p)\right) \quad \text{(eq. 10)}$$

where,

S_c = the critical value that defines the confidence contours ($\%^2$)
p = number of parameters (3 in this case)
α = the confidence level (0.50 in this case)
F(α, p, n-p) = F distribution with α level of confidence and degrees of freedom p and n-p