US EPA ARCHIVE DOCUMENT

Data Evaluation Report on the aerobic biotransformation of chlorothalonil in water-sediment system

PMRA Submission Number {.....} EPA MRID Number 45908001

Data Requirement: PMRA Data Code:
EPA DP Barcode: D301503
OECD Data Point:
EPA Guideline: 162-4

Test material:
Common name: Chlorothalonil.
Chemical name
IUPAC: Tetrachloroisophthalonitrile.
CAS name: 2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile.
CAS No: 1897-45-6.
Synonyms: 2,4,5,6-Tetrachloro-1,3-dicyanobenzene.
Bravo, Daconil 2787, Exotherm termil, Forturf, Tuffcide.
SMILES string: Clc1c(c(c(c(c1C#N)Cl)C#N)Cl)Cl.

Primary Reviewer: Lynne Binari
Dynamac Corporation

Signature:
Date:

QC Reviewer: Kathleen Ferguson
Dynamac Corporation

Signature:
Date:

Secondary Reviewer: Lucy Shanaman
EPA

Signature: Lucy Shanaman
Date: September 19, 2005

Company Code:
Active Code:
Use Site Category:
EPA PC Code: 081901

CITATION: Kirkpatrick, D. 1996. Chlorothalonil degradability and fate in water/sediment systems. Unpublished study performed by Huntingdon Life Sciences Ltd., Cambridgeshire, England; prepared by Technology Sciences Group Inc., Washington, D.C.; sponsored and submitted by Vischim S.r.L., Milan, Italy. Report No.: VCM 45/962245 (p.3). Experiment initiation December 6, 1994, and completion June 1996 (p.11). Final report issued September 19, 1996.

US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

EXECUTIVE SUMMARY:

The biotransformation of [phenyl-U-^{14}C]- labeled 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile (chlorothalonil) was studied in running ditch water-clay sediment (water pH 6.73, organic carbon 27.8 mg/L; sediment pH 7.3, organic carbon 5.8%) and pond water-clay loam sediment (water pH 5.24-5.46, organic carbon 12-19.6 mg/L; sediment pH 8.0-8.6, organic carbon 0.8-1.0%) systems from the United Kingdom for 100 days under aerobic conditions in darkness at 20°C. Based on the water volume, [^{14}C]chlorothalonil was applied at a nominal rate of 0.83 mg a.i./L. The sediment:water ratios used were 1:2.7 (60 g wet wt. sediment:160 mL water) for the ditch water-clay systems and 1:1.3 (100 g wet wt. sediment:130 mL water) for the pond water-clay loam systems. This experiment was conducted in accordance with BBA Guidelines for the Official Testing of Plant Protectants (Part IV, 5-1, 1990) and in compliance with 40 CFR Part 160 GLP standards. The test systems consisted of 250-mL vessels containing water-sediment incubated in darkness in a temperature controlled room. The vessels were connected to a flow-through trapping system for the continuous collection of CO_2 and volatile organic compounds. The water-sediment systems were pre-incubated *ca.* 1 month, then following treatment, duplicate systems were collected after 0, 0.25 (6 hours), 1, 2, 7, 14, 30/35, 59/61 and 100 days of incubation. Water layers were analyzed directly. Sediment samples were sequentially extracted twice with acetonitrile, twice with acetonitrile:water (3:1, v:v), reflux-extracted overnight with acetonitrile:water (3:1, v:v), followed by a final extraction with acetone. For each sediment sample, a single pooled extract was prepared by combining aliquots of each respective extract, then the resulting pooled sample was filtered and concentrated. Water layers, sediment extracts, extracted sediment and trapping materials were analyzed for total radioactivity using LSC. Water layers and sediment extracts were analyzed for [^{14}C]chlorothalonil and its transformation products by reverse-phase HPLC; parent [^{14}C]chlorthalonil was identified by comparison to the retention time of and/or co-chromatography with unlabeled reference standard. Four nonvolatile transformation products were identified. Trichloro-1,3-dicyanobenzene was tentatively identified through TLC co-chromatography. 2,4,5-Trichloro-6-mercapto-isophthalonitrile was identified via LC/MS, 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene via HPLC and LC/MS, and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or positional isomer) is a proposed structure based on LC/MS.

The test conditions outlined in the study appear to have been maintained throughout the 3-month incubation. For both test systems, conditions in the water layers of the treated systems were moderately reducing to moderately oxidizing, whereas conditions in the sediment layers were reducing to strongly reducing. In the ditch water-clay sediment systems, redox potentials, dissolved oxygen levels and pH in the water layers averaged +165 ± 58 mV, 2.7 ± 0.8 mg/L and 7.51 ± 0.40, respectively, while redox potentials in the sediment averaged -189 ± 40 mV. In the pond water-clay loam systems, redox potentials, oxygen saturation and pH in the water layers averaged +205 ± 44 mV, 3.4 ± 1.2 mg/L and 7.65 ± 0.21, respectively, while redox potentials in the sediment averaged -125 ± 53 mV.

Overall recoveries of radiolabeled material averaged 92.0 ± 2.4% (range 86.6-95.7%) of the applied for the ditch water-clay systems and 94.7 ± 5.4% (range 86.2-108.5%) for the pond water-clay loam systems. There were no consistent patterns of decline in material balances during the 3-month study for either system. However, material balances were <90% (86.6-89.9%) at the final interval for both systems. Following application of [^{14}C]chlorothalonil to the water layer of the ditch water-clay sediment systems, [^{14}C]residues partitioned from the water phase to the sediment with average (n = 2) distribution ratios (water:sediment) of 4:1 at time 0, 1:4 at 6 hours, 1:5 at 1 day, then decreased to 1:2 at 1-2 weeks and were 1:3 thereafter. For the pond water-clay loam systems, partitioning of [^{14}C]residues from the water to the sediment was highly variable with average (n = 2) distribution ratios (water:sediment) of 9:1 at time 0, 1:5 at 6 hours, 1:3 at 1 day, 2:1 at 2 days, 1:3 at 1 week, 1:1 at 2 weeks, 1:2 at 1-2 months and 1:4 at study termination.

In the ditch water-clay sediment systems, chlorothalonil appeared to degrade rapidly with an observed half-life in the total system of <6 hours. [^{14}C]Chlorothalonil in the water layer and total system decreased from 71.4-73.2% of the applied at time 0 posttreatment to 12.2-20.7% at 6 hours, 6.1-12.1% at 1 day, 2.5-6.6% at 1 week, 0.2-2.6% at 2-4 weeks and was 0.2-1.0% at study termination. In sediment extracts, [^{14}C]chlorothalonil was detected at a maximum 6.6% at 6 hours, decreasing to 1.9-5.1% at 1-2 days and was ≤1.2% thereafter. Based on nonlinear/normal (2-parameter, unweighted) regression analysis, [^{14}C]chlorothalonil dissipated in the water layer and total system with calculated half-lives of 2.6 and 3.3 hours, respectively, with an observed DT_{50} in the sediment of 2-7 days.

In the pond water-clay loam sediment systems, recovery of chlorothalonil was variable, consequently, observed dissipation half-lives were <7 days in the water layer and total system and 7-14 days in the sediment. [^{14}C]Chlorothalonil in the water layer and total system decreased from 83.7-88.0% of the applied at time 0 to 5.0-7.0% at 6 hours, then were 15.2-16.0% at 1 day, 51.7-70.0% at 2 days, 4.0-9.1% at 1 week, 1.5-3.7% at 4 weeks and ≤1.0% thereafter. In sediment extracts, [^{14}C]chlorothalonil was ≤1.9% at any sampling interval.

Four major nonvolatile transformation products, trichloro-1,3-dicyanobenzene (R_t 15-16 min.), 2,4,5-trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min.), 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t 12-13 min.) and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or positional isomer, R_t 9-10 min.) were detected in both systems. No minor products were identified. Two unidentified [^{14}C]compounds, A/C1 (R_t 8-9 min.) and P1 (R_t 2-3 min.), were detected as major products in both systems, plus G/C7 (R_t 14-15 min.) was a major product in the ditch water-clay systems and P2 (R_t 3-4 min.) a major product in the pond water-clay loam systems. In general, the levels of nonvolatile products were similar in the two test systems.

Trichloro-1,3-dicyanobenzene (R_t 15-16 min.) was detected at maximums of 3.9-4.7% (1 week), 23.3-25.9% (6 hours-1 day) and 24.0-28.3% (6 hours-1 day) of the applied in the

US EPA ARCHIVE DOCUMENT

water layer, sediment and total system, respectively, and was 0.2-0.5%, 0.8-1.2% and 1.0-1.7%, respectively, at study termination.

4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t 12-13 min.) was detected at maximums of 3.5-4.8% (1-4 weeks), 5.2-11.7% (2-3 months) and 6.9-16.2% (1-2 months) in the water layer, sediment and total system, respectively, and was 0.8-3.6%, 2.7-10.3% and 3.6-12.8%, respectively, at termination.

2,4,5-Trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min.) was detected at maximums of ≤3.4% (2 weeks), 14.1-18.3% (6 hours) and 14.1-18.7% (6 hours) in the water layer, sediment and total system, respectively, and was ≤0.6%, 0.7-4.1% and 0.7-4.7%, respectively, at termination.

2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (R_t 9-10 min.) was detected at maximums of 2.1-3.1% (2 weeks-2 months), 8.4-9.8% (6 hours-2 days) and 8.9-10.4% (6 hours-2 days) in the water, sediment and total system, respectively, and was 0.3-0.9%, 1.7-2.3% and 2.0-3.2%, respectively, at termination.

For both systems, unidentified A/C1 (R_t 8-9 min.) was detected at maximums of 2.0-7.5% (2-4 weeks), 18.9-23.0% (1 day) and 19.5-23.6% (1 day) in the water, sediment and total system, respectively, and was 0.4-1.1%, 1.4-3.7% and 1.8-4.8%, respectively, at termination. P1 (R_t 2-3 min.) was detected at maximums of 4.6-11.4% (1-2 months), 6.8-11.2% (1-7 days) and 11.3-13.7% (1 day-2 months) in the water, sediment and total system, respectively, and was 0.8-4.7%, 1.2-3.1% and 3.3-6.7%, respectively, at termination. G/C7 (R_t 14-15 min.) was detected at maximums of 3.0-5.0% (2-4 weeks), 5.5-6.8% (2 weeks-3 months) and 7.1-9.5% (1-3 months) in the water, sediment and total system, respectively, and was 0.3-0.5%, 0.8-6.8% and 1.2-7.1%, respectively, at termination. P2 (R_t 3-4 min.) was detected at maximums of 6.2-8.8% (1-3 months), 2.0-3.4% (2 days-2 months) and 7.3-9.7% (1-3 months) in the water, sediment and total system, respectively, and was 0.7-6.2%, 0.4-2.1% and 2.7-7.3%, respectively, at termination. All remaining unidentified components were minor in the total systems with C/C3 (R_t 10-11 min.) detected at a maximum 4.4-5.8%, D/C4 (R_t 11-12 min.) at 5.1-7.7%, P3 (R_t 4-5 min.) at 4.2-7.5%, P4 (R_t 5-6 min.) at 2.6-6.8%, and I (R_t 17-18 min.) at 1.5% in the water layer only.

For both systems, extractable [^{14}C]residues in the sediment increased from 8.8-20.5% of the applied at time 0 to 65.0-68.3% at 1 day and were 27.2-34.8% at study termination, while nonextractable [^{14}C]residues increased from 0.3-2.3% at time 0 to 30.5-42.2% at 3 months. Unidentified volatilized [^{14}C]residues were detected at maximums of 29.4% (2 months) and 9.5% (2 weeks and termination) of the applied for the ditch water-clay and pond water-clay loam systems, respectively. Separate results for $^{14}CO_2$ and volatile [^{14}C]organic compounds were not provided, but, rather, only stated that the majority of the volatilized [^{14}C]residues were primarily associated with the polyurethane foam plug and PVC tubing associated with the volatiles trapping system.

US EPA ARCHIVE DOCUMENT

Based on the results, the study author proposed a transformation pathway whereby processes involving de-chlorination, oxidation and/or sulphonation of chlorothalonil yielded trichloro-1,3-dicyanobenzene (maximums of 3.9-4.7%, 23.3-25.9% and 24.0-28.3% in water, sediment and total system, respectively), 2,4,5-trichloro-6-mercapto-isophthalonitrile (maximums of ≤3.4%, 14.1-18.3% and 14.1-18.7% in water, sediment and total system, respectively), 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (maximums of 3.5-4.8%, 5.2-11.7% and 6.9-16.2% in water, sediment and total system, respectively), and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or its positional isomer; maximums of 2.1-3.1%, 8.4-8.9% and 8.9-10.4% in water, sediment and total system, respectively). Additionally, chlorothalonil yielded nine unidentified nonvolatile [^{14}C]components (four detected at ≥ 10% of the applied) plus unidentified volatile [^{14}C]residues (CO_2 plus organic volatiles, maximums of 9.5-29.4% of applied).

In a supplemental experiment, the presence of chlorothalonil, at 0.8 mg/L, had no apparent impact on the microbial viability of the water-sediment systems after 3 months of incubation.

Results Synopsis:

Test system used: Running ditch water-clay sediment from United Kingdom.
Linear half-life (0- to 100-day data) in water: 16.8 days ($r^2 = 0.5254$).
Non-linear half-life (0- to 100-day data) in water: 2.6 hours ($r^2 = 0.9409$).
Half-life (DT_{50}) in sediment: 2-7 days.
Linear half-life (0- to 100-day data) in total system: 21.0 days ($r^2 = 0.4450$).
Non-linear half-life (0- to 100-day data) in total system: 3.3 hours ($r^2 = 0.9006$).
Major transformation products:
- Trichloro-1,3-dicyanobenzene (maximum of 24.0% in total system).
- 2,4,5-Trichloro-6-mercapto-isophthalonitrile (maximum of 14.1% in sediment only).
- 4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (maximum 16.2% in total system).
- Unidentified A/C1 (R_t 8-9 min.; maximum 23.6% in total system).
- Unidentified G/C7 (R_t 14-15 min.; maximum 9.5% in total system).
- Unidentified P1 (R_t 2-3 min.; maximum 11.3% in total system).
- Unidentified volatilized [^{14}C]residues (maximum 29.4%).

Minor identified transformation products:
- 2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate.

Test system used: Pond water-clay loam sediment from United Kingdom.
Linear half-life (0- to 100-day data) in water: 13.2 days ($r^2 = 0.6706$).
Non-linear half-life (0- to 100-day data) in water: 3.4 hours ($r^2 = 0.4280$).
Half-life (DT_{50}) in sediment: 7-14 days.
Linear half-life (0- to 100-day data) in total system: 13.4 days ($r^2 = 0.6699$).
Non-linear half-life (0- to 100-day data) in total system: 3.5 hours ($r^2 = 0.4185$).
Major transformation products:
- Trichloro-1,3-dicyanobenzene (maximum of 28.3% in total system).

US EPA ARCHIVE DOCUMENT

2,4,5-Trichloro-6-mercapto-isophthalonitrile (maximum of 18.7% in total system).
2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (or its positional isomer; maximum of 10.4% in total system).
Unidentified A/C1 (R_t 8-9 min.; maximum of 19.5% in total system).
Unidentified P1 (R_t 2-3 min.; maximum of 13.7% in total system).
Unidentified P2 (R_t 3-4 min.; maximum of 9.7% in total system).
Unidentified volatilized [^{14}C]residues (maximum 9.5%).

Minor identified transformation products:
4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene.

Study Acceptability: This study is classified as **supplemental**. This study, conducted with [phenyl-U-^{14}C]chlorothalonil, can not be used to fully meet the requirement for an aerobic aquatic metabolism study because the stability of parent chlorothalonil and its degradates during storage prior to analysis was not addressed.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with BBA Guidelines for the Official Testing of Plant Protectants (Part IV, 5-1, 1990; p.17). The following deviations from USEPA Subdivision N Guideline §162-4 were noted:

The stability of parent chlorothalonil and its degradates during storage prior to analysis was not addressed. This may affect the validity of the study.

Not all degradates detected at ≥10% of the applied were identified. This does not affect the validity of the study.

COMPLIANCE: This study was conducted in compliance with USEPA GLP Standards 40 CFR, Part 160 (1983, 1989), United Kingdom Compliance Programme GLP (1989), EC Council Directive 87/18 EEC (1986), OECD Principles of GLP (1992) and Japan Ministry of Agriculture, Forestry and Fisheries 59 NohSan (1984; p.3). Signed and dated Data Confidentiality, GLP and Quality Assurance statements were provided (pp.2-4).

A. MATERIALS:

US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

1. Test Material: [Phenyl-U-^{14}C]- labeled 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile (chlorothalonil; p.12).

Chemical Structure: See DER Attachment 2.

Description: Technical, crystalline solid (pp.12-13).

Purity: Radiochemical purity: ≥99.0% (Figure 1, p.57).
Lot No.: CFQ7386 (p.12).
Analytical purity: not reported.
Specific activity: 102.6 µCi/mg (3.8 MBq/mg, p.12).
Location of radiolabel: Uniformly in phenyl ring.

Storage conditions of test chemical: At <-15°C in darkness (Appendix 2, p.75).

Table 1: Physico-chemical properties of chlorothalonil.

Parameter	Values	Comments
Molecular weight:	265.9 g/mol.	
Molecular formula:	$C_8Cl_4N_2$.	
Water solubility:	0.6 mg/L.	At 20°C.
Solubility in acetone:	20 g/L.	At 20°C.
Melting point:	250-251°C.	
Vapor pressure/volatility:	Not reported.	
UV absorption:	Not reported.	
pK_a:	Not reported.	
K_{ow}/log K_{ow}:	Not reported.	
Stability of compound at room temperature:	Not reported.	

Data obtained from p.12 of the study report.

2. Water-sediment collection, storage and properties:

Table 2: Description of water-sediment collection and storage.

Description		Houghton Meadow	Bury Pond
Geographic location:		Running water ditch in Cambridgeshire, U.K. Ordinance survey map reference TL293715	Static pool in Cambridgeshire, U.K. Ordinance survey map reference TL281843.
Collection date:		Primary and repeat time 0 experiments: October 31, 1994.	Primary experiment: February 22, 1995. Repeat time 0 experiment: May 1, 1996.
Pesticide use history at the collection site:		Not reported.	
Collection procedures:	Water:	Not reported.	
	Sediment:	Not reported.	
Sampling depth:	Water:	Not reported.	
	Sediment:	Not reported.	
Storage conditions:		Water and sediment were stored at 4°C in darkness until use; not specified if water and sediment stored combined or separately.	
Storage length:		Primary experiment: 2 days after collection. Repeat time 0 experiment: 141 days after collection. Water-sediment systems were prepared and incubated for 33 (primary) or 34 (repeat) days prior to treatment.	Primary and repeat time 0 experiments: 1 day after collection, water-sediment systems were prepared and incubated for 27 (primary) or 32 days (repeat) days prior to treatment.
Preparation:	Water:	Water was filtered through a 212-µm sieve.	
	Sediment:	Sediment was passed through a 2-mm sieve.	

Data obtained from pp.16-17; Table III, p.35; Table V-VIII, pp.37-40; Appendix 2, p.76 of the study report.

US EPA ARCHIVE DOCUMENT

Table 3: Properties of the waters.

Property		Houghton Meadow		Bury Pond			
				Primary		Repeat time 0	
Temperature (C°)[1]:		11.5.		5.4		11	
pH[1]:		6.73		5.46		5.24	
Redox potential (mV):		Initial[1]:	Final[2]:	Initial[1]:	Final[3]:	Initial[1]:	Final[4]:
		+251	+170, +200	+240	+200, +250	+225	+160, +240
Oxygen concentration (%):		Initial[1]:	Final[2]:	Initial[1]:	Final[3]:	Initial[1]:	Final[4]:
	At surface:	40	25, 30	120	20, 26	92	36, 41
	Water-sediment interface:	37		50		38	
Dissolved organic carbon (mg/L):		27.8.		12		19.6	
Hardness (mg $CaCO_3$/L):		428		690		578	
Electrical conductivity (µmhos):		Not reported.					
Biomass (mg microbial C/100 g or CFU or other):		Not reported.					

[1]At collection site (Table III, p.35).
[2]At 100 days posttreatment for primary experiment. In water layers of repeat time 0 systems, redox potentials +230 mV, +250 mV and oxygen concentrations 20%, 25% (Table IX, p.41).
[3]At 100 days posttreatment (Table X, p.42).
[4]At day 0 posttreatment (Table X, p.42).
Data obtained from Tables III-IV, pp.35-36; Tables IX-X, pp.41-42 of the study report.

US EPA ARCHIVE DOCUMENT

Table 4: Properties of the sediments.

Property	Houghton Meadow		Bury Pond			
			Primary		Repeat time 0	
Textural classification:	Clay.		Clay loam.		Clay loam.	
% sand (2000-50 µm):	29.82		40.06		40.83	
% silt (50-2 µm):	23.61		29.43		28.48	
% clay (<2 µm):	46.57		30.50		30.69	
pH:	7.3		8.0		8.6	
Organic carbon (%):	5.8		0.8		1.0	
CEC (meq/100 g):	51.4		16.1		14.1	
Redox potential (mV):	Initial[1]:	Final[2]:	Initial[1]:	Final[3]:	Initial[1]:	Final[4]:
	-66	-120, -108	-406	-95, -70	-54	-60, -45
Bulk (particle) density:	Not reported.					
Biomass (µC/g):	163.34		40.14		nd[5]	

[1]At collection site (Table III, p.35).
[2]At 100 days posttreatment for primary experiment. In sediment of repeat time 0 systems, redox potentials -120 mV, -108 mV (Table IX, p.41).
[3]At 100 days posttreatment (Table X, p.42).
[4]At day 0 posttreatment (Table X, p.42).
[5]Not determined.
Data obtained from Table III, p.35; Table IV, p.36; Tables IX-X, pp.41-42 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None.

2. Experimental conditions:

Table 5: Study design.

Parameter	Houghton Meadow	Bury Pond
Duration of the test:	100 days.	
Water: Filtered/unfiltered water: Type and size of filter used, if any:	 Filtered. 0.2-mm sieve.	

US EPA ARCHIVE DOCUMENT

Parameter		Houghton Meadow	Bury Pond
Amount of sediment and water per treatment:	Water (6-cm depth over sediment):	160 mL.	130 mL.
	Sediment (2.0- to 2.5-cm depth):	*ca.* 60 g wet wt.	*ca.* 100 g wet wt.
Water/sediment ratio:		2.7:1 (160 mL:60 g wet wt.).	1.3:1 (130 mL:100 g wet wt).
Nominal application rate:		0.83 mg a.i./L.	
Actual application rate:		0.78-0.81 mg a.i./L (0.125-0.129 mg/160 mL).	0.85 mg a.i./L (0.11 mg a.i./130 mL).
Control conditions, if used:		Sterile controls were not used.	
No. of Replications:	Controls, if used:	Sterile controls were not used.	
	Treatments:	For each water-sediment type, twenty pre-incubated, nonsterile systems were treated with [^{14}C]chlorothalonil; eighteen for duplicate systems at each sampling interval, plus two reserves.	
Test apparatus (Type/material/volume):		Sediment and water were combined in 250-mL glass vessel (diameter *ca.* 5 cm) and incubated for 27-34 days at *ca.* 20°C in darkness prior to treatment. During pre-incubation, humidified air was purged (500-1,000 mL/minute) through the headspace of each vessel.	
Details of traps for CO_2 and organic volatiles, if any:		Humidified air was continuously purged (500-1,000 mL/minute) through each flask, then sequentially through a polyurethane foam (PUF) plug, and a single tube each of ethyl digol (2-(2-ethoxyethoxy)ethanol, Carbitol), 1M KOH and finally ethanolamine:2-ethoxyethanol. The KOH solution contained phenolphthalein indicator for CO_2.	
If no traps were used, is the system closed/open?		Volatiles traps were used with continuous air-flow (500-1,000 mL/minute).	
Identity and concentration of co-solvent:		Acetonitrile, final concentration *ca.* 0.06-0.07% based on water layer; 95-100 µL test solution in 130-160 mL water (specifics for each water-sediment system were not reported).	
Test material application:	Volume of test solution used/treatment:	95-100 µL of 1.1-1.3 mg/mL test solution.	
	Application method:	Applied to water layer; additional information not reported .	
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.	
Biomass (mg microbial C/100 g, CFU or other) of controls:		Sterile controls were not used.	
Biomass of treated (µC/g sediment):		Initial[1]:	Final[2]: Initial[1]: Final[2]:

US EPA ARCHIVE DOCUMENT

Parameter		Houghton Meadow		Bury Pond	
		163.34	515.02	40.14	100.37
Experimental conditions:	Temperature (°C):	20.3 ± 0.5°C; maintained in temperature-controlled room.			
	Continuous darkness (Yes/No):	Yes.			
Other details, if any:		For each system type, twelve additional water-sediment systems were prepared and pre-incubated as described above, then six of those systems were treated with unlabeled chlorothalonil (purity 99.8%, Batch No.: 14/09/93/1) for microbial biomass determinations at study termination .			

[1]Initial conducted with untreated sediment at day 0 following pre-incubation (Table IV, p.36; Appendix 2, p.79).
[2]Final at 100 days using sediment treated with unlabeled chlorothalonil.
Data obtained from pp.9-11, 13, 17-19, 21; Tables IV-VIII, pp.36-40; Figure 2, p.58; Appendix 2, p.79 of the study report.

3. Aerobic conditions: Humidified air was continuously purged (500-1,000 mL/minute) through the headspace of each system vessel during the 1-month pre-incubation and following treatment (pp.17-18). In Houghton Meadow water-clay sediment systems at day 0 posttreatment (repeat time 0 and primary experiment 0.25-day), redox potentials, oxygen concentrations and pH in the water layers were +210 to +250 mV, 1.8-3.6 mg/L and 7.39-7.76, respectively, with redox potentials in the sediment of -158 to -108 mV (Table IX, p.41). In Bury Pond water-clay loam sediment systems at day 0, redox potentials, oxygen concentrations and pH in the water layers were +160 to +240 mV, 2.8-3.8 mg/L and 7.56-7.91, respectively, with redox potentials in the sediment of -175 to -45 mV (Table X, p.42).

4. Supplementary experiment: High dose (2x) rate experiment. To facilitate identification of nonvolatile degradates of chlorothalonil, eight additional Bury Pond water-clay loam sediment systems were prepared as described above and pre-incubated for 119 days (Report Amendment No. 1, p.103). Following pre-incubation, the systems were treated with [^{14}C]chlorothalonil at 1.6 mg a.i./L (2x rate, 100 µL of 2.1 mg/mL test solution) then incubated as described above under continuous air flow (500 mL/minute), but with no volatiles trapping system. All eight treated systems were taken for analysis at 7 days posttreatment, then processed and analyzed as described below.

US EPA ARCHIVE DOCUMENT

5. Sampling:

Table 6: Sampling details.

Criteria	Houghton Meadow	Bury Pond
Sampling intervals:	0, 0.25, 1, 2, 7, 14, 30, 35[1], 59 and 100 days.	0, 0.25, 1, 2, 7, 14, 30, 61 and 100 days.
Sampling method:	Duplicate nonsterile systems (vessels) were collected at each interval[1].	
Method of collection of CO_2 and volatile organic compounds:	PUF plug and trapping solutions were collected and/or replaced at each sampling interval. Additionally, selected segments of the PVC tubing used to construct the volatiles trapping system were collected.	
Sampling intervals/times for: Sterility check, if sterile controls are used: Redox potential/dissolved oxygen/pH of water layer and redox potential of sediment:	Sterile controls were not used. Measured at each sampling interval	
Sample storage before analysis:	Water and sediment were separated and sediment extracted the day of collection. Water layers, sediment extracts, PUF plugs and PVC tubing were stored at -20°C prior to analysis. The study author reported that initial analysis of water layers and sediment extracts typically occurred within 1 and 3 months, respectively, of collection; specific storage intervals were not provided.	
Other observations, if any:	Additional nonsterile systems were incubated alongside the [^{14}C]chlorothalonil treated systems and used for microbial biomass determinations after 0 (untreated systems) and 100 days (treated with unlabeled chlorothalonil) of incubation.	

[1]One of the duplicate systems collected at 30 days posttreatment apparently had not been treated with [^{14}C]chlorothalonil; therefore, a single reserve system was taken at 35 days posttreatment (p.19).
Data obtained from pp.17, 19-21; Tables IX-XII, pp.41-44; Appendix 2, p.79 of the study report.

C. ANALYTICAL METHODS:

Separation of the sediment and water: The method used to separate the water layer from the sediment was not specified (p.19). Following separation, aliquots (1 mL x 2) of the water layer were analyzed for total radioactivity by LSC (p.19).

Extraction/clean up/concentration methods: Aliquots (volume not specified) of the water layers were analyzed directly by HPLC (p.24).

Sediment was sequentially extracted twice with acetonitrile (extracts 1 and 2) followed by twice with acetonitrile:water (3:1, v:v, extracts 3 and 4). All extraction solvent volumes were 150 mL (p.20). Each extraction was done using sonication for 15 minutes followed by shaking

US EPA ARCHIVE DOCUMENT

(mechanism not specified) for 15 minutes; sediment and extract were separated by centrifugation (2,000 rpm, 15 minutes). Extracted sediments were further reflux-extracted overnight with acetonitrile:water (3:1, v:v, volume not specified, extract 5), followed by a final extraction with acetone (150 mL, extract 6) via sonication and shaking (15 minutes each). Duplicate aliquots (volume not specified) of each extract were analyzed for total radioactivity using LSC. For each sediment sample, a single pooled extract were prepared by combining aliquots (10% by volume) of each respective extract (Extracts 1-6, p.24). The pooled extract sample was filtered (0.2 µm) and reduced to dryness via rotary evaporation (temperature not specified), with the resulting residues reconstituted in acetonitrile for HPLC and TLC analyses.

High dose (2x) rate experiment. Two pooled bulk samples (metabolite isolation A and B) were prepared, each consisting of four of the water-sediment systems (Report Amendment No. 1: p.103). Water and sediment were separated by centrifugation (2,000 rpm, 15 minutes), then the water layer was decanted and aliquots (1 mL x 2) were analyzed by LSC (Report Amendment: p.104). The sediment was sequentially extracted in the same manner as described above, expect all extraction solvent volumes were 400 mL.

To isolate degradates, metabolite isolation A extract 6 was concentrated to dryness via rotary evaporation, then the remaining extracts (1-5) were added to the residue and further concentrated to *ca.* 5 mL (Report Amendment No. 1: p.108). The sample was taken to volume (10 mL) with acetonitrile, filtered (13 mm, 0.45 µm PTFE syringe filter), then aliquots were analyzed by LSC (100 µL x 2), HPLC, LC/MS, MS and MS/MS (methods described below). Multiple injections and separation via HPLC was used to isolate degradates from the concentrated sample. Respective fractions were collected, combined and concentrated under nitrogen.

Nonextractable residue determination: Extracted sediments were air-dried, then aliquots (*ca.* 0.15-0.3 g x 3) were analyzed for total radioactivity by LSC following combustion (p.20).

If needed, extracted sediment was reflux-extracted overnight with ethanolamine (1:3, w:v; p.20). Aliquots (0.3 mL x 3) of the extract were combined with cellulose powder then analyzed by LSC following combustion (p.22).

Volatile residue determination: Aliquots (1 mL x 2) of the trapping solutions were analyzed for total radioactivity using LSC (p.20).

The PUF plug was extracted with acetone (volume not specified), then brought to volume (typically 20 mL) and aliquots (0.5 mL x 2) of the extract were analyzed by LSC (p.20). Possible nonextractable [^{14}C]residues associated with the PUF matrix were quantified by LSC either following combustion or dissolution in a tissue-solubilizer. For dissolution, an aliquot (*ca.* 0.05 g) of the plug was combined with NCS II solubilizer (1.5 mL) at *ca.* 55°C for *ca.* 45 minutes,

US EPA ARCHIVE DOCUMENT

after which the sample was combined with Optisorb S scintillation solution:methanol (10 mL:2 mL) and allowed to sit overnight in darkness prior to LSC analysis (p.22).

Selected segments of the PVC tubing used in the volatiles trapping system were extracted with acetone (volume not specified), then aliquots (0.5 mL x 2) of the extract were analyzed by LSC (p.20). Possible nonextractable [^{14}C]residues associated with the PVC tubing were quantified by LSC following combustion.

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the water layers, sediment extracts, extracted sediment and volatile trapping materials (Tables XI-XII, pp.43-44).

Derivatization method, if used: A derivatization method was not employed.

Identification and quantification of parent compound: Water layers and sediment extracts were analyzed by reverse-phase HPLC under the following conditions: Zorbax R_x-C8 column (4.6 x 250 mm, particle size not specified), gradient mobile phase combining (A) pH 3 20mM ammonium formate and (B) acetonitrile [percent A:B at 0 min. 75:25 (v:v), 20 min. 0:100], injection volume not reported, flow rate 1.5 mL/minute, UV detector (254 nm), either a Reeve Analytical Model 9700 radiodetector or Raytest Ramona 5 radiodetector equipped with a 400 µL calcium fluoride cell (p.22, 28; Report Amendment No. 1, p.105). Additionally, HPLC radiochromatograms were reconstructed following fraction collection (1-minute intervals) and LSC analysis (p.23). Parent [^{14}C]chlorthalonil was identified by comparison to the retention time of and/or co-chromatography with unlabeled reference standard (p.23; Table I, p.33).

Selected samples were reportedly also analyzed using one-dimensional TLC on silica gel plates (Merck, Kieselgel F-254) developed with toluene:acetone (4:1, v:v) and on reverse-phase plates (Whatman, LKC18F) developed with methanol:water (9:1, v:v; pp.23-24). Following development, areas of radioactivity were detected and quantified using a Berthold TLC Linear Analyzer (Models 2832 or 2842) and also via a Fuji BAS2000 Autoradiographic Imaging System (supporting results were not provided). [^{14}C]Chlorothalonil was identified by co-chromatography with unlabeled reference standard, which was visualized under UV light (Table II, p.34).

Identification and quantification of transformation products: Transformation products were separated, quantified and identified via HPLC and TLC as described for the parent.

High dose (2x) rate experiment. The concentrated metabolite isolation A extract was analyzed by HPLC as described above (Report Amendment No. 1: Figure 2, p.117). [^{14}C]Compounds isolated via HPLC were also co-chromatographed with normal dose (1x) rate Houghton Meadow 6-hour sediment extract (Report Amendment No. 1: Figure 3, p.118; Figure 6, p.121; Figure 9, p.124).

US EPA ARCHIVE DOCUMENT

Samples were also analyzed by LC/MS under the following conditions: LC conditions were as described above except the flow rate was 1.0 mL/minute and a Lablogic β-RAM (Model 2A) equipped with a radio-HPLC cell were used, split ratio *ca.* 9:1 (fraction collector:MS detector), Finnigan MAT TSQ7000 MS with electrospray ionization (ESI), positive and negative modes, 3 sec./scan (Report Amendment No. 1: 107-108).

For MS and MS/MS analyses, an aliquot (*ca.* 100 µL) of the sample was injected via syringe into the ESI interface at 5 µL/min., with ionization conditions optimized against the reference standard (Report Amendment No. 1: p.108).

Table 7: Reference compounds utilized for identifying transformation products of chlorothalonil.

Applicant's code, name	Chemical Name	Purity
Isophthalonitrile	1,3-Dicyanobenzene	99.8%
Batch No.: 21/9/93	4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene	–[1]
None	4-Methoxy-2,5,6-trichloroisophthalonitrile	97.2%
Monoamide of chlorothalonil	3-Cyano-2,4,5,6-tetrachlorobenzamide	–
Diamide of chlorothalonil	2,4,5,6-Tetrachloroisophthalamide	–
Trichloro-m-dicyanobenzene	4,5,6-Trichloro-m-dicyanobenzene 2,4,6-Trichloro-m-dicyanobenzene 2,4,5-Trichloro-m-dicyanobenzene	– – –
Dichloro-m-dicyanobenzene	2,5-Dichloro-m-dicyanobenzene 2,4-Dichloro-m-dicyanobenzene	– –
None	2-Chloro-m-dicyanobenzene	–
None	4-Chloro-m-dicyanobenzene	–
Batch No.: SPS/VCM 73/1	[Phenyl-^{14}C]-labeled 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene	>97%
Batch No.: VCM/14/01	2,4,5-Trichloro-6-mercapto-isophthalonitrile	–

[1]Not reported.
Data obtained from pp.13-16; Report Amendment No. 1: p.102 of the study report.

Detection limits (LOD, LOQ) for the parent compound and transformation products: Limits of determination for LSC analyses were reported as twice background levels, but were not quantified (p.21). Detection limits for HPLC and TLC analyses were not reported.

II. RESULTS AND DISCUSSION:

US EPA ARCHIVE DOCUMENT

A. TEST CONDITIONS: For both water-sediment systems during the 100-day study, conditions in water layers of the treated systems were moderately reducing (-50 to +200 mV) to moderately oxidizing (+200 to +400 mV), whereas conditions in the sediment layers were reducing (-200 to -50 mV) to strongly reducing (-400 to -200 mV; Tables IX-X, pp.41-42). Incubation temperatures were maintained at 20 ± 0°C during the study (Tables IX-X, pp.41-42).

In Houghton Meadow water-clay sediment systems, redox potentials, dissolved oxygen concentrations and pH in the water layers were +50 to +250 mV, 1.3-4.3 mg/L (14-45%) and 6.50-8.48 , respectively, with redox potentials in the sediment of -260 to -108 mV (Table IX, p.41).

In Bury Pond water-clay loam sediment systems, redox potentials, dissolved oxygen concentrations and pH in the water layers were +100 to +250 mV, 1.8-6.1 mg/L (20-66%) and 7.20-7.96, respectively, with redox potentials in the sediment of -233 to -45 mV (Table X, p.42).

B. MATERIAL BALANCE: For Houghton Meadow water-clay sediment systems, recoveries of radiolabeled material averaged 92.0 ± 2.4% (range 86.6-95.7%, n = 18) of the applied, with no consistent pattern of decline in material balances during the 100-day study (Table XI, p.43; DER Attachment 1). Following application of [^{14}C]chlorothalonil to the water layer, [^{14}C]residues appeared to partition from the water to the sediment with average (n = 2) distribution ratios (water:sediment) of 4:1 at time 0, 1:4 at 6 hours, 1:5 at 1 day, then decreased to 1:2 at 7-14 days and were 1:3 at 30-100 days (DER Attachment 1).

For Bury Pond water-clay loam sediment systems, recoveries of radiolabeled material averaged 94.7 ± 5.4% (range 86.2-108.5%, n = 18) of the applied, with no consistent pattern of decline in material balances during the 100-day study (Table XII, p.44). Following application of [^{14}C]chlorothalonil to the water layer, partitioning of [^{14}C]residues from the water to the sediment was variable with average (n = 2) distribution ratios (water:sediment) of 9:1 at time 0, 1:5 at 6 hours, 1:3 at 1 day, 2:1 at 2 days, 1:3 at 7 days, 1:1 at 14 days, 1:2 at 30-61 days and 1:4 at 100 days (DER Attachment 1).

US EPA ARCHIVE DOCUMENT

Table 8: Biotransformation of [phenyl-U-^{14}C]chlorothalonil, expressed as percentage of applied radioactivity (mean ± s.d., n = 2), in Houghton Meadow water-clay sediment under aerobic conditions.

Compound		Sampling times (days)								
		0	0.25	1	2	7	14	30/35	59	100
Chlorothalonil	water	72.1 ± 0.7	13.2 ± 1.0	8.2 ± 2.1	12.7 ± 1.6	4.0 ± 1.5	0.6 ± 0.4	1.4 ± 1.0	0.3 ± 0.2	0.3 ± 0.1
	sediment	0.6 ± 0.2	4.7 ± 2.0	2.9 ± 1.0	4.5 ± 0.7	0.6 ± 0.5	0.6 ± 0.5	0.2 ± 0.1	0.9 ± 0.3	0.6 ± 0.0
	system[3]	72.7 ± 0.5	17.9 ± 2.9	11.1 ± 1.0	17.2 ± 2.3	4.6 ± 0.7	1.2 ± 0.9	1.6 ± 1.1	1.2 ± 0.1	0.9 ± 0.2
Trichloro-1,3-dicyanobenzene (R, 15-16 min)	water	<0.1[4]	0.5 ± 0.1	0.6 ± 0.1	0.8 ± 0.4	2.9 ± 1.0	1.9 ± 0.3	0.9 ± 0.0	0.4 ± 0.1	0.3 ± 0.1
	sediment	5.4 ± 0.8	11.5 ± 5.6	20.0 ± 3.3	20.0 ± 0.3	15.3 ± 3.4	12.4 ± 1.5	5.0 ± 0.3	1.3 ± 0.3	0.9 ± 0.0
	system	5.4 ± 0.8	12.0 ± 5.5	20.6 ± 3.4	20.8 ± 0.8	18.2 ± 2.4	14.3 ± 1.3	5.9 ± 0.4	1.6 ± 0.2	1.2 ± 0.0
4-Hydroxy-2,5,6-trichloro-1,3-dicyano-benzene (R, 12-13 min)	water	<0.1	0.9 ± 0.1	1.2 ± 0.2	1.2 ± 0.6	4.0 ± 0.8	3.3 ± 1.4	2.7 ± 1.5	3.7 ± 0.9	3.1 ± 0.6
	sediment	1.2 ± 0.1	2.1 ± 0.3	4.2 ± 0.8	3.7 ± 0.1	3.5 ± 0.5	3.9 ± 1.5	3.7 ± 0.1	8.6 ± 3.2	9.6 ± 0.8
	system	1.2 ± 0.1	3.0 ± 0.3	5.3 ± 0.7	4.8 ± 0.4	7.5 ± 1.3	7.2 ± 2.9	6.4 ± 1.6	12.2 ± 4.0	12.6 ± 0.2
2,4,5-Trichloro-6-mercapto-isophthalonitrile (R, 13-14 min)	water	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1
	sediment	1.5 ± 1.3	12.2 ± 1.9	4.8 ± 0.2	3.6 ± 0.1	2.8 ± 0.9	2.9 ± 0.7	3.7 ± 0.0	1.1 ± 0.4	0.8 ± 0.1
	system	1.5 ± 1.3	12.2 ± 1.9	4.8 ± 0.2	3.6 ± 0.1	2.8 ± 0.9	2.9 ± 0.7	3.7 ± 0.0	1.1 ± 0.4	0.8 ± 0.1
2,5,6-Trichloro-1,3-dicyano-benzene-4-sulphonate (R, 9-10 min)	water	<0.1	0.5 ± 0.4	0.5 ± 0.1	0.3 ± 0.2	1.5 ± 0.2	0.9 ± 0.2	1.5 ± 0.3	1.4 ± 0.8	0.5 ± 0.2
	sediment	1.2 ± 0.5	2.4 ± 0.3	4.0 ± 1.9	5.6 ± 2.8	2.9 ± 0.3	1.3 ± 1.2	1.4 ± 0.1	0.1 ± 0.0	1.7 ± 0.0
	system	1.2 ± 0.5	2.8 ± 0.0	4.5 ± 1.8	5.9 ± 3.0	4.3 ± 0.1	2.1 ± 1.3	2.9 ± 0.5	1.4 ± 0.7	2.2 ± 0.2
Total Unidentified HPLC [^{14}C]Residues	water	3.0 ± 1.6	2.9 ± 0.2	4.6 ± 0.1	3.1 ± 1.4	16.5 ± 3.0	22.3 ± 1.0	18.4 ± 2.0	13.2 ± 5.5	15.7 ± 0.6
	sediment	7.0 ± 2.4	30.3 ± 4.4	31.4 ± 4.8	25.7 ± 2.1	23.9 ± 2.5	21.5 ± 0.1	26.1 ± 2.8	14.3 ± 1.3	14.5 ± 1.4
	system	10.0 ± 0.8	33.1 ± 4.6	36.0 ± 4.6	28.8 ± 0.7	40.4 ± 0.5	43.7 ± 1.2	44.5 ± 0.9	27.5 ± 6.8	30.2 ± 0.8
Total extractable sediment residues		16.9 ± 3.6	62.9 ± 2.8	67.0 ± 0.0	63.1 ± 0.1	48.9 ± 6.6	42.3 ± 0.9	39.9 ± 2.2	26.0 ± 4.1	28.0 ± 0.8
CO_2		ns[5]	--	--	--	--	--	--	--	--
Total volatile organics		ns	--	--	--	--	--	--	--	--
Total volatiles		ns	0.6 ± 0.0	0.6 ± 0.0	3.1 ± 0.9	1.7 ± 0.6	7.3 ± 3.2	6.3 ± 3.3	19.9 ± 9.6	4.8 ± 2.7
Nonextractable sediment residues		1.8 ± 0.5	9.9 ± 0.7	9.7 ± 0.1	8.1 ± 0.1	14.3 ± 2.1	13.2 ± 1.2	20.6 ± 4.5	28.3 ± 3.9	36.5 ± 5.7
Total % recovery	water	75.3 ± 2.4	18.0 ± 1.0	15.2 ± 1.7	17.9 ± 1.1	28.8 ± 3.1	28.9 ± 1.3	24.9 ± 4.8	18.8 ± 7.1	19.1 ± 0.7
	sediment	18.7 ± 4.2	72.7 ± 2.1	76.7 ± 0.1	71.2 ± 0.0	63.2 ± 4.5	55.5 ± 2.0	60.5 ± 6.7	54.3 ± 0.2	64.4 ± 5.0
	system	93.9 ± 1.8	91.2 ± 3.2	92.5 ± 1.6	92.1 ± 0.2	93.7 ± 2.0	91.6 ± 0.2	91.6 ± 1.3	93.0 ± 2.3	88.3 ± 1.6

[3]Entire system; water + sediment.
[4]Apparent limit of detection (Table XVII, p.49).
[5]No sample.
Data obtained from Table XI, p.43; Table XIII, p.45; Table XVII, pp.49-50; Table XIX, pp.53-54 of the study report and DER Attachment 1.

US EPA ARCHIVE DOCUMENT

Table 9: Biotransformation of [phenyl-U-^{14}C]chlorothalonil, expressed as percentage of applied radioactivity (mean ± s.d., n = 2), in Bury Pond water-clay loam sediment under aerobic conditions.

Compound		Sampling times (days)								
		0	0.25	1	2	7	14	30	61	100
Chlorothalonil	water	85.8 ± 2.1	5.6 ± 0.5	15.3 ± 0.1	60.6 ± 8.8	5.6 ± 1.6	2.2 ± 0.7	0.3 ± 0.2	0.4 ± 0.3	0.3 ± 0.2
	sediment	0.1 ± 0.1	1.0 ± 0.1	0.7 ± 0.1	0.3 ± 0.3	1.2 ± 0.7	0.6 ± 0.3	0.2 ± 0.1	0.2 ± 0.2	<0.1[2]
	system[3]	85.9 ± 2.0	6.6 ± 0.5	16.0 ± 0.0	60.9 ± 9.1	6.8 ± 2.3	2.8 ± 1.0	0.5 ± 0.1	0.6 ± 0.4	0.3 ± 0.2
Trichloro-1,3-dicyanobenzene (R_t 15-16 min)	water	<0.1	1.4 ± 1.0	0.4 ± 0.1	0.7 ± 0.2	2.9 ± 1.9	3.5 ± 0.4	1.0 ± 0.3	0.7 ± 0.2	0.4 ± 0.2
	sediment	2.3 ± 0.7	16.9 ± 9.1	17.4 ± 1.7	2.9 ± 2.2	9.5 ± 1.0	7.7 ± 0.3	6.5 ± 1.2	5.1 ± 0.5	1.0 ± 0.2
	system	2.3 ± 0.7	18.3 ±10.1	17.8 ± 1.6	3.6 ± 2.1	12.4 ± 0.9	11.1 ± 0.7	7.4 ± 0.9	5.8 ± 0.7	1.4 ± 0.3
4-Hydroxy-2,5,6-trichloro-1,3-dicyano-benzene (R_t 12-13 min)	water	<0.1	1.4 ± 0.0	0.9 ± 0.1	2.6 ± 0.8	1.9 ± 0.4	2.5 ± 0.3	3.5 ± 0.0	1.9 ± 0.5	0.9 ± 0.0
	sediment	0.3 ± 0.1	1.5 ± 0.3	2.9 ± 0.6	1.9 ± 0.5	3.4 ± 0.0	1.8 ± 0.2	3.4 ± 0.0	2.0 ± 0.2	4.0 ± 1.3
	system	0.3 ± 0.1	2.8 ± 0.3	3.8 ± 0.5	4.4 ± 1.2	5.3 ± 0.4	4.2 ± 0.4	6.9 ± 0.1	3.9 ± 0.7	4.8 ± 1.2
2,4,5-Trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min)	water	<0.1	0.4 ± 0.0	0.2 ± 0.1	0.4 ± 0.2	0.6 ± 0.1	3.2 ± 0.3	1.8 ± 0.9	1.3 ± 0.7	0.5 ± 0.2
	sediment	1.3 ± 0.1	10.6 ± 7.7	9.7 ± 4.2	1.3 ± 0.5	9.1 ± 3.1	2.4 ± 0.7	2.6 ± 0.9	1.3 ± 0.1	3.5 ± 0.6
	system	1.3 ± 0.1	11.0 ± 7.7	9.9 ± 4.2	1.6 ± 0.3	9.7 ± 3.0	5.5 ± 0.9	4.4 ± 0.1	2.6 ± 0.6	4.0 ± 0.8
2,5,6-Trichloro-1,3-dicyano-benzene-4-sulphonate (R_t 9-10 min)	water	<0.1	0.5 ± 0.2	0.3 ± 0.1	0.6 ± 0.2	1.3 ± 0.3	2.0 ± 1.1	1.8 ± 0.4	1.5 ± 0.3	0.8 ± 0.2
	sediment	0.3 ± 0.1	9.8 ± 0.0	6.0 ± 3.3	3.8 ± 1.1	8.3 ± 0.7	3.8 ± 1.1	3.4 ± 0.6	2.1 ± 1.0	2.2 ± 0.2
	system	0.3 ± 0.1	10.3 ± 0.2	6.3 ± 3.3	4.4 ± 1.3	9.5 ± 0.4	5.8 ± 2.2	5.2 ± 0.3	3.6 ± 1.3	2.9 ± 0.3
Total Unidentified HPLC [^{14}C]Residues	water	0.3 ± 0.2	7.0 ± 0.4	4.5 ± 0.3	6.5 ± 2.1	12.7 ± 0.8	26.4 ± 3.0	25.1 ± 0.6	25.7 ± 2.5	12.1 ± 0.2
	sediment	5.9 ± 0.3	24.4 ± 0.6	30.1 ± 0.3	19.0 ± 3.4	29.9 ± 0.4	19.7 ± 1.9	23.3 ± 1.2	22.1 ± 1.6	21.6 ± 2.7
	system	6.2 ± 0.0	31.4 ± 1.0	34.6 ± 0.1	25.5 ± 5.6	42.6 ± 1.2	46.1 ± 4.9	48.4 ± 0.6	47.8 ± 0.9	33.7 ± 2.5
Total extractable sediment residues		10.0 ± 1.2	64.0 ± 0.3	66.7 ± 1.6	29.1 ± 2.2	61.3 ± 1.7	35.8 ± 0.2	39.2 ± 1.2	32.7 ± 1.0	32.3 ± 2.5
CO_2		ns[4]	–	--	--	--	--	--	--	--
Total volatile organics		ns	--	--	--	--	--	--	--	--
Total volatiles		ns	0.2 ± 0.1	0.9 ± 0.0	1.8 ± 0.9	1.9 ± 0.1	7.8 ± 1.8	4.4 ± 0.9	9.3 ± 0.1	9.0 ± 0.5
Nonextractable sediment residues		0.3 ± 0.0	8.1 ± 0.5	8.3 ± 1.7	4.4 ± 0.6	8.5 ± 0.5	10.2 ± 1.3	14.2 ± 0.2	19.3 ± 1.0	32.7 ± 2.2
Total % recovery	water	86.1 ± 2.3	16.0 ± 1.1	21.5 ± 0.5	71.4 ± 5.5	24.9 ± 1.2	40.6 ± 0.4	33.6 ± 1.0	31.4 ± 2.1	14.8 ± 0.4
	sediment	10.3 ± 1.2	72.1 ± 0.8	75.0 ± 0.0	33.4 ± 2.7	69.8 ± 1.2	46.0 ± 1.1	53.3 ± 1.3	52.0 ± 1.9	65.0 ± 0.3
	system	96.4 ± 1.1	88.3 ± 2.0	97.4 ± 0.5	106.6±1.9	96.6 ± 0.1	94.3 ± 0.2	91.3 ± 0.5	92.7 ± 0.0	88.7 ± 0.3

[2]Apparent limit of detection (Table XIV, p.46; Table XVIII, pp.51-52; Table XX, pp.55-56).
[3]Entire system; water + sediment.
[4]No sample.
Data obtained from Table XII, p.44; Table XIV, p.46; Table XVIII, pp.51-52; Table XX, pp.55-56 of the study report and DER Attachment 1.

US EPA ARCHIVE DOCUMENT

C. TRANSFORMATION OF PARENT COMPOUND: In Houghton Meadow water-clay sediment systems, [^{14}C]chlorothalonil in the total system and water layer decreased from 72.2-73.2% and 71.4-72.8% of the applied, respectively, at time 0 posttreatment to 10.0-20.7% and 6.1-14.3%, respectively, at 0.25-2 days, 2.5-6.6% at 7 days, 0.2-2.6% at 14-35 days and was 0.2-1.0% at 100 days (Table XVII, pp.49-50; DER Attachment 1). In sediment extracts, [^{14}C]chlorothalonil increased from 0.4-0.8% at time 0 to 1.9-6.6% at 0.25-2 days and was ≤1.2% thereafter (Table XIX, pp.53-54).

In Bury Pond water-clay loam sediment systems, [^{14}C]chlorothalonil in the total system and water layer decreased from 83.9-88.0% and 83.7-87.9% of the applied, respectively, at time 0 posttreatment to 5.0-7.0% at 6 hours, then was 15.2-16.0% at 1 day, 51.7-70.0% at 2 days, 4.0-9.1% at 7 days, 1.5-3.7% at 14 days and ≤1.0% thereafter (Table XVIII, pp.51-52; DER Attachment 1). In sediment extracts, [^{14}C]chlorothalonil was detected at ≤1.9% at any sampling interval (Table XX, pp.55-56).

HALF-LIFE/DT50: Half-life values for the dissipation of [phenyl-U-^{14}C]chlorothalonil from the water layer and total system of the treated Houghton Meadow water-sediment systems and the Bury Pond water-sediment systems were determined using linear regression analysis based on first-order kinetics as calculated by Corel Quattro Pro version 8 (Attachment 1). Highly variable recoveries of [^{14}C]chlorothalonil in the water layer and total system in the Bury Pond water-sediment systems were driven by replicate data points at the day 2 sampling interval that appear to be out of sequence. Clarification form the resistrant is needed. Additionally, half-life values for chlorothalonil in the sediments of either system were not calculated as [^{14}C]chlorothalonil was detected at ≤6.6% and ≤1.9% of the applied in the Houghton Meadow and Bury Pond sediments, respectively.

Half-life/DT_{50} values were not determined by the study author (p.28).

US EPA ARCHIVE DOCUMENT

Table 10: Half-life ($t_{1/2}$) values for the dissipation of chlorothalonil in aerobic water-sediment.

Phase	Regression type	Half-life	3 x half-life and/or DT_{90}	y-intercept	p-value	r^2
Houghton Meadow water-clay sediment						
Water:	Empirical data	DT_{50} = <6 hours	DT_{90} = 2-7 days	--	--	--
	Linear/natural log[1]	16.8 days	50.4 days	2.12	0.0010	0.5254
	Nonlinear/normal[1]	2.6 hours	7.8 hours	71.93	<0.0001	0.9409
Sediment:	Empirical data	DT_{50} = 2-7 days	DT_{90} = >100 days	--	--	--
	Linear/natural log	nd[2]	--	--	--	--
	Nonlinear/normal	nd	--	--	--	--
Total system:	Empirical data	DT_{50} = <6 hours	DT_{90} = 2-7 days	--	--	--
	Linear/natural log	21.0 days	63 days	2.31	0.0025	0.4450
	Nonlinear/normal	3.3 hours	9.9 hours	72.18	<0.0001	0.9006
Bury Pond water-clay loam sediment						
Water:	Empirical data	DT_{50} = <7 days	DT_{90} = 2-7 days	--	--	--
	Linear/natural log	13.2 days	39.6 days	2.65	<0.0001	0.6706
	Nonlinear/normal	3.4 hours	10.2 hours	47.37	0.0010	0.4185
Sediment:	Empirical data	DT_{50} = 7-14 days	DT_{90} = >100 days	--	--	--
	Linear/natural log	nd	--	--	--	--
	Nonlinear/normal	nd	--	--	--	--
Total system:	Empirical data	DT_{50} = <7 days	DT_{90} = 2-7 days	--	--	--
	Linear/natural log	13.4 days	42.2 days	2.68	<0.0001	0.6699
	Nonlinear/normal	3.5 hours	10.5 hours	47.51	<0.0001	0.4281

[1]Determined using data obtained from Table XVII, pp.49-50; Table XIX, pp.53-54 of the study report (DER Attachment 1).

TRANSFORMATION PRODUCTS: Four nonvolatile transformation products, trichloro-1,3-dicyanobenzene (R_t 15-16 min.), 2,4,5-trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min.), 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t 12-13 min.) and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or positional isomer, R_t 9-10 min.) were detected in both systems. Trichloro-1,3-dicyanobenzene (R_t 15-16 min.) and 2,4,5-trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min.) were major products in both systems. 4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t 12-13 min.) was a major product in the Houghton Meadow systems, but a minor product in the Bury Pond systems, while the reverse occurred for 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or positional isomer, R_t 9-10 min.) in the two systems. Trichloro-1,3-dicyanobenzene (R_t 15-16 min.) was identified only through TLC co-chromatography (p.29).

US EPA ARCHIVE DOCUMENT

2,4,5-Trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min.) was identified via LC/MS, 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t 12-13 min.) via HPLC and LC/MS, and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or positional isomer, R_t 9-10 min.) is a proposed structure based on LC/MS (Report Amendment No. 1: pp.111-112; Figure 5, p.120). Additionally, two unidentified [^{14}C]compounds, A/C1 (R_t 8-9 min.) and P1 (R_t 2-3 min.), were detected as major transformation products in both systems, with G/C7 (R_t 14-15 min.) a major product in the Houghton Meadow systems and P2 (R_t 3-4 min.) a major product in the Bury Pond systems.

In Houghton Meadow water-clay sediment systems, trichloro-1,3-dicyanobenzene (R_t 15-16 min.) was detected at maximums of 3.9% (7 days), 23.3% (1 day) and 24.0% (1 day) of the applied in the water layer, sediment and total system, respectively, and was 0.2-0.4%, 0.8-0.9% and 1.1-1.2%, respectively, at 100 days (Table XVII, pp.49-50; Table XIX, pp.53-54; DER Attachment 1). 4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t 12-13 min.) was detected at maximums of 4.8% (7 days), 11.7% (59 days) and 16.2% (59 days) of the applied in the water layer, sediment and total system, respectively, and was 2.5-3.6%, 8.8-10.3% and 12.4-12.8%, respectively, at 100 days. 2,4,5-Trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min.) was detected at a maximum 14.1% at 6 hours in the sediment and was 0.7-0.9% at 100 days, but was not detected (<0.1% of applied) in the water layer at any interval. 2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (R_t 9-10 min.) was detected at maximums of 2.1% (59 days), 8.4% (2 days) and 8.9% (2 days) in the water, sediment and total system, respectively.

Unidentified [^{14}C]residues (nine components plus "Others") totaled a maximum 23.3% (14 days), 36.1% (1 day) and 45.3% (35 days) in the water, sediment and total system, respectively and were 15.1-16.2%, 13.1-15.9% and 29.3-31.0%, respectively, at 100 days (DER Attachment 1). A/C1 (R_t 8-9 min.) was detected at maximums of 7.5% (14 days), 23.0% (1 day) and 23.6% (1 day) in the water, sediment and total system, respectively, and was 0.4-0.5%, 1.4-3.5% and 1.8-4.0%, respectively, at 100 days. P1 (R_t 2-3 min.) was detected at maximums of 4.6% (30 days), 11.2% (1 day) and 11.3% (1 day) in the water, sediment and total system, respectively, and was 0.8-1.4%, 2.5-3.1% and 3.3-4.5%, respectively, at 100 days. G/C7 (R_t 14-15 min.) was detected at maximums of 5.0% (35 days), 5.5% (14 days) and 9.5% (35 days) in the water, sediment and total system, respectively, and was 0.4-0.5%, 0.8% and 1.2-1.3%, respectively, at 100 days. All remaining unidentified components were minor in the total system with C/C3 (R_t 10-11 min.) detected at a maximum 5.8% (maximums of 3.0% in water, 2.8% in sediment), D/C4 (R_t 11-12 min.) at 7.7% (5.6% in water, 6.3% in sediment), P2 (R_t 3-4 min.) at 7.3% (6.2% in water, 2.0% in sediment), P3 (R_t 4-5 min.) at 4.2% (2.4% in water, 3.7% in sediment), P4 (R_t 5-6 min.) at 2.6% (1.7% in water, 1.6% in sediment), I (R_t 17-18 min.) at 1.5% in the water layer only and Others at 5.0% (4.6% in water, 3.7% in sediment).

In Bury Pond water-clay loam sediment systems, trichloro-1,3-dicyanobenzene (R_t 15-16 min.) was detected at maximums of 4.7% (7 days), 25.9% (6 hours) and 28.3% (6 hours) of the applied in the water layer, sediment and total system, respectively, and was 0.2-0.5%, 0.8-1.2% and 1.0-

US EPA ARCHIVE DOCUMENT

1.7%, respectively, at 100 days (Table XVIII, pp.51-52; Table XX, pp.55-56; DER Attachment 1). 2,4,5-Trichloro-6-mercapto-isophthalonitrile (R_t 13-14 min.) was detected at maximums of 3.4% (14 days), 18.3% (6 hours) and 18.7% (6 hours) in the water, sediment and total system, respectively, and was 0.3-0.6%, 2.9-4.1% and 3.2-4.7%, respectively, at 100 days. 2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (R_t 9-10 min.) was detected at maximums of 3.1% (14 days), 9.8% (6 hours) and 10.4% (6 hours) in the water, sediment and total system, respectively, and was 0.6-0.9%, 2.0-2.3% and 2.6-3.2%, respectively, at 100 days. 4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t 12-13 min.) was detected at maximums of 3.5% (30 days), 5.2% (100 days) and 6.9% (30 days) of the applied in the water layer, sediment and total system, respectively.

Unidentified [^{14}C]residues totaled a maximum 29.3% (14 days), 30.4% (1 day) and 50.9% (14 days) in the water, sediment and total system, respectively and were 11.9-12.3%, 18.8-24.3% and 31.1-36.2%, respectively, at 100 days (DER Attachment 1). A/C1 (R_t 8-9 min.) was detected at maximums of 2.0% (30 days), 18.9% (1 day) and 19.5% (1 day) in the water, sediment and total system, respectively, and was 0.8-1.1%, 2.2-3.7% and 3.0-4.8%, respectively, at 100 days. P1 (R_t 2-3 min.) was detected at maximums of 11.4% (61 days), 6.8% (7 days) and 13.7% (61 days) in the water, sediment and total system, respectively, and was 3.4-4.7%, 1.2-2.0% and 4.6-6.7%, respectively, at 100 days. P2 (R_t 3-4 min.) was detected at maximums of 8.8% (30 days), 3.4% (61 days) and 9.7% (30 days) in the water, sediment and total system, respectively, and was 0.7-2.3%, 0.4-2.1% and 2.7-2.8%, respectively, at 100 days. All remaining unidentified components were minor in the total system with C/C3 (R_t 10-11 min.) detected at a maximum 4.4% (maximums of 2.1% in water, 3.0% in sediment), D/C4 (R_t 11-12 min.) at 5.1% (2.5% in water, 4.9% in sediment), G/C7 (R_t 14-15 min.) at 7.1% (3.0% in water, 6.8% in sediment), P3 (R_t 4-5 min.) at 7.5% (5.7% in water, 3.5% in sediment), P4 (R_t 5-6 min.) at 6.8% (5.0% in water, 2.3% in sediment), I (R_t 17-18 min.) at 1.5% in the water layer only and Others at 5.2% (3.3% in water, 3.0% in sediment).

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: In the Houghton Meadow clay sediment, extractable [^{14}C]residues increased from 13.2-20.5% of the applied at time 0 to 67.0% at 1 day then decreased to 21.9-30.1% at 59 days and were 27.2-28.7% at 100 days (Table XI, p.43). Nonextractable residues increased from 1.3-2.3% at time 0 to 30.7-42.2% at 100 days.

In the Bury Pond clay loam sediment, extractable [^{14}C]residues increased from 8.8-11.2% at time 0 to 65.0-68.3% at 1 day, ranged from 26.9-63.0% at 2-61 days and were 29.8-34.8% at 100 days (Table XII, p.44). Nonextractable residues increased from 0.3% at time 0 to 30.5-34.8% at 100 days.

VOLATILIZATION: Unidentified volatilized [^{14}C]residues were detected at maximums of 29.4% (59 days) and 9.5% (14 and 100 days) of the applied for the Houghton Meadow and Bury Pond systems, respectively (Tables XI-XII, pp.43-44. Separate results for $^{14}CO_2$ and volatile [^{14}C]organic compounds were not provided, but, rather, only stated that the majority of the

US EPA ARCHIVE DOCUMENT

volatilized [^{14}C]residues were primarily associated with the polyurethane foam plug and PVC tubing associated with the volatiles trapping system (p.27).

TRANSFORMATION PATHWAY: The following transformation pathway was proposed by the study author: through processes involving de-chlorination, oxidation and/or sulphonation, chlorothalonil in aerobic water-sediment systems was found to form trichloro-1,3-dicyanobenzene, 2,4,5-trichloro-6-mercapto-isophthalonitrile, 4-hydroxy-2,5,6-trichloro-1,3-dicyanobenzene and 2,5,6-trichloro-1,3-dicyanobenzene-4-sulphonate (or its positional isomer; Report No. 1: Figure 11, p.126). Additionally, chlorothalonil yielded nine unidentified nonvolatile [^{14}C]components plus unidentified volatile [^{14}C]residues.

Table 11: Chemical names for identified transformation products of chlorothalonil in aerobic water-sediment.

Applicant's code	CAS Number	Chemical Name(s)	Chemical formula	Molecular weight	SMILES string
H/C-1 (R_t 15-16 min)	--[1]	Trichloro-1,3-dicyanobenzene[2]	--	--	--
F/C6 (R_t 13-14 min.)	--	2,4,5-Trichloro-6-mercapto-isophthalonitrile[3]	--	--	--
E/C5 (R_t 12-13 min.)	--	4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene[4]	--	--	--
B/C2 (R_t 9-10 min.)	--	2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (or positional isomer)[5]	--	--	--

[1]Not reported.
[2]Identification via one-dimensional, normal phase TLC co-chromatography with reference standard (p.29).
[3]Identification via LC/MS against reference standard (Report Amendment No. 1: p.112).
[4]Identification via HPLC co-elution and LC/MS against reference standard (Report Amendment No. 1: p.111).
[5]Proposed structure based on LC/MS (Report Amendment No. 1: p.111).

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Microbial viability. The presence of chlorothalonil, at *ca.* 0.8 mg/L, appeared to have no significant impact on the microbial viability of the water-sediment systems after *ca.* 3 months of incubation (Table IV, p.36). Microbial biomass values were 163 and 40 µg C/g sediment in untreated Houghton Meadow clay and Bury Pond clay loam sediments, respectively, at study initiation, and 515 and 100 µg C/g, respectively, in the chlorothalonil-treated sediments at study termination.

III. STUDY DEFICIENCIES:

1. The stability of parent chlorothalonil and its degradates during storage prior to analysis was not addressed. The study author reported that initial analysis of water layers and sediment

US EPA ARCHIVE DOCUMENT

extracts typically occurred within 1 and 3 months, respectively, of collection. However, specific storage intervals for the various samples were not provided. Given the significant amount of degradation which occurred even in the day 0 (time 0 and 6-hour) samples and the variable recoveries of parent chlorothalonil in the Bury Pond systems, the storage interval and conditions of each sample should be reported and storage stability experiments need to be conducted in order to demonstrate that degradation did not during storage prior to analysis.

2. Four nonvolatile transformation products, A/C1 (R_t 8-9 min.) and P1 (R_t 2-3 min.) in both systems, G/C7 (R_t 14-15 min.) in the Houghton Meadow systems and P2 (R_t 3-4 min.) in the Bury Pond systems, plus volatile transformation products were detected at ≥10% of the applied, but not identified. In the Houghton Meadow systems, A/C1, P1 and G/C7 were detected at maximums of 23.6%, 11.3% and 9.5% of the applied, respectively, and volatilized [^{14}C]residues were a maximum 29.4% of applied. In the Bury Pond systems, A/C1, P1 and P2 were detected at maximums of 19.5%, 13.7% and 9.7%, respectively, and volatilized [^{14}C]residues were a maximum 9.5% of applied.

IV. REVIEWER'S COMMENTS:

1. Due to rapid dissipation of [^{14}C]chlorothanonil, the time 0 water-sediment systems were repeated (pp.18, 26). There was sufficient water-sediment from the initial collection (October 31, 1994) for the repeat time 0 Houghton Meadow systems. However, additional water-sediment was collected (May 1, 1996) for the repeat time 0 Bury Pond systems (Table III, p.35). The study author reported that the repeat time 0 systems were "treated in a fashion to ensure the quickest possible separation of water and sediment" (p.26), but did not specify how treatment of the repeat time 0 systems differed from the remaining systems.

2. Limits of determination for LSC analyses were reported as twice background levels. Accepted Analytical Chemistry practices normally consider limits of detection for analytical methods to be three times the background noise levels.

3. It appears that the two replicates from the day 2 sampling interval were out of sequence. Parent concentrations rose sharply and degradation products dropped dramatically. At the next sampling interval, concentrations once again fell, or rose, to expected levels. Clarification from the registrant is required. Recoveries of parent [^{14}C]chlorothalonil in the Bury Pond systems were too variable to accurately assess the dissipation of chlorothalonil from the water layer/total system. Recovery of [^{14}C]chlorothalonil appeared to correlate with recovery of total radioactivity in the water layer. At time 0, 6 hours, 1, 2 and 7 days posttreatment, [^{14}C]chlorothalonil in the water layer and total system was detected at 83.7-88.0%, 5.0-7.0%, 15.2-16.0%, 51.7-70.0% and 4.0-9.1% of

US EPA ARCHIVE DOCUMENT

the applied, respectively, and total radioactivity recovered in the water layer was 83.8-88.4%, 14.9-17.1%, 21.0-22.0%, 65.9-76.9% and 23.7-26.1% of applied, respectively.

4. The test substance was incompletely characterized; physico-chemical characteristics including the vapor pressure/volatility, UV absorption, dissociation constant (pK_a), octanol-water partition coefficient (K_{ow}/log K_{ow}) and stability at room temperature should have been reported.

5. The study author reported that parent [^{14}C]chlorthalonil and its degradates were identified by co-chromatography with unlabeled reference standards (p.23). However, no comparative UV chromatograms were provided for review.

6. The study author reported that selected water layer and sediment extract samples were analyzed using one-dimensional normal-phase (silica gel plates) and reverse-phase (C-18 plates) TLC with identifications of [^{14}C]residues made by co-chromatography with unlabeled reference standards (pp.23-24). However, no supporting quantitative (linear analyzer results) or qualitative (chromatogram showing locations of labeled and unlabeled areas) TLC results were provided.

7. Quantitative detection limits for LSC, HPLC and TLC analyses were not provided. The reported results indicate that the HPLC LOD was 0.1% of the applied (Tables XVII-XX, pp.49-56).

8. According to N. Wolfe, *et al.* (see reference below), redox potentials in the range of +400 to +800 mV are considered strongly oxidizing, +200 to +400 mV moderately oxidizing, -50 to +200 mV moderately reducing, -200 to -50 mV reducing, and -400 to -200 mV strongly reducing.

9. The study author reported that the nominal 0.83 mg a.i./kg treatment rate selected for this study was based on a field application rate of 2.5 kg a.i./ha disbursed over water with a depth of 30 cm (pp.9-10).

10. Tetrachloroisophthalonitrile and 2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile were identified as the IUPAC and CAS names, respectively, of chlorothalonil by the Compendium of Pesticide Common Names (http://www.hclrss.demon.co.uk/chlorothalonil.html). The synonym 2,4,5,6-tetrachloro-1,3-dicyanobenzene and trade names Bravo, Daconil 2787, Exotherm termil, Forturf and Tuffcide were obtained from the USEPA/OPP Chemical Database (http://www.cdpr.ca.gov/cgi-bin/epa/chemidetriris.pl?pccode=081901) and/or the California Department of Pesticide Registration (CA DPR) database (http://www.cdpr.ca.gov/cgi-bin/mon/bycode.pl?p_chemcode=677). The CAS Reg No. 1897-45-6 was confirmed for chlorothalonil at the USEPA/OPP Chemical Database.

US EPA ARCHIVE DOCUMENT

11. The following typographical errors/discrepancies were noted:

    i) In RESULTS, OXYGEN CONCENTRATIONS, pH AND REDOX POTENTIALS FOLLOWING APPLICATION OF THE TEST SUBSTANCE (p.26), it was reported that the pH range in the Houghton Meadow systems was **6.83**-8.48; however, the actual range was **6.50**-8.48 (Table IX, p.41).

    ii) In Table IV (p.36), the Houghton Meadow sediment was classified as a silt loam by the study author. However, the sediment should have been classified as a clay according to the USDA Soil Textural Triangle.

    iii) In the Proposed degradation pathway of Chlorothalonil in sediment, the chemical name for 4-hydroxy-**2,5,6**-trichloro-1,3-dicyanobenzene was incorrectly written as 4-hydroxy-**2,4,5**-trichloro-1,3-dicyanobenzene (Figure 11, p.126).

V. REFERENCES:

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-4, Aerobic Aquatic Metabolism Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

4. Wolfe, N., *et al.* 1990. Abiotic transformations in water, sediments and soil. *In* Pesticides in the Soil Environment, Soil Science Society of America, pp.103-110.

US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

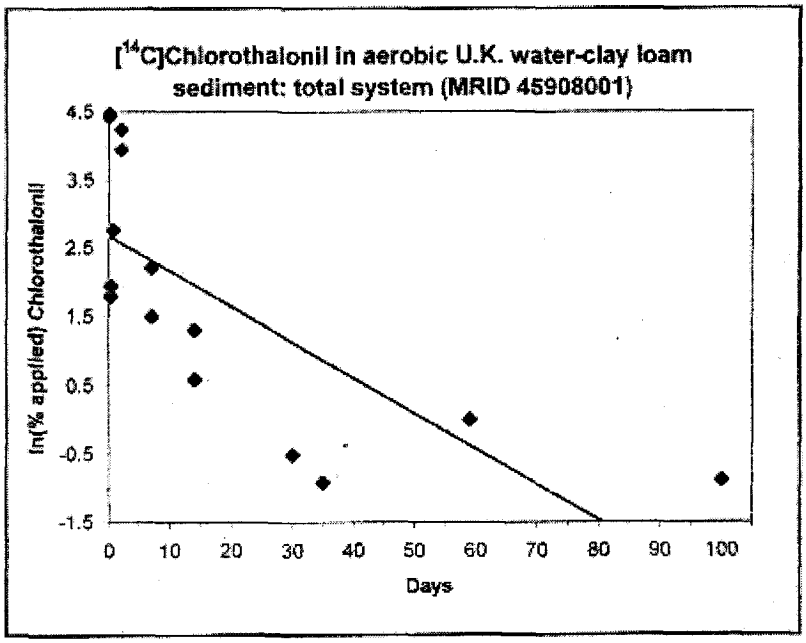
Attachment 1

Excel Spreadsheets
SigmaPlot Spreadsheets

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Bury Pond water-clay loam sediment
Half-life determination
Total system

Hours	Chlorothalonil	
	%AR	Ln(%AR)
0	88.0	4.477337
0	83.9	4.429626
0.25	7.0	1.94591
0.25	6.0	1.791759
1	15.9	2.766319
1	16.0	2.772589
2	51.8	3.94739
2	70.0	4.248495
7	9.1	2.208274
7	4.5	1.504077
14	3.7	1.308333
14	1.8	0.587787
30	0.6	-0.510826
35	0.4	-0.916291
59	1.0	0
59	0.2	-1.609438
100	0.4	-0.891598
100	0.1	-2.207275



SUMMARY OUTPUT

Linear half-life = 13.4 days

Regression Statistics	
Multiple R	0.8185
R Square	0.6699
Adjusted R Sc	0.6493
Standard Erro	1.2609
Observations	18

Nonlinear (exponential decay/single, 2 parameter)
half-life = 3.5 hours R squared: 0.4280
See SigmaPlot 45908001 162-4 Parent BP Tot sys nonlinear.

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	51.62152	51.622	32.468704	3.297E-05
Residual	16	25.43817	1.5899		
Total	17	77.05969			

	Coefficient	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.675	0.368218	7.2646	1.893E-06	1.8943641	3.4555371	1.894364146	3.455537086
X Variable 1	-0.052	0.009082	-5.698	3.297E-05	-0.071006	-0.0324987	-0.07100605	-0.03249867

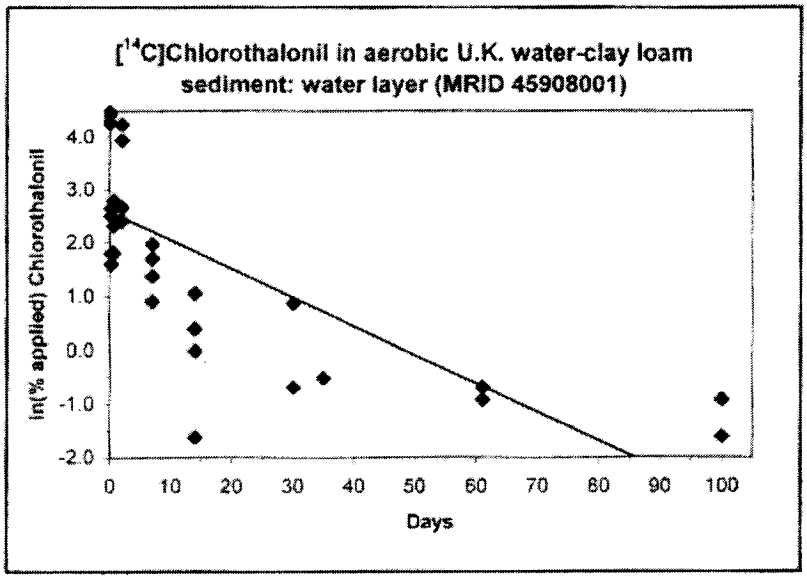
US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Bury Pond water-clay loam sediment
Half-life determination
Water layer

Hours	Chlorothalonil	
	%AR	Ln(%AR)
0	87.9	4.4762
0	83.7	4.427239
0.25	6.1	1.808289
0.25	5.0	1.609438
1	15.2	2.721295
1	16.4	2.797281
2	51.7	3.945458
2	69.4	4.239887
7	7.2	1.974081
7	4.0	1.386294
14	2.9	1.064711
14	1.5	0.405465
30	0.5	-0.693147
61	0.6	-0.510826
61	0.1	-2.302585
100	0.4	-0.916291
100	0.1	-2.302585



Linear half-life = 13.2 days

SUMMARY OUTPUT

Nonlinear (exponential decay/single, 2 parameter)
half-life = 3.4 hours R squared: 0.4185
See SigmaPlot 45908001 162-4 Parent BP H2O nonlinear.

Regression Statistics	
Multiple R	0.8189
R Square	0.6706
Adjusted R Sc	0.6487
Standard Erro	1.3198
Observations	17

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	53.19369	53.194	30.53897	5.813E-05
Residual	15	26.12744	1.7418		
Total	16	79.32113			

	Coefficien	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.6498	0.389913	6.7959	6.03E-06	1.8187376	3.4808996	1.818737632	3.48089956
X Variable 1	-0.052	0.009466	-5.526	5.81E-05	-0.072491	-0.0321363	-0.07249085	-0.0321363

Linear regression analysis performed using Microsoft Excel 2000.
Results (% of applied radioactivity) from Table XVIII, pp. 45-52 pp. 53-54 of the study report

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Determination of means/standard deviations of system parameters (pH, O_2 and redox potentials).

Houghton Meadow water-clay sediment.

	Water layer				Sediment
Day	pH	O_2 (mg/L)	O_2 (%)	Redox (mV)	Redox (mV)
0	7.48	1.8	20	250	-120
	7.71	2.3	25	230	-108
0.25	7.39	3.4	37	220	-146
	7.76	3.6	39	210	-158
1	7.46	3.2	35	210	-180
	7.81	2.0	22	195	-193
2	7.55	4.1	45	180	-160
	7.42	3.4	37	150	-176
7	7.64	1.3	14	150	-195
	7.49	2.5	27	180	-185
14	7.10	1.8	20	150	-219
	7.59	3.7	40	170	-202
30	6.83	2.3	25	50	-209
35	6.50	4.3	47	50	-184
59	7.64	2.3	25	60	-256
	7.78	2.1	23	140	-228
100	7.59	2.3	25	170	-215
	8.48	2.8	30	200	-260
Mean	7.51	2.7	30	165	-189
std.dev.	0.40	0.8	9	58	40
n =	18	18	18	18	18

Results from Table IX, p. 41 of the study report.

Bury Pond water-clay loam sediment.

	Water layer				Sediment
Day	pH	O_2 (mg/L)	O_2 (%)	Redox (mV)	Redox (mV)
0	7.88	3.8	41	240	-60
	7.56	3.3	36	160	-45
0.25	7.91	2.8	30	200	-175
	7.62	3.7	40	230	-145
1	7.50	3.2	35	250	-146
	7.96	4.1	45	100	-233
2	7.83	5.7	62	180	-205
	7.86	6.1	66	165	-213
7	7.20	3.7	40	180	-125
	7.53	3.2	35	130	-130
14	7.47	2.3	25	200	-124
	7.33	4.6	50	250	-108
30	7.48	3.7	40	250	-106
	7.62	1.8	20	240	-120
61	7.73	2.6	28	220	-92
	7.65	2.3	25	240	-50
100	7.67	1.8	20	200	-95
	7.94	2.4	26	250	-70
Mean	7.65	3.4	37	205	-125
std.dev.	0.21	1.2	13	44	53
n =	18	18	18	18	18

Results from Table X, p. 42 of the study report.

Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation of summations (sediment extracts and material balances) and determination of means/standard deviations for applied radioactivity.

Houghton Meadow water-clay sediment.

	Water layer			Sediment						CO_2 + Organic vol.			Material Balance		
				Extract			Nonextractable								
Day	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	77.6			13.2			1.3						92.1		
	72.9	75.3	2.4	20.5	16.9	3.6	2.3	1.8	0.5		#####	#####	95.7	93.9	1.8
0.25	19.0			65.6			9.2			0.6			94.4		
	16.9	18.0	1.0	60.1	62.9	2.8	10.5	9.9	0.7	0.5	0.6	0.0	88.0	91.2	3.2
1	16.9			67.0			9.6			0.6			94.1		
	13.5	15.2	1.7	67.0	67.0	0.0	9.8	9.7	0.1	0.6	0.6	0.0	90.9	92.5	1.6
2	16.8			63.0			8.2			3.9			91.9		
	19.0	17.9	1.1	63.2	63.1	0.1	7.9	8.1	0.1	2.2	3.1	0.9	92.3	92.1	0.2
7	31.9			42.2			16.4			1.1			91.6		
	25.7	28.8	3.1	55.5	48.9	6.6	12.2	14.3	2.1	2.3	1.7	0.6	95.7	93.7	2.0
14	27.6			41.4			12.0			10.4			91.4		
	30.2	28.9	1.3	43.2	42.3	0.9	14.3	13.2	1.2	4.1	7.3	3.2	91.8	91.6	0.2
30	29.6			37.7			16.1			9.5			92.9		
35	20.1	24.9	4.8	42.1	39.9	2.2	25.1	20.6	4.5	3.0	6.3	3.3	90.3	91.6	1.3
59	25.9			30.1			24.4			10.3			90.7		
	11.7	18.8	7.1	21.9	26.0	4.1	32.2	28.3	3.9	29.4	19.9	9.6	95.2	93.0	2.3
100	19.8			28.7			30.7			7.4			86.6		
	18.4	19.1	0.7	27.2	28.0	0.8	42.2	36.5	5.7	2.1	4.8	2.7	89.9	88.3	1.6
													Overall:	92.0	2.4

Results from Table XI, p. 43 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation of summations (sediment extracts and material balances) and determination of means/standard deviations for applied radioactivity.

Bury Pond water-clay loam sediment.

	Water layer			Sediment						CO_2 + Organic vol.			Material Balance		
				Extract			Nonextractable								
Day	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	88.4			8.8			0.3						97.5		
	83.8	86.1	2.3	11.2	10.0	1.2	0.3	0.3	0.0		#####	#####	95.3	96.4	1.1
0.25	17.1			64.3			8.6			0.3			90.3		
	14.9	16.0	1.1	63.6	64.0	0.3	7.6	8.1	0.5	0.1	0.2	0.1	86.2	88.3	2.0
1	21.0			68.3			6.6			0.9			96.8		
	22.0	21.5	0.5	65.0	66.7	1.6	10.0	8.3	1.7	0.9	0.9	0.0	97.9	97.4	0.5
2	65.9			31.2			4.9			2.7			104.7		
	76.9	71.4	5.5	26.9	29.1	2.2	3.8	4.4	0.6	0.9	1.8	0.9	108.5	106.6	1.9
7	26.1			59.6			9.0			2.0			96.7		
	23.7	24.9	1.2	63.0	61.3	1.7	8.0	8.5	0.5	1.8	1.9	0.1	96.5	96.6	0.1
14	40.2			35.9			8.9			9.5			94.5		
	41.0	40.6	0.4	35.6	35.8	0.2	11.5	10.2	1.3	6.0	7.8	1.8	94.1	94.3	0.2
30	32.6			40.3			14.3			3.5			90.7		
	34.5	33.6	1.0	38.0	39.2	1.2	14.0	14.2	0.2	5.3	4.4	0.9	91.8	91.3	0.5
61	29.3			33.6			20.3			9.4			92.6		
	33.5	31.4	2.1	31.7	32.7	1.0	18.3	19.3	1.0	9.2	9.3	0.1	92.7	92.7	0.0
100	15.2			34.8			30.5			8.5			89.0		
	14.3	14.8	0.4	29.8	32.3	2.5	34.8	32.7	2.2	9.5	9.0	0.5	88.4	88.7	0.3
													Overall:	94.7	5.4

Results from Table XII, p. 44 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Determination of means/standard deviations for total applied radioactivity in sediment.

Houghton Meadow water-clay sediment.

	Sediment								
	Extract			Nonextractable			Total		
Day	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	13.2			1.3			14.5		
	20.5	16.9	3.6	2.3	1.8	0.5	22.8	18.7	4.2
0.25	65.6			9.2			74.8		
	60.1	62.9	2.8	10.5	9.9	0.7	70.6	72.7	2.1
1	67.0			9.6			76.6		
	67.0	67.0	0.0	9.8	9.7	0.1	76.8	76.7	0.1
2	63.0			8.2			71.2		
	63.2	63.1	0.1	7.9	8.1	0.1	71.1	71.2	0.0
7	42.2			16.4			58.6		
	55.5	48.9	6.6	12.2	14.3	2.1	67.7	63.2	4.5
14	41.4			12.0			53.4		
	43.2	42.3	0.9	14.3	13.2	1.2	57.5	55.5	2.0
30	37.7			16.1			53.8		
35	42.1	39.9	2.2	25.1	20.6	4.5	67.2	60.5	6.7
59	30.1			24.4			54.5		
	21.9	26.0	4.1	32.2	28.3	3.9	54.1	54.3	0.2
100	28.7			30.7			59.4		
	27.2	28.0	0.8	42.2	36.5	5.7	69.4	64.4	5.0

Extract results imported from **Mat bal HM** worksheet.
All other results from Table XI, p. 43 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

[14C]Residue water phase:soil ratios.

	Water	Sed.	Ratio	Ratio	W:S ratio		S:W ratio	
Day	% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
0	77.6	14.5	5	0				
	72.9	22.8	3	0	4	1	0	0
0.25	19.0	74.8	0	4				
	16.9	70.6	0	4	0	0	4	0
1	16.9	76.6	0	5				
	13.5	76.8	0	6	0	0	5	1
2	16.8	71.2	0	4				
	19.0	71.1	0	4	0	0	4	0
7	31.9	58.6	1	2				
	25.7	67.7	0	3	0	0	2	0
14	27.6	53.4	1	2				
	30.2	57.5	1	2	1	0	2	0
30	29.6	53.8	1	2				
35	20.1	67.2	0	3	0	0	3	1
59	25.9	54.5	0	2				
	11.7	54.1	0	5	0	0	3	1
100	19.8	59.4	0	3				
	18.4	69.4	0	4	0	0	3	0

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Determination of means/standard deviations for total applied radioactivity in sediment.

Bury Pond water-clay loam sediment.

Day	Sediment								
	Extract			Nonextractable			Total		
	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	8.8			0.3			9.1		
	11.2	10.0	1.2	0.3	0.3	0.0	11.5	10.3	1.2
0.25	64.3			8.6			72.9		
	63.6	64.0	0.3	7.6	8.1	0.5	71.2	72.1	0.8
1	68.3			6.6			74.9		
	65.0	66.7	1.6	10.0	8.3	1.7	75.0	75.0	0.0
2	31.2			4.9			36.1		
	26.9	29.1	2.2	3.8	4.4	0.6	30.7	33.4	2.7
7	59.6			9.0			68.6		
	63.0	61.3	1.7	8.0	8.5	0.5	71.0	69.8	1.2
14	35.9			8.9			44.8		
	35.6	35.8	0.2	11.5	10.2	1.3	47.1	46.0	1.1
30	40.3			14.3			54.6		
	38.0	39.2	1.2	14.0	14.2	0.2	52.0	53.3	1.3
61	33.6			20.3			53.9		
	31.7	32.7	1.0	18.3	19.3	1.0	50.0	52.0	1.9
100	34.8			30.5			65.3		
	29.8	32.3	2.5	34.8	32.7	2.2	64.6	65.0	0.3

Extract results imported from **Mat bal BP** worksheet.
All other results from Table XII, p. 44 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

[14C]Residue water phase:soil ratios.

Day	Water	Sed.	Ratio	Ratio	W:S ratio		S:W ratio	
	% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
0	88.4	9.1	10	0				
	83.8	11.5	7	0	9	1	0	0
0.25	17.1	72.9	0	4				
	14.9	71.2	0	5	0	0	5	0
1	21.0	74.9	0	4				
	22.0	75.0	0	3	0	0	3	0
2	65.9	36.1	2	1				
	76.9	30.7	3	0	2	0	0	0
7	26.1	68.6	0	3				
	23.7	71.0	0	3	0	0	3	0
14	40.2	44.8	1	1				
	41.0	47.1	1	1	1	0	1	0
30	32.6	54.6	1	2				
	34.5	52.0	1	2	1	0	2	0
61	29.3	53.9	1	2				
	33.5	50.0	1	1	1	0	2	0
100	15.2	65.3	0	4				
	14.3	64.6	0	5	0	0	4	0

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment.

	Chlorothalonil									Trichloro-1,3-dicyanobenzene (R_t=15-16 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	72.8			0.4			73.2						6.2			6.2		
	71.4	72.1	0.7	0.8	0.6	0.2	72.2	72.7	0.5		#####	#####	4.6	5.4	0.8	4.6	5.4	0.8
0.25	14.1			6.6			20.7			0.6			5.9			6.5		
	12.2	13.2	1.0	2.7	4.7	2.0	14.9	17.8	2.9	0.4	0.5	0.1	17.0	11.5	5.6	17.4	12.0	5.5
1	10.2			1.9			12.1			0.7			23.3			24.0		
	6.1	8.2	2.1	3.9	2.9	1.0	10.0	11.1	1.0	0.5	0.6	0.1	16.7	20.0	3.3	17.2	20.6	3.4
2	14.3			5.1			19.4			0.4			19.6			20.0		
	11.1	12.7	1.6	3.8	4.5	0.7	14.9	17.2	2.3	1.2	0.8	0.4	20.3	20.0	0.3	21.5	20.8	0.8
7	2.5			0.05			2.6			3.9			11.9			15.8		
	5.5	4.0	1.5	1.1	0.6	0.5	6.6	4.6	2.0	1.9	2.9	1.0	18.7	15.3	3.4	20.6	18.2	2.4
14	0.2			0.1			0.3			1.6			13.9			15.5		
	1.0	0.6	0.4	1.0	0.6	0.5	2.0	1.2	0.9	2.2	1.9	0.3	10.8	12.4	1.5	13.0	14.3	1.3
30	2.4			0.2			2.6			0.9			5.3			6.2		
35	0.4	1.4	1.0	0.1	0.2	0.1	0.5	1.6	1.1	0.8	0.9	0.0	4.7	5.0	0.3	5.5	5.9	0.4
59	0.5			0.6			1.1			0.3			1.5			1.8		
	0.05	0.3	0.2	1.2	0.9	0.3	1.3	1.2	0.1	0.4	0.4	0.1	1.0	1.3	0.3	1.4	1.6	0.2
100	0.2			0.5			0.7			0.4			0.8			1.2		
	0.4	0.3	0.1	0.6	0.6	0.0	1.0	0.9	0.2	0.2	0.3	0.1	0.9	0.9	0.0	1.1	1.2	0.0

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment (continued).

	2,4,5-Trichloro-6-mercapto-isophthalonitrile (R_t=13-14 min.)									4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t=12-13 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.2 2.7	1.5	1.3	0.2 2.7	1.5	1.3		#####	#####	1.1 1.3	1.2	0.1	1.1 1.3	1.2	0.1
0.25		#####	#####	14.1 10.3	12.2	1.9	14.1 10.3	12.2	1.9	1.0 0.8	0.9	0.1	1.7 2.4	2.1	0.3	2.7 3.2	3.0	0.3
1		#####	#####	4.6 5.0	4.8	0.2	4.6 5.0	4.8	0.2	1.0 1.3	1.2	0.2	5.0 3.3	4.2	0.8	6.0 4.6	5.3	0.7
2		#####	#####	3.6 3.5	3.6	0.1	3.6 3.5	3.6	0.1	0.6 1.7	1.2	0.6	3.8 3.5	3.7	0.1	4.4 5.2	4.8	0.4
7		#####	#####	1.9 3.7	2.8	0.9	1.9 3.7	2.8	0.9	4.8 3.2	4.0	0.8	4.0 3.0	3.5	0.5	8.8 6.2	7.5	1.3
14		#####	#####	3.6 2.2	2.9	0.7	3.6 2.2	2.9	0.7	1.9 4.7	3.3	1.4	2.4 5.4	3.9	1.5	4.3 10.1	7.2	2.9
30 35		#####	#####	3.6 3.7	3.7	0.0	3.6 3.7	3.7	0.0	4.1 1.2	2.7	1.5	3.8 3.6	3.7	0.1	7.9 4.8	6.4	1.6
59		#####	#####	0.7 1.4	1.1	0.4	0.7 1.4	1.1	0.4	4.5 2.8	3.7	0.9	11.7 5.4	8.6	3.2	16.2 8.2	12.2	4.0
100		#####	#####	0.9 0.7	0.8	0.1	0.9 0.7	0.8	0.1	3.6 2.5	3.1	0.6	8.8 10.3	9.6	0.8	12.4 12.8	12.6	0.2

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev, for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment (continued).

	2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (R_t=9-10 min.)									A/C1 (R_t=8-9 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.7 1.7	1.2	0.5	0.7 1.7	1.2	0.5		#####	#####	2.5 6.0	4.3	1.8	2.5 6.0	4.3	1.8
0.25	0.1 0.8	0.5	0.4	2.7 2.0	2.4	0.3	2.8 2.8	2.8	0.0	1.1 0.3	0.7	0.4	21.8 12.2	17.0	4.8	22.9 12.5	17.7	5.2
1	0.4 0.6	0.5	0.1	5.8 2.1	4.0	1.9	6.2 2.7	4.5	1.8	1.7 0.6	1.2	0.6	4.2 23.0	13.6	9.4	5.9 23.6	14.8	8.9
2	0.1 0.5	0.3	0.2	2.8 8.4	5.6	2.8	2.9 8.9	5.9	3.0	0.4 1.5	1.0	0.6	16.6 11.3	14.0	2.7	17.0 12.8	14.9	2.1
7	1.3 1.6	1.5	0.2	3.1 2.6	2.9	0.3	4.4 4.2	4.3	0.1	4.5 3.2	3.9	0.7	11.0 13.6	12.3	1.3	15.5 16.8	16.2	0.7
14	0.7 1.0	0.9	0.2	0.1 2.4	1.3	1.2	0.8 3.4	2.1	1.3	7.5 5.2	6.4	1.2	3.1 8.5	5.8	2.7	10.6 13.7	12.2	1.6
30 35	1.8 1.2	1.5	0.3	1.5 1.2	1.4	0.1	3.3 2.4	2.9	0.5	0.8 0.6	0.7	0.1	9.1 8.1	8.6	0.5	9.9 8.7	9.3	0.6
59	2.1 0.6	1.4	0.8	0.05 0.1	0.1	0.0	2.2 0.7	1.4	0.7	2.0 0.3	1.2	0.9	3.5 3.9	3.7	0.2	5.5 4.2	4.9	0.7
100	0.6 0.3	0.5	0.2	1.7 1.7	1.7	0.0	2.3 2.0	2.2	0.2	0.5 0.4	0.5	0.1	3.5 1.4	2.5	1.1	4.0 1.8	2.9	1.1

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment (continued).

	C/C3 (R_t=10-11 min.)									D/C4 (R_t=11-12 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.5	0.5	0.0	0.5	0.5	0.0		#####	#####	0.1	0.2	0.1	0.1	0.2	0.1
				0.5			0.5						0.3			0.3		
0.25	0.2			2.7			2.9			0.4			2.0			2.4		
	0.6	0.4	0.2	1.7	2.2	0.5	2.3	2.6	0.3	0.05	0.2	0.2	0.9	1.5	0.6	1.0	1.7	0.7
1	0.2			1.1			1.3			0.4			2.0			2.4		
	0.3	0.3	0.1	1.9	1.5	0.4	2.2	1.8	0.5	0.6	0.5	0.1	1.4	1.7	0.3	2.0	2.2	0.2
2	0.1			0.9			1.0			0.2			2.4			2.6		
	0.05	0.1	0.0	2.5	1.7	0.8	2.6	1.8	0.8	0.5	0.4	0.2	1.4	1.9	0.5	1.9	2.3	0.4
7	1.3			1.1			2.4			2.9			1.3			4.2		
	1.1	1.2	0.1	2.2	1.7	0.6	3.3	2.9	0.5	0.8	1.9	1.1	2.8	2.1	0.8	3.6	3.9	0.3
14	0.3			1.8			2.1			3.2			1.7			4.9		
	0.8	0.6	0.3	2.0	1.9	0.1	2.8	2.5	0.3	1.9	2.6	0.7	0.05	0.9	0.8	2.0	3.4	1.5
30	1.3			1.7			3.0			5.6			2.1			7.7		
35	2.0	1.7	0.4	2.0	1.9	0.1	4.0	3.5	0.5	0.8	3.2	2.4	6.3	4.2	2.1	7.1	7.4	0.3
59	1.5			2.3			3.8			0.6			1.6			2.2		
	0.9	1.2	0.3	1.1	1.7	0.6	2.0	2.9	0.9	0.5	0.6	0.0	1.9	1.8	0.2	2.4	2.3	0.1
100	3.0			2.8			5.8			0.8			1.4			2.2		
	1.6	2.3	0.7	2.7	2.8	0.0	4.3	5.1	0.7	0.9	0.9	0.0	0.1	0.8	0.7	1.0	1.6	0.6

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev, for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment (continued).

	G/C7 (R_t=14-15 min.)									P1 (R_t=2-3 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.3	0.3	0.0	0.3	0.3	0.0		#####	#####	0.2	0.3	0.1	0.2	0.3	0.1
				0.3			0.3						0.4			0.4		
0.25	0.2	0.5	0.3	2.2	1.9	0.3	2.4	2.4	0.0		#####	#####	2.5	3.2	0.7	2.5	3.2	0.7
	0.7			1.6			2.3						3.8			3.8		
1	0.2	0.6	0.4	2.4	3.2	0.8	2.6	3.8	1.2	0.05	0.2	0.1	11.2	7.3	3.9	11.3	7.5	3.8
	1.0			4.0			5.0			0.3			3.4			3.7		
2	0.1	0.5	0.4	2.9	3.1	0.2	3.0	3.6	0.6		#####	#####	0.05	1.6	1.6	0.1	1.6	1.6
	0.9			3.2			4.1						3.2			3.2		
7	1.5	1.4	0.1	1.5	2.1	0.6	3.0	3.5	0.5	3.8	3.3	0.5	2.7	2.3	0.4	6.5	5.6	0.9
	1.3			2.7			4.0			2.8			1.9			4.7		
14	2.8	2.7	0.2	5.5	4.8	0.7	8.3	7.5	0.9	3.4	3.7	0.2	4.9	3.9	1.1	8.3	7.5	0.8
	2.5			4.1			6.6			3.9			2.80			6.7		
30	1.8	3.4	1.6	3.7	4.1	0.4	5.5	7.5	2.0	4.6	3.2	1.4	1.7	1.6	0.2	6.3	4.8	1.6
35	5.0			4.5			9.5			1.8			1.4			3.2		
59	3.0	1.7	1.3	2.3	2.2	0.1	5.3	3.9	1.4	0.9	1.5	0.6	1.9	1.5	0.4	2.8	3.0	0.1
	0.4			2.1			2.5			2.0			1.1			3.1		
100	0.5	0.5	0.1	0.8	0.8	0.0	1.3	1.3	0.1	0.8	1.1	0.3	2.5	2.8	0.3	3.3	3.9	0.6
	0.4			0.8			1.2			1.4			3.1			4.5		

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev, for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment (continued).

	P2 (R_t=3-4 min.)									P3 (R_t=4-5 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		######	######	0.3 0.5	0.4	0.1	0.3 0.5	0.4	0.1		######	######	0.2 0.4	0.3	0.1	0.2 0.4	0.3	0.1
0.25	0.3 0.2	0.3	0.1	1.8 0.9	1.4	0.5	2.1 1.1	1.6	0.5	0.3 0.3	0.3	0.0	0.9 0.6	0.8	0.2	1.2 0.9	1.1	0.2
1	1.0 0.3	0.7	0.4	1.7 0.8	1.3	0.5	2.7 1.1	1.9	0.8	0.6 0.5	0.6	0.0	1.2 0.5	0.9	0.4	1.8 1.0	1.4	0.4
2	0.2 0.5	0.4	0.2	2.0 0.7	1.4	0.7	2.2 1.2	1.7	0.5	0.3 0.5	0.4	0.1	1.8 0.3	1.1	0.8	2.1 0.8	1.5	0.7
7	1.5 1.4	1.5	0.0	1.1 1.5	1.3	0.2	2.6 2.9	2.8	0.2	1.2 0.8	1.0	0.2	1.6 0.9	1.3	0.4	2.8 1.7	2.3	0.6
14	2.3 2.2	2.3	0.0	0.8 0.9	0.9	0.0	3.1 3.1	3.1	0.0	1.7 1.5	1.6	0.1	0.9 1.0	1.0	0.1	2.6 2.5	2.6	0.1
30 35	2.8 0.8	1.8	1.0	1.3 0.4	0.9	0.5	4.1 1.2	2.7	1.5	1.5 0.5	1.0	0.5	1.9 3.7	2.8	0.9	3.4 4.2	3.8	0.4
59	4.5 1.4	3.0	1.6	0.2 1.1	0.7	0.5	4.7 2.5	3.6	1.1	2.3 0.3	1.3	1.0	1.4 1.0	1.2	0.2	3.7 1.3	2.5	1.2
100	5.4 6.2	5.8	0.4	1.1 1.1	1.1	0.0	6.5 7.3	6.9	0.4	2.4 2.1	2.3	0.2	1.7 1.5	1.6	0.1	4.1 3.6	3.9	0.3

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment (continued).

	P4 (R_t=5-6 min.)									I (R_t=17-18 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.1			0.1				#####	#####		#####	#####	0.0		
				0.2	0.2	0.1	0.2	0.2	0.1							0.0	0.0	0.0
0.25	0.1			0.2			0.3			0.1				#####	#####	0.1		
	0.1	0.1	0.0	0.5	0.4	0.2	0.6	0.5	0.2	0.1	0.1	0.0				0.1	0.1	0.0
1	0.2			0.9			1.1			0.1				#####	#####	0.1		
	0.1	0.2	0.1	0.2	0.6	0.4	0.3	0.7	0.4	0.4	0.3	0.2				0.4	0.3	0.2
2	0.1			0.5			0.6			0.1				#####	#####	0.1		
	0.1	0.1	0.0	0.1	0.3	0.2	0.2	0.4	0.2	0.01	0.1	0.0				0.0	0.1	0.0
7	0.6			0.5			1.1				#####	#####		#####	#####	0.0		
	0.6	0.6	0.0	0.3	0.4	0.1	0.9	1.0	0.1							0.0	0.0	0.0
14	0.7			0.8			1.5			0.1				#####	#####	0.1		
	1.0	0.9	0.2	0.8	0.8	0.0	1.8	1.7	0.2	0.2	0.2	0.1				0.2	0.2	0.1
30	1.7			0.8			2.5			0.2				#####	#####	0.2		
35	1.0	1.4	0.3	1.6	1.2	0.4	2.6	2.6	0.1	2.0	1.1	0.9				2.0	1.1	0.9
59	1.2			1.0			2.2			0.05				#####	#####	0.1		
	0.4	0.8	0.4	0.05	0.5	0.5	0.5	1.3	0.9	0.6	0.3	0.3				0.6	0.3	0.3
100	0.4			0.8			1.2			0.3				#####	#####	0.3		
	0.9	0.7	0.3	0.6	0.7	0.1	1.5	1.4	0.2	1.5	0.9	0.6				1.5	0.9	0.6

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Houghton Meadow water-clay sediment (continued).

	Others									Total Unidentified [^{14}C]Residues								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	4.6			0.4			5.0			4.6			4.6			9.2		
	1.4	3.0	1.6	0.8	0.6	0.2	2.2	3.6	1.4	1.4	3.0	1.6	9.4	7.0	2.4	10.8	10.0	0.8
0.25	0.4			0.5			0.9			3.1			34.6			37.7		
	0.3	0.4	0.1	3.7	2.1	1.6	4.0	2.5	1.6	2.7	2.9	0.2	25.9	30.3	4.4	28.6	33.1	4.6
1	0.3			1.9			2.2			4.8			26.6			31.4		
	0.4	0.4	0.1	0.9	1.4	0.5	1.3	1.8	0.5	4.5	4.6	0.1	36.1	31.4	4.8	40.6	36.0	4.6
2	0.2			0.6			0.8			1.7			27.8			29.5		
	0.4	0.3	0.1	0.9	0.8	0.2	1.3	1.1	0.3	4.5	3.1	1.4	23.6	25.7	2.1	28.1	28.8	0.7
7	2.2			0.6			2.8			19.5			21.4			40.9		
	1.5	1.9	0.4	0.5	0.6	0.0	2.0	2.4	0.4	13.5	16.5	3.0	26.4	23.9	2.5	39.9	40.4	0.5
14	1.3			2.1			3.4			23.3			21.6			44.9		
	2.0	1.7	0.4	1.2	1.7	0.5	3.2	3.3	0.1	21.2	22.3	1.0	21.4	21.5	0.1	42.6	43.7	1.2
30	0.1			0.9			1.0			20.4			23.2			43.6		
35	1.9	1.0	0.9	0.9	0.9	0.0	2.8	1.9	0.9	16.4	18.4	2.0	28.9	26.1	2.8	45.3	44.5	0.9
59	2.6			1.4			4.0			18.7			15.6			34.3		
	0.9	1.8	0.9	0.7	1.1	0.4	1.6	2.8	1.2	7.7	13.2	5.5	13.0	14.3	1.3	20.7	27.5	6.8
100	1.0			1.3			2.3			15.1			15.9			31.0		
	0.8	0.9	0.1	1.8	1.6	0.3	2.6	2.5	0.1	16.2	15.7	0.6	13.1	14.5	1.4	29.3	30.2	0.8

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Bury Pond water-clay loam sediment.

	Chlorothalonil									Trichloro-1,3-dicyanobenzene (R_t=15-16 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	87.9			0.05			88.0						1.6			1.6		
	83.7	85.8	2.1	0.2	0.1	0.1	83.9	85.9	2.0		#####	#####	2.9	2.3	0.7	2.9	2.3	0.7
0.25	6.1			0.9			7.0			2.4			25.9			28.3		
	5.0	5.6	0.5	1.0	1.0	0.1	6.0	6.5	0.5	0.4	1.4	1.0	7.8	16.9	9.1	8.2	18.3	10.1
1	15.2			0.7			15.9			0.3			19.1			19.4		
	15.4	15.3	0.1	0.6	0.7	0.1	16.0	16.0	0.0	0.4	0.4	0.1	15.7	17.4	1.7	16.1	17.8	1.6
2	51.7			0.05			51.8			0.8			0.7			1.5		
	69.4	60.6	8.8	0.6	0.3	0.3	70.0	60.9	9.1	0.5	0.7	0.2	5.1	2.9	2.2	5.6	3.6	2.1
7	7.2			1.9			9.1			1.0			10.5			11.5		
	4.0	5.6	1.6	0.5	1.2	0.7	4.5	6.8	2.3	4.7	2.9	1.9	8.5	9.5	1.0	13.2	12.4	0.9
14	2.9			0.8			3.7			3.9			7.9			11.8		
	1.5	2.2	0.7	0.3	0.6	0.3	1.8	2.8	1.0	3.0	3.5	0.4	7.4	7.7	0.3	10.4	11.1	0.7
30	0.5			0.05			0.6			0.7			7.6			8.3		
	0.05	0.3	0.2	0.3	0.2	0.1	0.4	0.5	0.1	1.2	1.0	0.3	5.3	6.5	1.2	6.5	7.4	0.9
61	0.6			0.4			1.0			0.9			5.5			6.4		
	0.1	0.4	0.3	0.05	0.2	0.2	0.2	0.6	0.4	0.5	0.7	0.2	4.6	5.1	0.5	5.1	5.8	0.7
100	0.4						0.4			0.5			1.2			1.7		
	0.1	0.3	0.2		#####	#####	0.1	0.3	0.2	0.2	0.4	0.2	0.8	1.0	0.2	1.0	1.4	0.3

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Bury Pond water-clay loam sediment (continued).

	2,4,5-Trichloro-6-mercapto-isophthalonitrile (R_t=13-14 min.)									4-Hydroxy-2,5,6-trichloro-1,3-dicyanobenzene (R_t=12-13 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	1.4			1.4				#####	#####	0.2			0.2		
				1.2	1.3	0.1	1.2	1.3	0.1				0.4	0.3	0.1	0.4	0.3	0.1
0.25	0.4			2.9			3.3			1.4			1.1			2.5		
	0.4	0.4	0.0	18.3	10.6	7.7	18.7	11.0	7.7	1.3	1.4	0.0	1.8	1.5	0.3	3.1	2.8	0.3
1	0.2			5.5			5.7			0.8			3.4			4.2		
	0.1	0.2	0.1	13.9	9.7	4.2	14.0	9.9	4.2	1.0	0.9	0.1	2.3	2.9	0.6	3.3	3.8	0.5
2	0.5			0.8			1.3			3.3			2.3			5.6		
	0.2	0.4	0.2	1.7	1.3	0.5	1.9	1.6	0.3	1.8	2.6	0.8	1.4	1.9	0.5	3.2	4.4	1.2
7	0.7			6.0			6.7			2.3			3.3			5.6		
	0.5	0.6	0.1	12.1	9.1	3.1	12.6	9.7	3.0	1.5	1.9	0.4	3.4	3.4	0.0	4.9	5.3	0.4
14	3.4			3.0			6.4			2.2			1.6			3.8		
	2.9	3.2	0.3	1.7	2.4	0.7	4.6	5.5	0.9	2.7	2.5	0.3	1.9	1.8	0.2	4.6	4.2	0.4
30	0.9			3.4			4.3			3.4			3.4			6.8		
	2.7	1.8	0.9	1.7	2.6	0.9	4.4	4.4	0.1	3.5	3.5	0.0	3.4	3.4	0.0	6.9	6.9	0.1
61	2.0			1.2			3.2			1.4			1.8			3.2		
	0.6	1.3	0.7	1.4	1.3	0.1	2.0	2.6	0.6	2.3	1.9	0.5	2.2	2.0	0.2	4.5	3.9	0.7
100	0.6			4.1			4.7			0.9			2.7			3.6		
	0.3	0.5	0.2	2.9	3.5	0.6	3.2	4.0	0.8	0.8	0.9	0.0	5.2	4.0	1.3	6.0	4.8	1.2

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev, for [^{14}C]chlorothalonil and its degradates.

Bury Pond water-clay loam sediment (continued).

	2,5,6-Trichloro-1,3-dicyanobenzene-4-sulphonate (R_t=9-10 min.)									A/C1 (R_t=8-9 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.2 0.3	0.3	0.1	0.2 0.3	0.3	0.1		#####	#####	1.1 1.8	1.5	0.3	1.1 1.8	1.5	0.3
0.25	0.3 0.6	0.5	0.2	9.8 9.8	9.8	0.0	10.1 10.4	10.3	0.2	0.8 0.8	0.8	0.0	8.4 14.4	11.4	3.0	9.2 15.2	12.2	3.0
1	0.2 0.3	0.3	0.1	9.3 2.7	6.0	3.3	9.5 3.0	6.3	3.3	0.4 0.6	0.5	0.1	18.4 18.9	18.7	0.3	18.8 19.5	19.2	0.3
2	0.7 0.4	0.6	0.2	4.9 2.7	3.8	1.1	5.6 3.1	4.4	1.3	0.5 0.3	0.4	0.1	4.9 7.1	6.0	1.1	5.4 7.4	6.4	1.0
7	1.5 1.0	1.3	0.3	7.6 8.9	8.3	0.7	9.1 9.9	9.5	0.4	0.9 0.7	0.8	0.1	13.2 15.2	14.2	1.0	14.1 15.9	15.0	0.9
14	3.1 0.9	2.0	1.1	4.8 2.7	3.8	1.1	7.9 3.6	5.8	2.2	1.3 0.5	0.9	0.4	6.1 5.4	5.8	0.4	7.4 5.9	6.7	0.7
30	1.4 2.1	1.8	0.4	4.0 2.8	3.4	0.6	5.4 4.9	5.2	0.3	2.0 1.2	1.6	0.4	6.0 4.9	5.5	0.6	8.0 6.1	7.1	0.9
61	1.2 1.8	1.5	0.3	1.1 3.0	2.1	1.0	2.3 4.8	3.6	1.3	0.8 1.4	1.1	0.3	4.7 3.0	3.9	0.9	5.5 4.4	5.0	0.5
100	0.9 0.6	0.8	0.2	2.3 2.0	2.2	0.2	3.2 2.6	2.9	0.3	1.1 0.8	1.0	0.2	3.7 2.2	3.0	0.8	4.8 3.0	3.9	0.9

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev, for [^{14}C]chlorothalonil and its degradates.

Bury Pond water-clay loam sediment (continued).

	C/C3 (R_t=10-11 min.)									D/C4 (R_t=11-12 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.5 0.2	0.4	0.2	0.5 0.2	0.4	0.2		#####	#####	0.4 0.4	0.4	0.0	0.4 0.4	0.4	0.0
0.25	0.5 1.0	0.8	0.3	1.2 1.5	1.4	0.1	1.7 2.5	2.1	0.4	0.2 0.5	0.4	0.2	2.1 1.6	1.9	0.3	2.3 2.1	2.2	0.1
1	0.4 0.5	0.5	0.1	0.9 1.2	1.1	0.2	1.3 1.7	1.5	0.2	0.1 0.2	0.2	0.1	1.4 0.9	1.2	0.3	1.5 1.1	1.3	0.2
2	0.8 0.5	0.7	0.2	1.2 0.2	0.7	0.5	2.0 0.7	1.4	0.7	0.7 0.4	0.6	0.2	1.6 1.2	1.4	0.2	2.3 1.6	2.0	0.4
7	0.9 1.4	1.2	0.3	1.0 1.1	1.1	0.0	1.9 2.5	2.2	0.3	0.8 1.5	1.2	0.4	1.0 2.9	2.0	1.0	1.8 4.4	3.1	1.3
14	0.8 1.1	1.0	0.2	0.9 1.4	1.2	0.3	1.7 2.5	2.1	0.4	2.5 1.6	2.1	0.5	2.5 1.3	1.9	0.6	5.0 2.9	4.0	1.1
30	2.1 1.4	1.8	0.4	0.9 3.0	2.0	1.1	3.0 4.4	3.7	0.7	1.5 1.8	1.7	0.2	2.6 3.0	2.8	0.2	4.1 4.8	4.5	0.4
61	1.8 2.0	1.9	0.1	2.2 1.7	2.0	0.2	4.0 3.7	3.9	0.1	1.7 1.4	1.6	0.2	2.6 3.4	3.0	0.4	4.3 4.8	4.6	0.3
100	0.8 1.0	0.9	0.1	2.5 1.0	1.8	0.8	3.3 2.0	2.7	0.7	0.2 0.2	0.2	0.0	4.9 1.3	3.1	1.8	5.1 1.5	3.3	1.8

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Bury Pond water-clay loam sediment (continued).

	G/C7 (R_t=14-15 min.)									P1 (R_t=2-3 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.2			0.2				#####	#####	1.5			1.5		
				0.2	0.2	0.0	0.2	0.2	0.0				2.2	1.9	0.4	2.2	1.9	0.4
0.25	1.3			2.6			3.9			1.0			2.1			3.1		
	1.1	1.2	0.1	0.7	1.7	1.0	1.8	2.9	1.1	0.8	0.9	0.1	1.5	1.8	0.3	2.3	2.7	0.4
1	0.7			2.6			3.3			1.1			1.6			2.7		
	0.8	0.8	0.1	1.8	2.2	0.4	2.6	3.0	0.3	0.8	1.0	0.2	1.8	1.7	0.1	2.6	2.7	0.0
2	1.1			4.3			5.4			1.4			6.0			7.4		
	0.7	0.9	0.2	1.0	2.7	1.7	1.7	3.6	1.9	0.7	1.1	0.4	2.1	4.1	2.0	2.8	5.1	2.3
7	2.3			1.6			3.9			1.6			6.8			8.4		
	1.8	2.1	0.3	1.7	1.7	0.1	3.5	3.7	0.2	2.1	1.9	0.3	0.6	3.7	3.1	2.7	5.6	2.9
14	1.8			2.0			3.8			7.4			1.0			8.4		
	3.0	2.4	0.6	3.8	2.9	0.9	6.8	5.3	1.5	5.0	6.2	1.2	2.9	2.0	1.0	7.9	8.2	0.3
30	1.9			2.7			4.6			3.6			2.7			6.3		
	2.9	2.4	0.5	3.1	2.9	0.2	6.0	5.3	0.7	3.7	3.7	0.0	1.1	1.9	0.8	4.8	5.6	0.8
61	2.3			4.3			6.6			5.9			3.1			9.0		
	1.1	1.7	0.6	3.0	3.7	0.7	4.1	5.4	1.3	11.4	8.7	2.8	2.3	2.7	0.4	13.7	11.4	2.4
100	0.5			4.8			5.3			4.7			2.0			6.7		
	0.3	0.4	0.1	6.8	5.8	1.0	7.1	6.2	0.9	3.4	4.1	0.7	1.2	1.6	0.4	4.6	5.7	1.1

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Bury Pond water-clay loam sediment (continued).

	P2 (R_t=3-4 min.)									P3 (R_t=4-5 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.1 0.1	0.1	0.0	0.1 0.1	0.1	0.0		#####	#####	1.0 0.3	0.7	0.4	1.0 0.3	0.7	0.4
0.25	0.6 0.4	0.5	0.1	2.8 1.9	2.4	0.5	3.4 2.3	2.9	0.6	1.1 1.3	1.2	0.1	2.9 1.5	2.2	0.7	4.0 2.8	3.4	0.6
1	0.2 0.2	0.2	0.0	0.7 1.1	0.9	0.2	0.9 1.3	1.1	0.2	0.6 0.7	0.7	0.1	1.3 1.8	1.6	0.3	1.9 2.5	2.2	0.3
2	0.7 0.2	0.5	0.3	1.1 0.8	1.0	0.2	1.8 1.0	1.4	0.4	1.6 0.7	1.2	0.5	1.2 1.5	1.4	0.1	2.8 2.2	2.5	0.3
7	1.8 2.3	2.1	0.3	1.7 3.0	2.4	0.7	3.5 5.3	4.4	0.9	2.1 0.7	1.4	0.7	2.2 3.0	2.6	0.4	4.3 3.7	4.0	0.3
14	2.7 3.9	3.3	0.6	0.7 2.2	1.5	0.8	3.4 6.1	4.8	1.4	2.0 4.4	3.2	1.2	1.7 1.6	1.7	0.1	3.7 6.0	4.9	1.2
30	8.8 4.7	6.8	2.1	0.9 2.6	1.8	0.9	9.7 7.3	8.5	1.2	1.9 2.8	2.4	0.5	3.0 3.5	3.3	0.3	4.9 6.3	5.6	0.7
61	1.5 1.8	1.7	0.2	0.8 3.4	2.1	1.3	2.3 5.2	3.8	1.5	2.7 5.7	4.2	1.5	1.6 1.8	1.7	0.1	4.3 7.5	5.9	1.6
100	0.7 2.3	1.5	0.8	2.1 0.4	1.3	0.9	2.8 2.7	2.8	0.0	2.4 2.4	2.4	0.0	1.6 2.6	2.1	0.5	4.0 5.0	4.5	0.5

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev. for [^{14}C]chlorothalonil and its degradates.

Bury Pond water-clay loam sediment (continued).

	P4 (R_t=5-6 min.)									I (R_t=17.5-18 min.)								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0		#####	#####	0.4 0.8	0.6	0.2	0.4 0.8	0.6	0.2		#####	#####		#####	#####	0.0 0.0	0.0	0.0
0.25	0.3 0.6	0.5	0.2	1.0 0.6	0.8	0.2	1.3 1.2	1.3	0.0	0.2 0.2	0.2	0.0		#####	#####	0.2 0.2	0.2	0.0
1	0.2 0.2	0.2	0.0	2.1 0.6	1.4	0.8	2.3 0.8	1.6	0.8	0.1 0.2	0.2	0.1		#####	#####	0.1 0.2	0.2	0.1
2	0.9 0.2	0.6	0.4	1.0 0.7	0.9	0.2	1.9 0.9	1.4	0.5	0.2 0.2	0.2	0.0		#####	#####	0.2 0.2	0.2	0.0
7	0.8 0.3	0.6	0.3	1.3 0.6	1.0	0.4	2.1 0.9	1.5	0.6	1.1 0.4	0.8	0.4		#####	#####	1.1 0.4	0.8	0.4
14	1.6 5.0	3.3	1.7	1.8 1.8	1.8	0.0	3.4 6.8	5.1	1.7	1.0 1.5	1.3	0.3		#####	#####	1.0 1.5	1.3	0.3
30	2.4 3.3	2.9	0.5	1.9 2.3	2.1	0.2	4.3 5.6	5.0	0.7	0.2 0.6	0.4	0.2		#####	#####	0.2 0.6	0.4	0.2
61	3.3 1.3	2.3	1.0	1.4 0.4	0.9	0.5	4.7 1.7	3.2	1.5	1.0 0.3	0.7	0.4		#####	#####	1.0 0.3	0.7	0.4
100	0.8 1.1	1.0	0.2	1.4 2.0	1.7	0.3	2.2 3.1	2.7	0.5	0.4 0.1	0.3	0.2		#####	#####	0.4 0.1	0.3	0.2

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Confirmation/determination means/std.dev, for [^{14}C]chlorothalonil and its degradates.

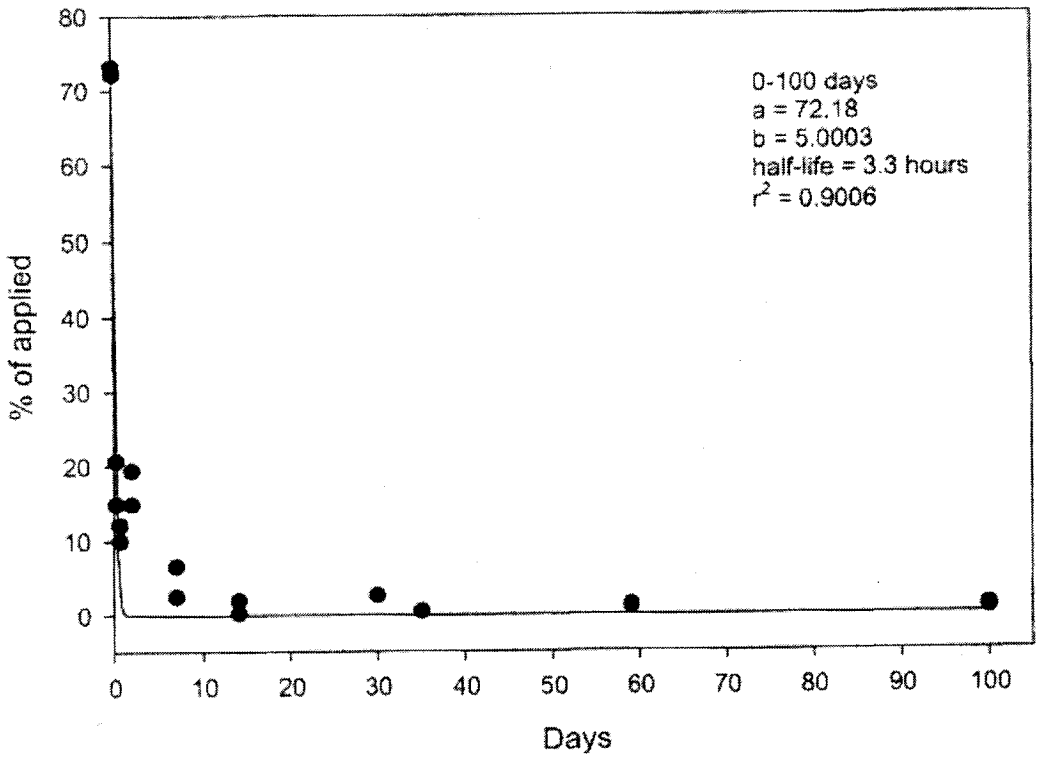
Bury Pond water-clay loam sediment (continued).

	Others									Total Unidentified [^{14}C]Residues								
	Water			Sediment			Total System			Water			Sediment			Total System		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	0.5			0.4			0.9			0.5			5.6			6.1		
	0.1	0.3	0.2	0.1	0.3	0.2	0.2	0.6	0.4	0.1	0.3	0.2	6.1	5.9	0.3	6.2	6.2	0.0
0.25	0.6			0.7			1.3			6.6			23.8			30.4		
	0.6	0.6	0.0	1.3	1.0	0.3	1.9	1.6	0.3	7.3	7.0	0.4	25.0	24.4	0.6	32.3	31.4	1.0
1	0.4			1.4			1.8			4.2			30.4			34.6		
	0.6	0.5	0.1	1.6	1.5	0.1	2.2	2.0	0.2	4.8	4.5	0.3	29.7	30.1	0.3	34.5	34.6	0.1
2	0.7			1.1			1.8			8.6			22.4			31.0		
	0.5	0.6	0.1	0.9	1.0	0.1	1.4	1.6	0.2	4.4	6.5	2.1	15.5	19.0	3.4	19.9	25.5	5.6
7	1.1			1.5			2.6			13.4			30.3			43.7		
	0.7	0.9	0.2	1.4	1.5	0.0	2.1	2.4	0.3	11.9	12.7	0.8	29.5	29.9	0.4	41.4	42.6	1.2
14	2.3			1.1			3.4			23.4			17.8			41.2		
	3.3	2.8	0.5	1.2	1.2	0.1	4.5	4.0	0.5	29.3	26.4	3.0	21.6	19.7	1.9	50.9	46.1	4.9
30	1.3			1.3			2.6			25.7			22.0			47.7		
	2.1	1.7	0.4	1.0	1.2	0.2	3.1	2.9	0.3	24.5	25.1	0.6	24.5	23.3	1.2	49.0	48.4	0.6
61	2.2			3.0			5.2			23.2			23.7			46.9		
	1.7	2.0	0.2	1.5	2.3	0.8	3.2	4.2	1.0	28.1	25.7	2.5	20.5	22.1	1.6	48.6	47.8	0.9
100	0.3			1.3			1.6			11.9			24.3			36.2		
	0.7	0.5	0.2	1.3	1.3	0.0	2.0	1.8	0.2	12.3	12.1	0.2	18.8	21.6	2.7	31.1	33.7	2.5

LOD appears to have been 0.1% of the applied for HPLC analyses, consequently, 0.05 was used for a nondetect with a detect at the same sampling interval for determining a mean and std. dev.
Results from Table XVIII, pp. 51-52; Table XX, pp. 55-56 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevpa(A1:A2).

US EPA ARCHIVE DOCUMENT

[Phenyl-^{14}C]Chlorothalonil in U.K. water-clay sediment: total system, nonlinear regression (MRID 45908001)



Aerobic aquatic metabolism of [phenyl-^{14}C]chlorothalonil in U.K. Houghton Meadow water-clay sediment.
MRID 45908001
Total system
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 72.1787}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 5.00033}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.94900683 Rsqr = 0.90061396 Adj Rsqr = 0.89440233

Standard Error of Estimate = 7.2624

	Coefficient	Std. Error	t	P
a	72.1787	5.1268	14.0788	<0.0001
b	5.0003	0.9713	5.1479	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	7647.0196	7647.0196	144.9884	<0.0001
Residual	16	843.8765	52.7423		
Total	17	8490.8961	499.4645		

PRESS = 940.2376

Durbin-Watson Statistic = 0.7747

Normality Test: K-S Statistic = 0.4459 Significance Level = 0.0009

Constant Variance Test: Passed (P = 0.5408)

Power of performed test with alpha = 0.0500: 1.0000

US EPA ARCHIVE DOCUMENT

Aerobic aquatic metabolism of [phenyl-^{14}C]chlorothalonil in U.K. Houghton Meadow water-clay sediment.
MRID 45908001
Total system

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	72.1787	1.0213	0.1406	0.1985	0.1925
2	72.1787	0.0213	0.0029	0.0041	0.0040
3	20.6779	0.0221	0.0030	0.0041	0.0040
4	20.6779	-5.7779	-0.7956	-1.0720	-1.0774
5	2.5743	9.5257	1.3116	1.3474	1.3856
6	2.5743	7.4257	1.0225	1.0504	1.0540
7	0.0033	19.3967	2.6708	2.6708	3.4739
8	0.0033	14.8967	2.0512	2.0512	2.3134
9	0.0000	2.5500	0.3511	0.3511	0.3413
10	0.0000	6.6000	0.9088	0.9088	0.9036
11	0.0000	0.3000	0.0413	0.0413	0.0400
12	0.0000	2.0000	0.2754	0.2754	0.2673
13	0.0000	2.6000	0.3580	0.3580	0.3480
14	0.0000	0.5000	0.0688	0.0688	0.0667
15	0.0000	1.1000	0.1515	0.1515	0.1468
16	0.0000	1.2500	0.1721	0.1721	0.1668
17	0.0000	0.7000	0.0964	0.0964	0.0934
18	0.0000	1.0000	0.1377	0.1377	0.1334

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.0196	0.4983	0.1918
2	0.0000	0.4983	0.0040
3	0.0000	0.4493	0.0036
4	0.4687	0.4493	-0.9731
5	0.0502	0.0524	0.3258
6	0.0305	0.0524	0.2479
7	0.0000	0.0000	0.0032
8	0.0000	0.0000	0.0021
9	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000

US EPA ARCHIVE DOCUMENT

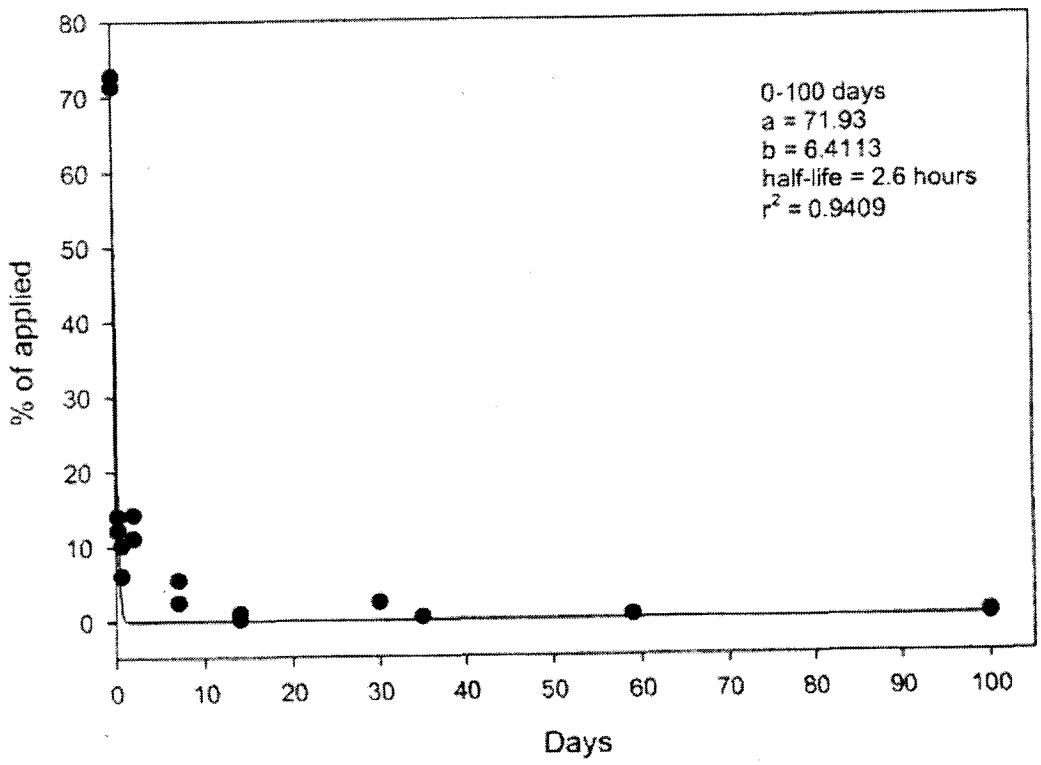
Aerobic aquatic metabolism of [phenyl-^{14}C]chlorothalonil in U.K. Houghton Meadow water-clay sediment.
MRID 45908001
Total system
95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	72.1787	61.3105	83.0470	53.3335	91.0240
2	72.1787	61.3105	83.0470	53.3335	91.0240
3	20.6779	10.3588	30.9970	2.1439	39.2118
4	20.6779	10.3588	30.9970	2.1439	39.2118
5	2.5743	-0.9499	6.0986	-13.2195	18.3681
6	2.5743	-0.9499	6.0986	-13.2195	18.3681
7	0.0033	-0.0110	0.0176	-15.3923	15.3989
8	0.0033	-0.0110	0.0176	-15.3923	15.3989
9	0.0000	-0.0000	0.0000	-15.3956	15.3956
10	0.0000	-0.0000	0.0000	-15.3956	15.3956
11	0.0000	-0.0000	0.0000	-15.3956	15.3956
12	0.0000	-0.0000	0.0000	-15.3956	15.3956
13	0.0000	-0.0000	0.0000	-15.3956	15.3956
14	0.0000	-0.0000	0.0000	-15.3956	15.3956
15	0.0000	-0.0000	0.0000	-15.3956	15.3956
16	0.0000	-0.0000	0.0000	-15.3956	15.3956
17	0.0000	0.0000	0.0000	-15.3956	15.3956
18	0.0000	0.0000	0.0000	-15.3956	15.3956

US EPA ARCHIVE DOCUMENT

US EPA ARCHIVE DOCUMENT

[Phenyl-^{14}C]Chlorothalonil in U.K. water-clay sediment: water layer, nonlinear regression (MRID 45908001)



Aerobic aquatic metabolism of [phenyl-^{14}C]chlorothalonil in U.K. Houghton Meadow water-clay sediment.
MRID 45908001
Water layer
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x) "Auto {{previous: 71.9315}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 6.41132}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.97001897 Rsqr = 0.94093680 Adj Rsqr = 0.93699926

Standard Error of Estimate = 5.7073

	Coefficient	Std. Error	t	P
a	71.9315	4.0346	17.8288	<0.0001
b	6.4113	1.1122	5.7645	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	7783.8267	7783.8267	238.9653	<0.0001
Residual	15	488.5957	32.5730		
Total	16	8272.4224	517.0264		

PRESS = 510.2500

Durbin-Watson Statistic = 0.7509

Normality Test: K-S Statistic = 0.3952 Significance Level = 0.0067

Constant Variance Test: Passed (P = 0.1510)

Power of performed test with alpha = 0.0500: 1.0000

US EPA ARCHIVE DOCUMENT

Aerobic aquatic metabolism of [phenyl-^{14}C]chlorothalonil in U.K. Houghton Meadow water-clay sediment.
MRID 45908001
Water layer

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	71.9315	0.8685	0.1522	0.2152	0.2082
2	71.9315	-0.5315	-0.0931	-0.1317	-0.1273
3	14.4817	-0.3817	-0.0669	-0.0930	-0.0899
4	14.4817	-2.2817	-0.3998	-0.5562	-0.5429
5	1.0015	9.1985	1.6117	1.6256	1.7302
6	1.0015	5.0985	0.8933	0.9010	0.8950
7	0.0002	14.2998	2.5055	2.5055	3.1743
8	0.0002	11.0998	1.9449	1.9449	2.1727
9	0.0000	2.5000	0.4380	0.4380	0.4259
10	0.0000	5.5000	0.9637	0.9637	0.9612
11	0.0000	0.2000	0.0350	0.0350	0.0339
12	0.0000	1.0000	0.1752	0.1752	0.1694
13	0.0000	2.4000	0.4205	0.4205	0.4087
14	0.0000	0.4000	0.0701	0.0701	0.0677
15	0.0000	0.5000	0.0876	0.0876	0.0847
16	0.0000	0.2000	0.0350	0.0350	0.0339
17	0.0000	0.4000	0.0701	0.0701	0.0677

Influence Diagnostics:

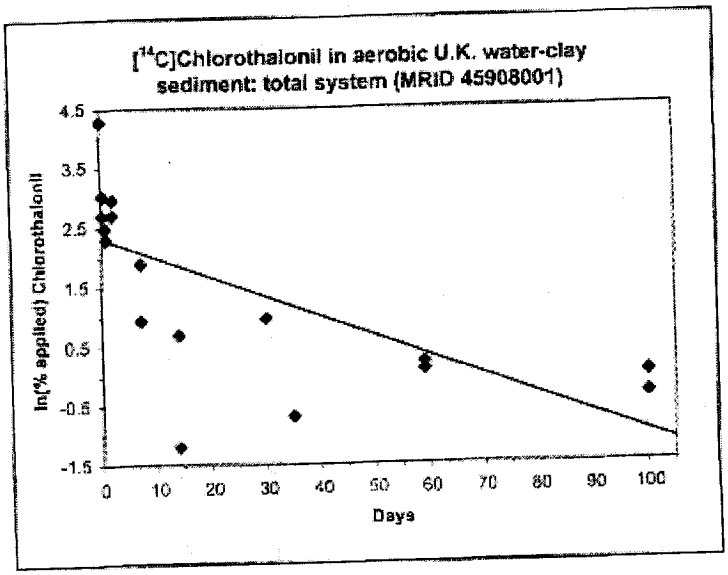
Row	Cook'sDist	Leverage	DFFITS
1	0.0231	0.4997	0.2081
2	0.0087	0.4997	-0.1272
3	0.0040	0.4833	-0.0869
4	0.1446	0.4833	-0.5251
5	0.0228	0.0170	0.2275
6	0.0070	0.0170	0.1177
7	0.0000	0.0000	0.0002
8	0.0000	0.0000	0.0002
9	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Houghton Meadow water-clay sediment
Half-life determination
Total system

Hours	Chlorothalonil	
	%AR	Ln(%AR)
0	73.2	4.293195
0	72.2	4.27944
0.25	20.7	3.030134
0.25	14.9	2.701361
1	12.1	2.493205
1	10.0	2.302585
2	19.4	2.965273
2	14.9	2.701361
7	2.6	0.936093
7	6.6	1.88707
14	0.3	-1.203973
14	2.0	0.693147
30	2.6	0.955511
35	0.5	-0.693147
59	1.1	0.09531
59	1.3	0.223144
100	0.7	-0.356675
100	1.0	0



Linear half-life = 21.0 days

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.6671
R Square	0.4450
Adj R Sq	0.4104
Std Error	1.2817
Observations	18

Nonlinear (exponential decay/single, 2 parameter)
half-life = 3.3 hours R squared: 0.9006
See SigmaPlot file 081901 45908001 162-4 Parent HM Tot sys nonlinear.

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	21.07936	21.079	12.83095	0.002492
Residual	16	26.28565	1.6429		
Total	17	47.36501			

	Coeffs	*Std Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.3084	0.374301	6.1672	1.353E-05	1.5149062	3.1018716	1.5149062	3.101871574
X Variable 1	-0.033	0.009232	-3.582	0.002492	-0.052642	-0.0134989	-0.0526425	-0.01349892

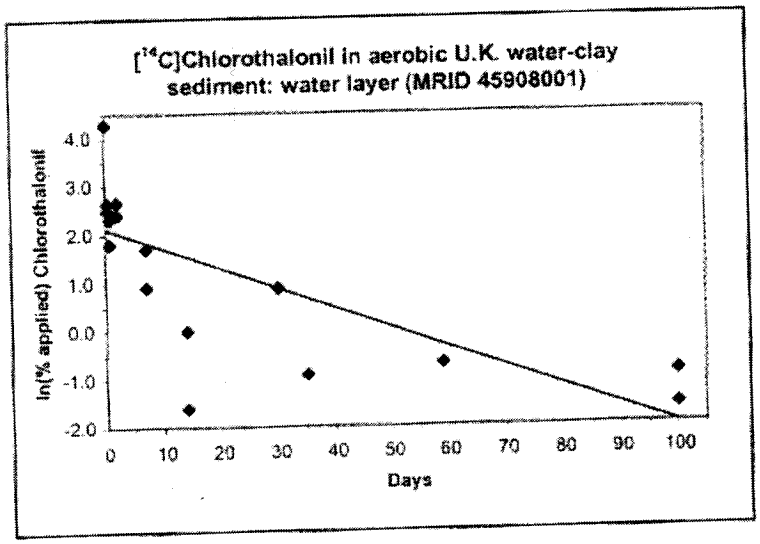
Linear regression analysis performed using Microsoft Excel 2000.
Results (% of applied radioactivity) from Table XVII, pp. 49-50; Table XIX, pp. 53-54 of the study report and DER Attachment 1.

US EPA ARCHIVE DOCUMENT

Aerobic Aquatic Metabolism of [Phenyl-14C]Chlorothalonil in two U.K. systems.
MRID 45908001

Houghton Meadow water-clay sediment
Half-life determination
Water layer

Hours	Chlorothalonil	
	%AR	Ln(%AR)
0	72.8	4.287716
0	71.4	4.268298
0.25	14.1	2.646175
0.25	12.2	2.501436
1	10.2	2.322388
1	6.1	1.808289
2	14.3	2.66026
2	11.1	2.406945
7	2.5	0.916291
7	5.5	1.704748
14	0.2	-1.60944
14	1.0	0
30	2.4	0.875469
35	0.4	-0.91629
59	0.5	-0.69315
100	0.2	-1.60944
100	0.4	-0.91629



SUMMARY OUTPUT

Linear half-life = 16.8 days

Nonlinear (exponential decay/single, 2 parameter)
half-life = 2.6 hours R squared: 0.9409
See SigmaPlot file 081901 45908001 162-4 Parent HM H2O nonlinear.

Regression Statistics	
Multiple R	0.7248
R Square	0.5254
Adj R Sq	0.4937
Std Error	1.3565
Observations	17

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	30.55414	30.554	16.60409	0.0009959
Residual	15	27.60237	1.8402		
Total	16	58.15651			

	Coeffs	*Std Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.1168	0.396521	5.3383	8.28E-05	1.271594	2.9619232	1.27159399	2.961923227
X Variable 1	-0.041	0.010119	-4.075	0.000996	-0.0628	-0.0196645	-0.06279985	-0.01966445

Linear regression analysis performed using Microsoft Excel 2000.
Results (% of applied radioactivity) from Table XVII, pp. 49-50 of the study report.

US EPA ARCHIVE DOCUMENT

Aerobic aquatic metabolism of [phenyl-^{14}C]chlorothalonil in U.K. Houghton Meadow water-clay sediment.

MRID 45908001

Water layer

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	71.9315	63.3320	80.5310	57.0341	86.8289
2	71.9315	63.3320	80.5310	57.0341	86.8289
3	14.4817	6.0249	22.9384	-0.3338	29.2972
4	14.4817	6.0249	22.9384	-0.3338	29.2972
5	1.0015	-0.5841	2.5871	-11.2662	13.2692
6	1.0015	-0.5841	2.5871	-11.2662	13.2692
7	0.0002	-0.0008	0.0011	-12.1646	12.1650
8	0.0002	-0.0008	0.0011	-12.1646	12.1650
9	0.0000	-0.0000	0.0000	-12.1648	12.1648
10	0.0000	-0.0000	0.0000	-12.1648	12.1648
11	0.0000	-0.0000	0.0000	-12.1648	12.1648
12	0.0000	-0.0000	0.0000	-12.1648	12.1648
13	0.0000	-0.0000	0.0000	-12.1648	12.1648
14	0.0000	-0.0000	0.0000	-12.1648	12.1648
15	0.0000	-0.0000	0.0000	-12.1648	12.1648
16	0.0000	0.0000	0.0000	-12.1648	12.1648
17	0.0000	0.0000	0.0000	-12.1648	12.1648

US EPA ARCHIVE DOCUMENT