Data Evaluation Report on the anaerobic biotransformation of pyrasulfotole (AE 0317309) in water-sediment system

PMRA Submission Number 2006-2445 EPA MRID Number 46801714

Data Requirement:	PMRA Data Code:	8.2.3.5.6
	EPA DP Barcode:	D328639
	OECD Data Point:	IIA 7.8.2
	EPA Guideline:	162-3

Test material:

Common name: Pyrasulfotole.

Chemical name:

IUPAC name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone.
(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl)-4(trifluoromethyl)phenyl]methanone.
Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

CAS No: 365400-11-9.

Synonyms: AE 0317309; K-1196; K-1267.

SMILES string: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C)(F)F (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.
CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.

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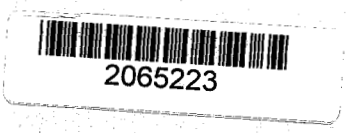

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CITATION: Shepherd, J. and E. Arthur. 2005. [Phenyl-UL-^{14}C]AE 0317309: anaerobic aquatic metabolism. Unpublished study performed by Bayer CropScience, Stilwell, Kansas; sponsored and submitted by Bayer CropScience, Research Triangle Park, North Carolina. BCS Study No.: A9042102 and Report No.: 200593. Experimental start date March 10, 2003 and termination date August 9, 2004 (p. 6). Final report issued May 4, 2005.

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EXECUTIVE SUMMARY

The biotransformation of [phenyl-U-^{14}C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone (pyrasulfotole, AE 0317309; radiochemical purity >97%) was studied in pond water-silty clay sediment (water pH 7.5, dissolved organic carbon 11.7 mg/L; sediment pH 6.6-7.0, organic carbon 1.1%) systems from Kansas for 365 days under anaerobic (static, nitrogen atmosphere) conditions in darkness at 20 ± 1°C. Based on the water volume, [^{14}C]pyrasulfotole was applied at a rate of 0.004 mg a.i./L. The sediment:water ratio used was 1:3 (50 g dry wt. sediment:150 mL water). This experiment was conducted in accordance with USEPA Subdivision N Guideline §162-3, and in compliance with USEPA GLP Standards 40 CFR, Part 160. The test system consisted of 250-mL, Pyrex, Erlenmeyer flasks sealed with either a mineral oil bubbler trap (pre-incubation) or a closeable, double-valve glass stopper (following treatment). To generate anaerobic conditions, the water-sediment systems were purged with nitrogen, then the sealed flasks were pre-incubated for 21 days prior to treatment. Following treatment, duplicate flasks were collected after 0, 3, 7, 10, 22, 31, 63, 92, 120, 183, 273 and 365 days of incubation. Upon collection, the metabolism flasks were attached to a flow-through (nitrogen, 40 mL/minute, 30 minutes) system with traps for the collection of CO_2 (2M KOH) and volatile organics (ethylene glycol, 1M H_2SO_4). Water layers were decanted, filtered (Whatman No. 1 paper), then concentrated via rotary evaporation for reverse-phase HPLC analysis. Sediment samples were extracted once with acetonitrile:water (9:1, v:v) via shaking, then further extracted with the acetonitrile:water solvent using an Accelerated Solvent Extraction (ASE) system (2 cycles, 80°C, 1,500 psi). Resulting sediment extracts were combined and concentrated in the same manner as the water samples for HPLC analysis. No major transformation products were detected and no minor products were identified.

The test conditions outlined in the study appear to have been maintained throughout the 365-day incubation. Conditions in untreated, control water-sediment systems incubated alongside the treated systems were moderately reducing with mean redox potentials of -39.5 to +33.2 mV and -28.2 to +35.6 mV in the water layer and sediment, respectively. In the water layer, mean dissolved oxygen and pH levels were ≤0.2 mg/L and 6.6-7.0, respectively.

Overall recovery of radiolabeled material averaged 96.6 ± 2.6% (range 92.6-103.7%) of the applied, with no pattern of decline in recoveries during the 365-day study. Following application of [^{14}C]pyrasulfotole to the water-sediment systems, [^{14}C]residues partitioned from the water layer to the sediment with average (n = 2) distribution ratios (water:sediment) of 100:1 at day 0, 4:1 at 3 days, 2:1 at 10 days and were 1:1 thereafter. [^{14}C]Pyrasulfotole dissipated slowly in the total system decreasing from a mean 99.2% of the applied at day 0 to 65.1% at 31 days and was 60.4%-65.6% thereafter. In the water layer, [^{14}C]pyrasulfotole decreased from a mean 99.2% at day 0 to 49.7% at 31 days and was 38.3-40.0% at 183-365 days. In the sediment, [^{14}C]pyrasulfotole increased to a mean 25.5% at study termination.

Calculated linear and nonlinear first-order half-lives (see below) for pyrasulfotole in the water layer and total system are of limited use given the low correlation coefficient values (r^2 = ≤0.51), and the half-lives for pyrasulfotole in the total system were extrapolated significantly beyond the final

sampling interval. Levels of [^{14}C]pyrasulfotole in the sediment were still increasing at study termination; consequently, calculated half-lives could not be determined. **Observed DT50** values of pyrasulfotole were 22-31 days in the water layer and >365 days in the sediment and total system. Non-first order DT50 and DT90 estimates for the total system were estimated at 6000 and 46000 days, respectively using a multi-compartment non-linear regression model ($r^2 = 0.95$). **Pyrasulfotole is considered stable in the whole system under these anaerobic aquatic conditions.**

Unidentified [^{14}C]residues, consisting of up to four [^{14}C]components, were detected at maximum totals of 1.7%, 2.6% and 3.4% of the applied in the water, sediment and total system, respectively, with no individual component detected at >2.9% of applied. Extractable and nonextractable sediment [^{14}C]residues increased to maximum means of 25.5% and 33.9% of applied, respectively, at 365 days. At study termination, organic matter fractionation of the nonextractable residues (33.9% of applied) found 31.6%, 66.3% and 2.1% of the recovered radioactivity associated with the humin, fulvic acids and humic acids, respectively. The maximum level of volatilized $^{14}CO_2$ detected at any sampling interval was 2.8% of the applied, with volatile [^{14}C]organic compounds <0.1%.

A transformation pathway was not provided as pyrasulfotole did not form any significant transformation products under the anaerobic aquatic conditions used in this study. Dissipation of parent pyrasulfotole primarily involved the formation of bound sediment residues with minimal levels of mineralization to CO_2 and the possible formation of several minor compounds.

In a supplementary experiment, pyrasulfotole remained stable in 365-day water layer and sediment extract samples after 153 days of frozen storage.

Results Synopsis:

Test system used: Pond water-silty clay sediment Kansas.

Linear half-life in water:	385 days ($r^2 = 0.5089$).
Linear half-life in sediment:	ND (not determined).
Linear half-life in the total system:	887 days ($r^2 = 0.3421$).
Non-linear half-life in water:	267 days ($r^2 = 0.4909$).
Non-linear half-life in sediment:	ND.
Non-linear half-life in total system:	770 days ($r^2 = 0.3489$).
Observed DT50 in water:	22-31 days.
Observed DT50 in sediment:	>365 days.
Observed DT50 in total system:	>365 days.
Non-linear DT50 in total system:	6000 days ($r^2 = 0.947$)
Non-linear DT90 in total system:	46000 days ($r^2 = 0.947$)

Note: Linear and non-linear first order models do not adequately describe dissipation pattern. Considered stable in anaerobic aquatic environments.

Major transformation products:
None.
Minor identified transformation products:
CO_2 (maximum mean 2.8% of applied).

Study Acceptability: This study is classified as **acceptable**. No significant deviations from good scientific practices were noted.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with USEPA Subdivision N Guideline §162-3 and PMRA Environmental Chemistry and Fate Guidelines for Registration of Pesticides in Canada (pp. 14-15, 31-32). No significant deviations from the objectives of Subdivision N guidelines were noted.

COMPLIANCE: This study was conducted in compliance with USEPA GLP Standards 40 CFR, Part 160 (pp. 3, 14, 32). Signed and dated Data Confidentiality, GLP, Quality Assurance and [study] Certification statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Material [Phenyl-U-^{14}C]pyrasulfotole (p. 16; Figure 1, p. 40).

Chemical Structure: See DER Attachment 1.

Description: Technical; pale, yellow solid (p. 16).

Purity:	Radiochemical purity:	>97% (p. 16; Figure 5A, p. 45).
	Lot/Batch No.	SEL/1006.
	Analytical purity:	Not reported.
	Specific activity:	194,959 dpm/µg (31.3 mCi/mmol, 3.19 MBq/mg).
	Location of the radiolabel:	Uniformly on phenyl ring.

Storage conditions of test chemicals: Not reported.

Physico-chemical properties of pyrasulfotole:

Parameter	Value	Comment
Molecular weight	362.3 g/mol	
Water Solubility (g/L) at 20°C	4.2 at pH 4 69.1 at pH 7 49.0 at pH 9	Very soluble
Vapor Pressure/Volatility	2.7×10^{-7} Pa at 20°C 6.8×10^{-7} Pa at 25°C	Non-volatile
UV Absorption	water $\lambda_{max} = 264$ 0.1M HCl $\lambda_{max} = 241$ 0.1M NaOH $\lambda_{max} = 216$	Not likely to undergo photolysis.
Pka	4.2 ± 0.15	
log K_{ow} at 23°C	0.276 at pH 4 -1.362 at pH 7 -1.58 at pH 9	Not likely to bioaccumulate
Stability of compound at room temperature, if provided		No significant degradation over 12 months at ambient temperatures.

Data obtained from pyrasulfatole chemistry review of Submission 2006-2445.

2. Water-sediment collection, storage and properties

Table 1: Description of water-sediment collection and storage.

Description		Details
Geographic location.		Nelson Environmental Study Area, Jefferson County, Lawrence, Kansas. Pond located in agricultural use area.
Coordinates	Latitude:	39.049°
	Longitude:	-95.193°
Pesticide use history at the collection sites		No pesticide applications for previous 5 years.
Collection date		January 21, 2003.
Collection procedures for:	Water:	Collected into 5-gallon buckets; no further description.
	Sediment:	Sediment collected with shovel into 5-gallon buckets and flooded with water.
Sampling depth for:	Water:	0- to 15.2-cm water depth.
	Sediment:	0- to 6-inch sediment layer taken at 15.2-cm water depth.
Storage conditions		Water and sediment transported at ambient temperature, then maintained at 25°C at test facility.
Storage length		27 days; water-sediment was collected on January 21, 2003, water-sediment systems were prepared and pre-incubated for 21 days prior to treatment, with the date of application March 10, 2003.
Preparation	Water:	None.
	Sediment:	Sieved (2-mm).

Data obtained from pp. 4, 18-19; Table 1, p. 33; Appendix 2, p. 58 of the study report.

Table 2: Properties of the water.

Property	Details	
Temperature (°C)	5.8°C	
pH	7.5	
Redox potential (mV)[1]	Initial[2]	Final
	-24.9	+16.9
Oxygen concentration (mg/L)[1]	Initial[2]	Final
	0.1	0.2
Dissolved organic carbon (mg/L)	11.7	
Hardness (mg $CaCO_3$/L)	200	
Electrical conductivity (units)	Not reported.	
Biomass (cells/mL water)[1]	Initial[3]	Final
	1.17×10^7	4.39×10^6

1 Measured in water layer of untreated, control systems prepared and incubated alongside treated systems (p. 19; Table 4, p. 37).
2 Initial and Final at 0 and 365 days posttreatment, respectively (Table 4, p. 37).
3 Initial and Final reported as "beginning" and "end" of study, respectively; sampling intervals were not specified (p. 19).
Data obtained from p. 19; Table 1, p. 34; Table 4, p. 37 of the study report.

Table 3: Properties of the sediment.

Property		Details	
Soil texture		Silty clay.	
% Sand (2000-50 Φm):		9.1	
% Silt (50-2 Φm):		47.5	
% Clay (<2 Φm):		43.4	
pH	soil:water (1:1):	7.0	
	saturated paste:	6.6	
	0.01M $CaCl_2$:	6.6	
Organic carbon (%)		1.1	
Organic matter (%)		2.0	
CEC (meq/100 g)		35.7	
Redox potential (mV)[1]		Initial[2]	Final
		-23.7	+6.3
Moisture at 1/3 bar (%)		40.2	
Bulk density (g/cm^3)		1.19	
Biomass (cells/g sediment)[1]		Initial[3]	Final
		2.89 x 10^8	1.42 x 10^8

1 Measured in sediment layer of untreated, control systems prepared and incubated alongside treated systems (p. 19; Table 4, p. 37).
2 Initial and Final at 0 and 365 days posttreatment, respectively (Table 4, p. 37).
3 Initial and Final reported as "beginning" and "end" of study; sampling intervals were not specified (p. 19).
Data obtained from p. 19; Table 1, p. 33; Table 4, p. 37 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None reported.

2. Experimental conditions:

Table 4: Experimental design.

Parameter		Details
Duration of the test		365 days.
Water: Filtered/unfiltered water: Type and size of filter used, if any:		Unfiltered.
Amount of sediment and water per treatment	Water:	150 mL
	Sediment:	50 g dry wt.
Water/sediment ratio		3:1 (mL:g dry wt.).
Application rates (mg a.i./L)	Nominal:	0.004 mg a.i./L
	Actual:	0.004 mg a.i./L (0.6 µg a.i./150 mL).

Parameter		Details	
Control conditions, if used		No sterile controls were used.	
No. of replications	Control, if used:	No sterile controls were used.	
	Treated:	Thirty-two nonsterile systems were treated with [^{14}C]pyrasulfotole to allow for duplicate flasks at each of twelve sampling intervals plus eight reserves.	
Test apparatus (type/material/volume):		Silanized, 250-mL side-arm Pyrex Erlenmeyer flask. During pre-incubation, flask sealed with mineral oil bubbler trap. Following treatment, flask sealed with closeable, double-valve glass stopper.	
Details of traps for CO_2 and organic volatile, if any:		2N potassium hydroxide (KOH) to trap CO_2 (two traps, each 30 mL). Ethylene glycol (one trap, 30 mL) and 1M sulfuric acid (H_2SO_4, one trap, 30 mL) to trap organic volatiles.	
If no traps were used, is the system closed?		Systems were incubated closed and attached to a flow-through volatiles trapping system upon collection.	
Identity and concentration of co-solvent		Acetonitrile (ACN); final concentration 0.07% based on water volume (100 µL.ACN in 150 mL water).	
Test material application method	Volume of the test solution used/treatment:	100 µL/system.	
	Application method (eg: mixed/not mixed):	Test solution was applied uniformly to the surface of the water layer using a 250-µL gas-tight Hamilton syringe without disturbing the water-sediment system.	
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated; however, flasks were silanized.	
Microbial biomass/microbial population of controls (units)		Initial	Final
	Water:	No sterile controls were used.	
	Sediment:		
Microbial biomass/microbial population of treated (units)		Initial	Final
	Water:	Treated systems were not analyzed for biomass.	
	Sediment:		
Experimental conditions:	Temperature (°C):	20 ± 1°C; maintained in a temperature-controlled incubator.	
	Continuous darkness (Yes/No):	Yes; system flasks wrapped with aluminum foil and maintained in darkness in an incubator.	
Other details, if any		None	

Data obtained from pp. 15, 19-21, 28; Table 2, p. 35; Figures 2-4, pp. 42-44; Appendix 2, p. 58 of the study report.

3. Anaerobic conditions: Water-sediment systems were prepared, purged with nitrogen (flow rate, interval not reported) and maintained in sealed (mineral oil bubbler trap) biometer flasks within a nitrogen-filled incubator for *ca.* 21 days prior to treatment to establish anaerobic conditions (p. 19). Following treatment, the mineral oil trap was replaced with a closeable, double-valve glass stopper, then the systems were purged with nitrogen (*ca.* 8 minutes, flow rate not reported) and returned to the nitrogen-filled incubator (p. 20). At day 0 posttreatment in untreated, control systems incubated alongside the treated systems, mean (n = 2) redox potential and dissolved oxygen in the water layer

were -24.9 mV and 0.1 mg/L, respectively, with a mean redox potential of -23.7 mV in the sediment (p. 21; Table 4, p. 37); individual replicate results were not provided.

4. Supplementary experiments: Metabolite identification (MID) samples. To facilitate identification of possible transformation products of pyrasulfotole, eight additional water-sediment systems were prepared and incubated as described above, but treated at 0.04 mg a.i./L or ten times the application rate (pp. 19-20).

5. Sampling:

Table 5: Sampling details.

Criteria	Details
Sampling intervals	0, 3, 7, 10, 22, 31, 63, 92, 120, 183, 273 and 365 days.
Sampling method	Duplicate treated systems at each interval.
Method of collection of CO_2 and organic volatile compounds	At each interval, the test flask was attached to a flow-through volatiles trapping system and purged with nitrogen (*ca.* 40 mL/minute, 30 minutes).
Sampling intervals/times for:	
Sterility check, if sterile controls are used:	Sterile controls were not prepared.
Redox potential, dissolved oxygen and pH in water layer and redox potential in sediment:	Measured in duplicate untreated, control systems at each sampling interval.
Sample storage before analysis	**Water layers and sediment** were separated and the **sediment** extracted the day of collection. **Water samples and sediment extracts** were stored frozen (≤-15°C) up to 137 days prior to analysis, with the majority of samples reportedly analyzed within an average of 17 days. However, specific extraction and analysis dates were not provided for review.
Other details, if any	None reported.

Data obtained from pp. 21, 31; Table 3, p. 36; Figure 4, p. 44 of the study report.

C. ANALYTICAL METHODS:

Separation of the water and sediment: The water layer was decanted and filtered (Whatman No. 1 filter paper), then triplicate aliquots (1 mL) were analyzed for total radioactivity by LSC (p. 22; Appendix 9, pp. 67-68).

Extraction/clean up/concentration methods for water and sediment samples: Prior to HPLC analysis, an aliquot (sufficient to characterize 2% of the applied radioactivity) of the water layer was concentrated to near dryness using rotary evaporation (*ca.* 30-35°C, under vacuum; p. 22).

Resulting residues were reconstituted to 9 mL with water:acetonitrile (9:1, v:v) and centrifuged (2,100 *g*, 20 minutes).

Sediment was transferred to a Teflon bottle using acetonitrile:water (9:1, v:v; *ca.* 100 mL), then extracted via shaking (bench-top shaker, 20 minutes, speed not reported; p. 22; Figure 6, p. 46). Extract was separated from sediment by filtration through diatomaceous earth (12 g, Hydromatrix sorbent) and filter paper (Whatman No. 541). The extracted sediment-sorbent sample was transferred to a 100-g extraction cell of an Accelerated Solvent Extraction (ASE) system (Model ASE 300, Dionex; Appendix 1, p. 57) and further extracted with acetonitrile:water (9:1, v:v) under the following conditions: 2 cycles, cell temperature 80°C, heating time 5 minutes, static time 5 minutes, flush volume 50%, purge time 120 seconds, pressure 1,500 psi. All sediment extracts were combined and triplicate aliquots (1 mL) were analyzed for total radioactivity. Prior to HPLC analysis, an aliquot of the combined extract was concentrated as described above for the water layer samples.

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 solutions (Table 5, p. 38).

Determination of nonextractable residues: Extracted sediment was air-dried and homogenized (method not reported, p. 22). Triplicate aliquots (*ca.* 0.25 g) were analyzed for total radioactivity by LSC following combustion (p. 22; Appendix 9, pp. 67-68).

Organic matter fractionation. Aliquots (*ca.* 50 g) of 365-day extracted sediment were further extracted with 0.5N sodium hydroxide (NaOH, 100 mL) via shaking (bench-top shaker, 1 hour, speed not reported), with the resulting extract separated from sediment by centrifugation (1,300 *g*, 20 minutes; pp. 22-23, 28). The supernatant was decanted, analyzed for total radioactivity by LSC, then acidified to pH 1 with hydrochloric acid with the resulting precipitate (humic acids) removed by centrifugation (1,300 *g*, 10 minutes). The resulting supernatant (fulvic acids) was analyzed for total radioactivity using LSC. [^{14}C]Residues remaining in the precipitate (humic acids) and extracted sediment (humin) were not analyzed, but quantified by subtraction.

Determination of volatile residues: Triplicate aliquots (1 mL) of the KOH, ethylene glycol and sulfuric acid trapping solutions were analyzed for total radioactivity by LSC (p. 21).

Derivatization method, if used: None was reported.

Identification and quantification of parent compound: Concentrated water and sediment extract samples were analyzed by reverse-phase HPLC under the following conditions: Supelco Supelcosil LC-ABZ (4.6 x 250 mm, 5 µm) column, Phenomenex C18 Security Guard pre-column, gradient mobile phase combining (A) 25mM potassium phosphate, dibasic and (B) acetonitrile [percent A:B at 0-3 min. 90:10 (v:v), 30-33 min. 0:100, 35 min. 90:10], injection volume 4.5 mL, flow rate 1 mL/minute, UV detector (wavelength not specified), and Ramona Classic or Ramona 90 radioactivity detector (Method I; pp. 22-23).

To confirm results from HPLC Method I, selected samples were also analyzed by reverse HPLC under the following conditions: Phenomenex C18(2) (10 x 250 mm, 10 µm) column, Phenomenex C18 Security Guard pre-column, gradient mobile phase combining (A) 30 mM triethylamine adjusted to pH 2.5 with phosphoric acid and (B) acetonitrile [percent A:B at 0-5 min. 90:10 (v:v), 5-33 min. 67:33], injection volume 4.5 mL, flow rate 3 mL/minute, Ramona radioactivity detector (Method II, p. 24).

Parent [^{14}C]pyrasulfotole was identified by co-chromatography with and comparison to the retention time of unlabeled reference standard (pp. 24-25, 29; Figure 7, p. 47; Figure 11, p. 51; Figures 13-14, pp. 53-54). Column recoveries were monitored through the collection and LSC analysis of selected bulk column eluates, with the average recovery reported as 92.2% (pp. 24, 28).

To confirm identification, [^{14}C]pyrasulfotole was isolated from a 128-day MID sediment extract sample via HPLC separation and fraction collection (p. 24). Fractions were concentrated (method not specified), then analyzed by LC/MS under the following conditions: either a Zorbax Rx or a Phenomenex Luna C-8 (4.6 x 250 mm, 5 µm) LC column, linear gradient mobile phase combining (A) 0.1% aqueous formic acid and (B) methanol [percent A:B at 0 min. 95:5 (v:v), 15 min. 5:95], flow rate 800 µL/minute, post-column split ratio 200:600 µL/min. (MS:radioactivity detector), Raytest Star radioactivity detector, Finnigan-MAT TSQ 7000 MS, electrospray ionization (ESI), negative ion mode, scan range generally 150-600 amu, scan time 1 second (pp. 24, 29). Identification of [^{14}C]pyrasulfotole in sample extract was made against labeled test substance (p. 29; Figure 5, p. 45; Figure 12, p. 52).

Identification and quantification of transformation products: Transformation products were separated and quantified using HPLC as described for the parent compound; however, no major transformation products were detected and minor products were not identified (pp. 23-24, 30-31; Figure 7, p. 47; Figure 11, p. 51; Figures 13-14, pp. 53-54).

Table 6: Reference compounds available for identifying transformation products of pyrasulfotole (AE 0317309).

Applicant codes	Chemical Name	Purity[1]
AE B197555, K-1367	2-(Methylsulfonyl)-4-(trifluoromethyl)benzoic acid	99.6%
AE 0317309 N-desmethyl, K-1385	(5-Hydroxy-3-methyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone	99.2%

1 Purity w/w unless otherwise designated.
Data obtained from p. 17; Figure 1, pp. 40-41 of the study report.

Detection limits (LOD, LOQ) for the parent compound and transformation products: For HPLC analyses, limits of detection (LOD) and quantitation (LOQ) were reported as 500 dpm and 2.0% of the applied radioactivity, respectively (p. 27). HPLC detector (Ramona Classic and Ramona 90) responses were linear from *ca.* 500-100,000 dpm (r^2 = 0.999-1.0; p. 28; Appendix 5, p. 61).

For LSC analyses, minimum sensitivities (MSP) were reported as 2.38% of the applied for water layer samples, 6.12% for sediment extracts and 3.66% for sediment combustions (Appendices 3-4, pp. 59-60).

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: Conditions in untreated, control water-sediment systems incubated alongside the treated systems were moderately reducing (-50 to +200 mV) throughout the 1-year incubation with mean (n = 2) redox potentials of -39.5 to +33.2 mV and -28.2 to +35.6 mV in the water layer and sediment, respectively (Table 4, p. 37). In the water layer, mean dissolved oxygen and pH levels were ≤0.2 mg/L and 6.6-7.0, respectively.

B. MATERIAL BALANCE: Overall recovery of radiolabeled material averaged 96.6 ± 2.6% (range 92.6-103.7%, n = 24) of the applied, with no pattern of decline in recoveries during the 1-year incubation (DER Attachment 2, Reviewer's Comment No. 1). Following application of [^{14}C]pyrasulfotole to the water-sediment systems, [^{14}C]residues partitioned from the water layer to the sediment with average (n = 2) distribution ratios (water:sediment) of 100:1 at day 0, 4:1 at 3 days, 2:1 at 10 days and were 1:1 thereafter (DER Attachment 2).

Table 7. Biotransformation of [phenyl-U-^{14}C]pyrasulfotole (AE 0317309), expressed as percentage of applied radioactivity (mean ± s.d., n = 2[1]), in Kansas pond water-silty clay sediment under anaerobic conditions.

Compound		Sampling times (days)											
		0	**3**	**7**	**10**	**22**	**31**	**63**	**92**	**120**	**183**	**273**	**365**
Pyrasulfotole	water	99.2 ± 0.5	77.1 ± 1.0	68.3 ± 1.0	62.2 ± 1.2	51.4 ± 0.1	49.7 ± 0.2	44.9 ± 0.6	44.2 ± 0.8	43.2 ± 0.1	40.0 ± 0.5	38.3 ± 0.7	40.0 ± 0.4
	sed.[2]	0.0 ± 0.0	8.7 ± 0.4	11.4 ± 0.5	13.2 ± 0.6	19.3 ± 0.0	15.5 ± 0.3	17.2 ± 0.5	21.4 ± 0.6	18.7 ± 1.3	20.9 ± 0.6	22.1 ± 3.5	25.5 ± 3.5
	system	99.2 ± 0.5	85.8 ± 0.6	79.6 ± 1.6	75.4 ± 1.8	70.7 ± 0.1	65.1 ± 0.5	62.1 ± 1.0	65.6 ± 0.1	61.9 ± 1.4	60.9 ± 1.1	60.4 ± 2.8	65.5 ± 3.9
Unidentified [^{14}C]residues[3]	water	0.0, 1.7	0.0 ± 0.0	0.0 ± 0.0	1.4, 0.0	1.0 ± 0.2	1.1 ± 0.3	0.9 ± 0.1	0.6, 0.0	0.0, 0.2	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0
	sed.	0.0, 0.9	0.0 ± 0.0	0.0 ± 0.0	0.0, 0.7	0.0, 1.0	1.9 ± 0.8	0.0, 1.2	0.0, 0.3	0.0, 0.1	0.0 ± 0.0	0.0, 2.5	0.0 ± 0.0
	system	0.0, 2.6	0.0 ± 0.0	0.0 ± 0.0	1.1 ± 0.4	1.4 ± 0.3	3.0 ± 0.5	1.5 ± 0.5	0.5 ± 0.2	0.0, 0.3	0.0 ± 0.0	0.0, 2.5	0.0 ± 0.0
CO_2		0.0 ± 0.0	1.7 ± 0.2	2.2 ± 0.1	1.9 ± 0.0	2.7 ± 0.2	2.5 ± 0.0	2.4 ± 0.1	2.1 ± 0.1	2.3 ± 0.1	2.2 ± 0.0	2.6 ± 0.0	2.8 ± 0.0
Volatile organics		0.0 ± 0.0	0.0 ± 0.00	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0
Extractable sediment residues		0.0 ± 0.0	9.4 ± 0.3	12.8 ± 0.5	14.7 ± 0.7	19.3 ± 0.0	17.5 ± 0.7	18.2 ± 0.7	21.4 ± 0.6	19.9 ± 1.1	20.9 ± 0.6	24.2 ± 1.4	25.5 ± 3.5
Nonextractable sediment residues		0.0 ± 0.0	8.5 ± 0.9	12.3 ± 1.2	17.0 ± 0.3	19.5 ± 1.1	25.8 ± 1.4	28.2 ± 2.1	26.8 ± 0.6	31.2 ± 0.2	32.7 ± 1.3	32.0 ± 1.2	33.9 ± 2.4
Total recovery	water	100.0 ± 0.3	77.1 ± 1.0	68.3 ± 1.0	63.0 ± 0.4	52.3 ± 0.2	50.8 ± 0.1	45.7 ± 0.4	44.5 ± 0.5	43.3 ± 0.0	40.0 ± 0.5	38.3 ± 0.7	40.0 ± 0.4
	sed.	0.0 ± 0.0	17.9 ± 0.6	25.1 ± 1.6	31.7 ± 1.0	38.8 ± 1.2	43.3 ± 2.0	46.3 ± 1.4	48.1 ± 1.3	51.1 ± 0.9	53.6 ± 0.7	56.1 ± 0.1	59.4 ± 1.1
	system	100.0 ± 0.3	96.8 ± 0.3	95.5 ± 2.9	96.5 ± 1.4	93.8 ± 1.1	96.5 ± 2.0	94.4 ± 0.9	94.8 ± 0.8	96.7 ± 0.7	95.7 ± 0.2	97.0 ± 0.6	102.1 ± 1.6

1 Reviewer's Comment No. 1.

2 Sediment.

3 Consisting of up to four [^{14}C]components (Unknowns A, B, C and D), each comprising ≤2.9% of the applied in the total system (DER Attachment 2).

Data obtained from DER Attachment 2.

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Pyrasulfotole dissipated slowly in the total system decreasing from 98.6-99.7% of the applied at day 0 to 61.0-63.1% at 63 days and was 57.6-69.4% thereafter (DER Attachment 2). In the water layer, [^{14}C]pyrasulfotole decreased from 98.6-99.7% at day 0 to 49.4-49.9% at 31 days and was 37.6-40.5% at 183-365 days. In the sediment, [^{14}C]pyrasulfotole increased to 20.7-22.0% at 92 days and was 22.0-29.0% at 365 days.

HALF-LIFE/DT50/DT90: Observed DT50 values of pyrasulfotole were 22-31 days in the water layer and >365 days in the sediment and total system. Based on first order linear regression analysis (Excel 2000, all intervals), the half-lives of pyrasulfotole were 385 days in the water layer and 887 days in the total system (DER Attachment 2). Based on nonlinear analysis (SigmaPlot v 8), half-lives were 267 and 770 days in the water and total system, respectively. However, the calculated half-lives are of limited use given the low correlation coefficient values ($r^2 = \leq 0.51$), and the half-lives for pyrasulfotole in the total system were extrapolated significantly beyond the final sampling interval. Levels of [^{14}C]pyrasulfotole in the sediment were still increasing at study termination; consequently, calculated half-lives could not be determined.

Using first order regression nonlinear analysis (Excel Solver/General Reduced Gradient optimization, all intervals), the study author determined half-lives for [^{14}C]pyrasulfotole of 84 days ($r^2 = 0.6344$) in the water layer and 273 days ($r^2 = 0.4008$) in the total system (pp. 25-26, 30; Appendices 10-11, pp. 70-71). Using nonlinear bi-exponential analysis (Model Maker v 3.0), the study author determined [^{14}C]pyrasulfotole dissipated in the total system with an initial half-life of 6.2 days ($r^2 = 0.95$) and a secondary half-life of >1 year (pp. 26, 30; Appendix 12, p. 72).

Half-lives/DT50/DT90

Phase	Half-life/DT50 [1] (days)	Regression equation	r^2	DT50 (days)	DT90[2] (days)
Pond water					
Linear/natural log	385	y = -0.0018x + 4.1355	0.5089	--	--
Nonlinear/normal	267	y = 67.8*exp(-0.0026*x)	0.4909	--	279
Observed DT50	22-31	--	--	--	--
Silty clay sediment					
Linear/natural log	--[3]	--	--	--	--
Nonlinear/normal	--[3]	--	--	--	--
Observed DT50	>365	--	--	--	--
Total system					
Linear/natural log	887	y = -0.0008x + 4.3266	0.3421	--	--
Nonlinear/normal[4]	770	y = 77.38*exp(-0.0009*x)	0.3489	--	906
		y = 33.8391*exp(-0.1017*x)+63.7288*exp(-0.00004*x)	0.95	6000	46000
Observed DT50	>365	--	--	--	--

1 Determined by the primary reviewer using Excel 2000 (linear) and Sigmaplot v 8.0 (nonlinear) and individual sample data obtained from Appendix 7, pp. 63-64 of the study report (DER Attachment 2).
2 DT90 (90% decline times) values determined by the study author using degradation rate constant (k) obtained via Excel Solver (pp. 25-26; Appendices 10-11, pp. 70-71).
3 Levels of parent pyrasulfotole were still increasing in the sediment at study termination.
4 Two-compartment, 4 parameter model determined by secondary reviewer (PMRA).

TRANSFORMATION PRODUCTS: No major transformation products were detected and no minor products were identified. Unidentified [^{14}C]residues, consisting of up to four [^{14}C]components (Unknowns A, B, C and D), were detected at maximum totals of 1.7%, 2.6% and 3.4% of the applied in the water, sediment and total system, respectively, with no individual component detected at >2.9% of applied (DER Attachment 2).

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: Extractable and nonextractable sediment [^{14}C]residues increased from <MSP (minimum sensitivity; 6.12% and 3.66% of applied, respectively) at day 0 posttreatment to 22.0-29.0% and 31.5-36.2% of applied, respectively, at 365 days (DER Attachment 2). At study termination, organic matter fractionation of nonextractable [^{14}C]residues, comprising a mean 33.9% of the applied, found 31.6%, 66.3% and 2.1% of the recovered radioactivity associated with the humin, fulvic acids and humic acids, respectively (p. 28, DER Attachment 2).

VOLATILIZATION: The maximum level of volatilized $^{14}CO_2$ (identity not confirmed) detected at any sampling interval was 2.8% of the applied, with volatile [^{14}C]organic compounds <0.1% (Table 5, p. 38).

TRANSFORMATION PATHWAY: A transformation pathway was not provided as pyrasulfotole did not form any significant transformation products under the anaerobic aquatic conditions used in this study (p. 30). Dissipation of parent pyrasulfotole primarily involved the formation of bound sediment residues with minimal levels of mineralization to CO_2 and the possible formation of several minor compounds.

Table 8: Chemical names and CAS numbers for the transformation products of pyrasulfotole.

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
No transformation products were identified.					

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Microbial biomass counts in water and sediment from untreated, control systems were 1.17×10^7 cells/mL water and 2.89×10^8 cells/g sediment, respectively, at study initiation, 4.56×10^6 cells/mL and 2.75×10^8 cells/g, respectively, at the study mid-point, and 4.39×10^6 cells/mL and 1.42×10^8 cells/g, respectively, at the study end; specific sampling intervals were not reported (Table 1, pp. 33-34).

Storage stability. HPLC re-analysis found no quantitative differences in the chromatographic profile of 365-day water layer and sediment extract samples after 153 days of frozen storage (p. 31; Figure 15, pp. 55-56).

III. STUDY DEFICIENCIES

No significant deviations from good scientific practices or Subdivision N guidelines were noted.

IV. REVIEWER'S COMMENTS

1. Mean results and standard deviations presented in this review were determined by the primary reviewer using Microsoft Excel 2000 (9.0.2720) software (DER Attachment 2). Standard deviations were determined using the "biased" or "n" method which determines the standard deviation of the entire sample population. Mean results and summations reported by the study author (Tables 5-6, pp. 38-39) were verified by the primary reviewer and there was consistent agreement (within ± 0.1% of applied) between the study author's reported values and those determined by the primary reviewer (DER Attachment 2). Standard deviations presented in the study report differed from those determined by the primary reviewer because the study author determined standard deviations using the "nonbiased" or "n-1" method which bases the standard deviation on a sample of the population rather than the entire population.

2. The test application rate of 0.004 mg a.i./L used in this study was based on a proposed maximum single use rate of 75 g a.i./ha (p. 15). Assuming direct over-spray of a 1-ha body of water with diffusion to a depth of 200 cm, the 75 g a.i./acre field rate converts to a test application rate of 0.004 mg a.i./L.

3. Observed DT50 values for total residues (days posttreatment).

Phase	[Phenyl-U-^{14}C]-pyrasulfotole	
	Parent +nonvolatile [^{14}C]products[1]	Total [^{14}C]residues[2]
Water	*ca.* 31	*ca.* 31
Sediment	>365	>365
Total system	>365	>365

1 Parent pyrasulfotole plus identified/unidentified [^{14}C]transformation products.
2 All [^{14}C]residues other than volatilized $^{14}CO_2$.
Data obtained from DER Attachment 2.

4. The study authors conclude that an anaerobic aquatic environment will have limited contribution to the overall degradation of pyrosulfotole.

5. The secondary reviewer from the PMRA fit a 2 compartment, 4 parameter non-linear regression model to the whole system data: y = 33.8391*exp(-0.1017*x)+63.7288*exp(-0.00004*x); r2 = 0.95. This model is nearly identical to the non-linear model proposed by the study authors. Due to the lack of dissipation after 63 days, the model produces DT50 and DT90 estimates of 6000 and 46000 days, respectively (Sigma Plot, equation solver module).

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-3, Anaerobic 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.

Attachment 1: Structures of Parent Compound and Transformation Products

Pyrasulfotole [AE 0317309; K-1196; K-1267]

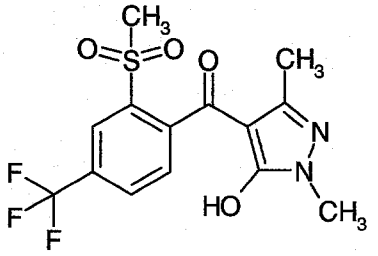
IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone.
(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS Name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl)-4(trifluoromethyl)phenyl]methanone.
Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

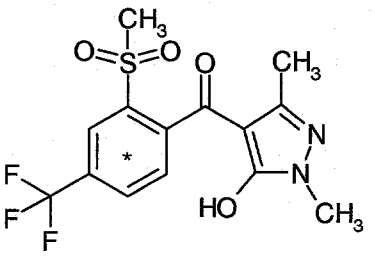
CAS Number: 365400-11-9.

SMILES String: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C)(F)F (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.
CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.

Unlabeled



[Phenyl-U-^{14}C]pyrasulfotole



^{14}C = Position of radiolabel.

Identified Compounds

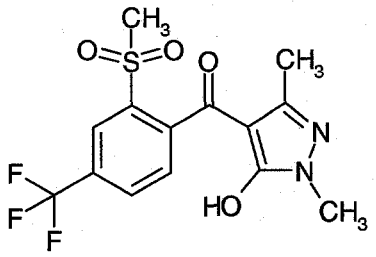
Pyrasulfotole [AE 0317309; K-1196; K-1267]

IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone.
(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

CAS Name: (5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-methylsulfonyl)-4(trifluoromethyl)phenyl]methanone.
Methanone, (5-hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].

CAS Number: 365400-11-9.

SMILES String: FC(c1cc(c(cc1)C(=O)c1c(n(nc1C)C)O)S(=O)(=O)C)(F)F (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
Cc1nn(C)c(O)c1C(=O)c2ccc(C(F)(F)F)cc2S(C)(=O)=O.
CS(=O)(=O)c1c(ccc(c1)C(F)(F)F)C(=O)c1c(n(nc1C)C)O.



Carbon Dioxide

IUPAC Name: Not reported.

CAS Name: Not reported.

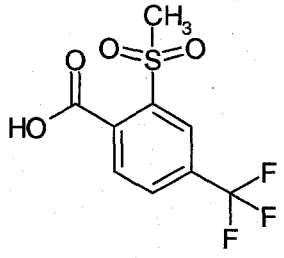
CAS Number: Not reported.

O=C=O

Unidentified Reference Compounds

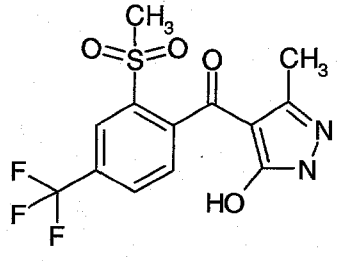
RPA 203328 [AE B197555-benzoic acid; AE B197555; K-1198; K-1367]

IUPAC Name: 2-Mesyl-4-trifluoromethylbenzoic acid.
CAS Name: Benzoic acid, 2-(methylsulfonyl)-4-(trifluoromethyl)-.
CAS Number: 142994-06-7.
SMILES String: O=C(c1ccc(cc1S(=O)(=O)C)C(F)(F)F)O (ISIS v2.3/Universal SMILES).
No EPI Suite, v3.12 SMILES String found as of 6/7/06.
CS(=O)(=O)c1cc(C(F)(F)F)ccc1C(=O)O.
CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F.



AE 1073910 [AE 0317309 N-Desmethyl; K-1385; K-1197]

IUPAC Name: (5-Hydroxy-3-methyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl]methanone.
CAS Name: Methanone, (5-hydroxy-3-methyl-1H-pyrazol-4-yl)[2-(methylsulfonyl)-4-(trifluoromethyl)phenyl].
CAS Number: Not reported.
SMILES String: O=C(C2=C(O)NN=C2C)C1=C(S(=O)(C)=O)C=C(C(F)(F)F)C=C1.
CS(=O)(=O)c1cc(ccc1C(=O)c1c([nH]nc1C)O)C(F)(F)F.



Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801714
Guideline: 162-3

Nonlinear half-lives (exponential decay/single, 2 parameter)

Kansas silty clay
[Phenyl-U-^{14}C]-label

Phase	water	sediment	system
Half-life (days)	266.6	ND[1]	770.2
R squared	0.4909		0.3489

[1]Calculated half-life not determined.

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801714
Guideline: 162-3

Anaerobic metabolism of [phenyl-U-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.

Day	Water			Sediment						CO_2			Material Balance			Study Reported Material Balance		
				Extracts			Nonextractable											
	% 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	99.7			0.0			0.0			0.0			99.7			99.7		
	100.3	100.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	100.3	100.0	0.3	100.3	100.0	0.3
3	76.1			9.1			9.4			1.8			96.4			96.5		
	78.1	77.1	1.0	9.7	9.4	0.3	7.6	8.5	0.9	1.5	1.7	0.2	96.9	96.7	0.3	97.0	96.8	0.3
7	67.2			12.3			11.1			2.1			92.7			92.6		
	69.3	68.3	1.0	13.3	12.8	0.5	13.4	12.3	1.2	2.3	2.2	0.1	98.3	95.5	2.8	98.3	95.5	2.9
10	62.5			14.0			16.7			1.9			95.1			95.1		
	63.4	63.0	0.4	15.3	14.7	0.7	17.3	17.0	0.3	1.8	1.9	0.0	97.8	96.5	1.4	97.8	96.5	1.4
22	52.5			19.3			18.3			2.5			92.6			92.7		
	52.1	52.3	0.2	19.3	19.3	0.0	20.6	19.5	1.1	2.8	2.7	0.2	94.8	93.7	1.1	94.8	93.8	1.1
31	50.7			18.2			27.1			2.5			98.5			98.5		
	50.9	50.8	0.1	16.8	17.5	0.7	24.4	25.8	1.4	2.5	2.5	0.0	94.6	96.6	1.9	94.5	96.5	2.0
63	45.3			17.5			30.2			2.3			95.3			95.3		
	46.1	45.7	0.4	18.8	18.2	0.7	26.1	28.2	2.1	2.4	2.4	0.1	93.4	94.4	1.0	93.5	94.4	0.9
92	44.0			22.0			27.4			2.0			95.4			95.5		
	45.0	44.5	0.5	20.7	21.4	0.6	26.1	26.8	0.6	2.1	2.1	0.1	93.9	94.7	0.8	94.0	94.8	0.8
120	43.3			21.0			31.0			2.2			97.5			97.4		
	43.3	43.3	0.0	18.8	19.9	1.1	31.4	31.2	0.2	2.4	2.3	0.1	95.9	96.7	0.8	95.9	96.7	0.7
183	40.5			21.5			31.4			2.1			95.5			95.5		
	39.5	40.0	0.5	20.3	20.9	0.6	33.9	32.7	1.3	2.2	2.2	0.0	95.9	95.7	0.2	95.9	95.7	0.2
273	37.6			25.5			30.7			2.6			96.4			96.4		
	39.0	38.3	0.7	22.8	24.2	1.4	33.2	32.0	1.2	2.6	2.6	0.0	97.6	97.0	0.6	97.6	97.0	0.6
365	39.6			22.0			36.2			2.8			100.6			100.5		
	40.4	40.0	0.4	29.0	25.5	3.5	31.5	33.9	2.4	2.8	2.8	0.0	103.7	102.2	1.6	103.7	102.1	1.6

Results from Table 5, p. 38 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Overall	96.6	2.6		96.6	2.6
maximum	103.7			103.7	
minimum	92.6			92.6	
n =	24			24	

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801714
Guideline: 162-3

Anaerobic metabolism of [phenyl-U-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Total [^{14}C]residues in sediment.

	Sediment				
	Ext.	Nonext.	Total in Sediment		
Day	% AR	% AR	% AR	Mean	s.d.
0	0.0	0.0	0.0		
	0.0	0.0	0.0	0.0	0.0
3	9.1	9.4	18.5		
	9.7	7.6	17.3	17.9	0.6
7	12.3	11.1	23.4		
	13.3	13.4	26.7	25.1	1.6
10	14.0	16.7	30.7		
	15.3	17.3	32.6	31.7	1.0
22	19.3	18.3	37.6		
	19.3	20.6	39.9	38.8	1.2
31	18.2	27.1	45.3		
	16.8	24.4	41.2	43.3	2.0
63	17.5	30.2	47.7		
	18.8	26.1	44.9	46.3	1.4
92	22.0	27.4	49.4		
	20.7	26.1	46.8	48.1	1.3
120	21.0	31.0	52.0		
	18.8	31.4	50.2	51.1	0.9
183	21.5	31.4	52.9		
	20.3	33.9	54.2	53.6	0.7
273	25.5	30.7	56.2		
	22.8	33.2	56.0	56.1	0.1
365	22.0	36.2	58.2		
	29.0	31.5	60.5	59.4	1.1

[14C]Residue water phase:sediment 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	99.7	0.0						
	100.3	0.0						
3	76.1	18.5	4	0				
	78.1	17.3	5	0	4	0	0	0
7	67.2	23.4	3	0				
	69.3	26.7	3	0	3	0	0	0
10	62.5	30.7	2	0				
	63.4	32.6	2	1	2	0	1	0
22	52.5	37.6	1	1				
	52.1	39.9	1	1	1	0	1	0
31	50.7	45.3	1	1				
	50.9	41.2	1	1	1	0	1	0
63	45.3	47.7	1	1				
	46.1	44.9	1	1	1	0	1	0
92	44.0	49.4	1	1				
	45.0	46.8	1	1	1	0	1	0
120	43.3	52.0	1	1				
	43.3	50.2	1	1	1	0	1	0
183	40.5	52.9	1	1				
	39.5	54.2	1	1	1	0	1	0
273	37.6	56.2	1	1				
	39.0	56.0	1	1	1	0	1	0
365	39.6	58.2	1	1				
	40.4	60.5	1	1	1	0	1	0

Results imported from **Mat bal** worksheet.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801714
Guideline: 162-3

Anaerobic metabolism of [phenyl-U-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Confirmation/determination of means/std.dev. for pyrasulfotole.

Day	Pyrasulfotole								
	Water			Sediment			Total system		
	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	99.7			0.0			99.7		
	98.6	99.2	0.5	0.0	0.0	0.0	98.6	99.2	0.5
3	76.1			9.1			85.2		
	78.1	77.1	1.0	8.3	8.7	0.4	86.4	85.8	0.6
7	67.2			10.8			78.0		
	69.3	68.3	1.0	11.9	11.4	0.5	81.2	79.6	1.6
10	61.0			12.6			73.6		
	63.4	62.2	1.2	13.8	13.2	0.6	77.2	75.4	1.8
22	51.4			19.3			70.7		
	51.3	51.4	0.1	19.3	19.3	0.0	70.6	70.7	0.1
31	49.9			15.7			65.6		
	49.4	49.7	0.2	15.2	15.5	0.3	64.6	65.1	0.5
63	44.3			16.7			61.0		
	45.4	44.9	0.6	17.7	17.2	0.5	63.1	62.1	1.0
92	43.4			22.0			65.4		
	45.0	44.2	0.8	20.7	21.4	0.6	65.7	65.6	0.1
120	43.3			20.0			63.3		
	43.1	43.2	0.1	17.4	18.7	1.3	60.5	61.9	1.4
183	40.5			21.5			62.0		
	39.5	40.0	0.5	20.3	20.9	0.6	59.8	60.9	1.1
273	37.6			25.5			63.1		
	39.0	38.3	0.7	18.6	22.1	3.5	57.6	60.4	2.8
365	39.6			22.0			61.6		
	40.4	40.0	0.4	29.0	25.5	3.5	69.4	65.5	3.9

Results from Appendix 7, pp. 63-64 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801714
Guideline: 162-3

Anaerobic metabolism of [phenyl-U-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Determination of total unidentified [^{14}C] following HPLC analyses.

	Unknown A		Unknown B		Unknown C		Unknown D		Total Uknowns								
	Water	Sed	Water	Sed	Water	Sed	Water	Sed	Water			Sediment			Total system		
Day	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	1.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	0.9	0.9	0.9	0.4	0.4	2.6	1.3	1.3
3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	1.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7	0.0	1.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	1.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	0.8	1.4	0.6	0.0	0.0	0.0	0.0	0.0	1.4			0.0			1.4		
	0.0	1.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.7	0.7	0.4	0.4	0.7	1.1	0.4
22	1.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.1			0.0			1.1		
	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	1.0	0.2	1.0	0.5	0.5	1.8	1.4	0.3
31	0.8	0.0	0.0	0.0	0.0	2.6	0.0	0.0	0.8			2.6			3.4		
	1.4	1.5	0.0	0.0	0.0	0.0	0.0	0.0	1.4	1.1	0.3	1.1	1.9	0.8	2.5	3.0	0.5
63	1.0	0.8	0.0	0.0	0.0	0.0	0.0	0.0	1.0			0.0			1.0		
	0.8	0.8	0.0	0.3	0.0	0.0	0.0	0.0	0.8	0.9	0.1	1.2	0.6	0.6	2.0	1.5	0.5
92	0.0	0.0	0.0	0.0	0.0	0.0	0.6	0.0	0.6			0.0			0.6		
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.3	0.3	0.2	0.2	0.3	0.5	0.2
120	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	1.4	0.2	0.0	0.0	0.0	0.0	0.0	0.2	0.1	0.1	0.1	0.1	0.1	0.3	0.2	0.2
183	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
273	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	1.6	0.0	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	1.3	1.3	2.5	1.3	1.3
365	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

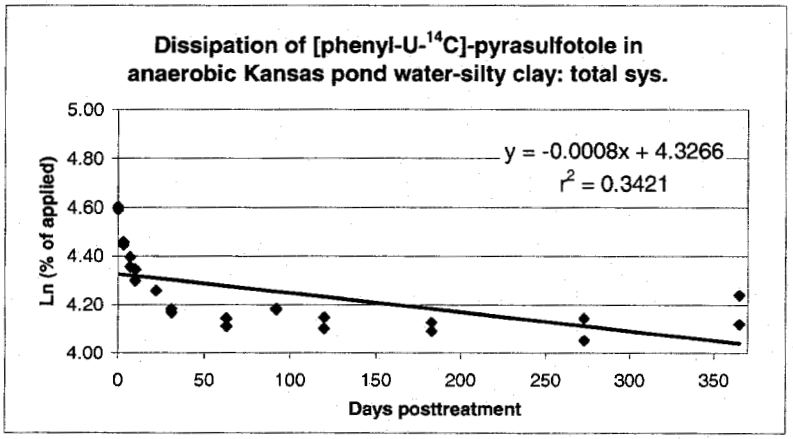
Results from Appendix 7, pp. 63-64 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801714
Guideline: 162-3

Anaerobic metabolism of [phenyl-U-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Half-life determination/total system
Half-life (days) 886.9 (0- to 365-day data)

	Pyrasolfotole	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	99.7	4.602165677
0	98.6	4.591071262
3	85.2	4.445001434
3	86.4	4.458987676
7	78.0	4.356708827
7	81.2	4.396915247
10	73.6	4.298645026
10	77.2	4.346399457
22	70.7	4.258445573
22	70.6	4.257030144
31	65.6	4.183575696
31	64.6	4.168214411
63	61.0	4.110873864
63	63.1	4.14472077
92	65.4	4.180522258
92	65.7	4.185098925
120	63.3	4.147885329
120	60.5	4.102643365
183	62.0	4.127134385
183	59.8	4.091005661
273	63.1	4.14472077
273	57.6	4.053522568
365	61.6	4.120661871
365	69.4	4.239886868

Results imported from **Profile** worksheet.



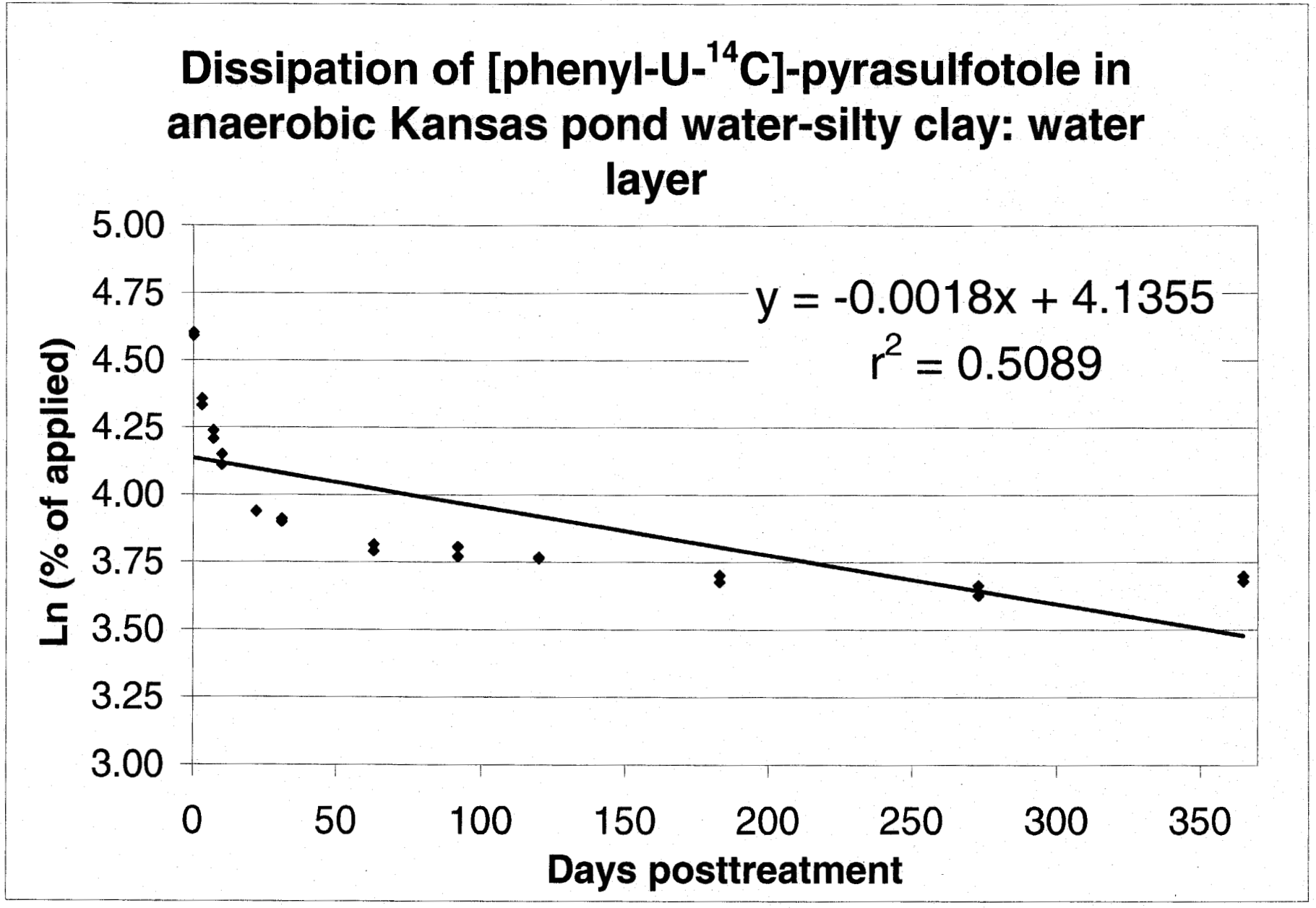
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.584857689
R Square	0.342058517
Adjusted R Square	0.312152086
Standard Error	0.12899717
Observations	24

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.190325152	0.19033	11.43762411	0.0026844
Residual	22	0.366085938	0.01664		
Total	23	0.55641109			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.326628174	0.034643033	124.892	7.28201E-33	4.2547828	4.3984735	4.25478284	4.3984735
X Variable 1	-0.000781539	0.000231091	-3.382	0.0026844	-0.001261	-0.0003023	-0.0012608	-0.0003023


Dissipation of [phenyl-U-14C]-pyrasulfotole in anaerobic Kansas pond water-silty clay: water layer
y = -0.0018x + 4.1355
r2 = 0.5089
Ln (% of applied)
5.00
4.75
4.50
4.25
4.00
3.75
3.50
3.25
3.00
0
50
100
150
200
250
300
350
Days posttreatment

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801714
Guideline: 162-3

Anaerobic metabolism of [phenyl-U-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Half-life determination/total system
Half-life (days) 886.9 (0- to 365-day data)

	Pyrasolfotole	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	99.7	4.602165677
0	98.6	4.591071262
3	85.2	4.445001434
3	86.4	4.458987676
7	78.0	4.356708827
7	81.2	4.396915247
10	73.6	4.298645026
10	77.2	4.346399457
22	70.7	4.258445573
22	70.6	4.257030144
31	65.6	4.183575696
31	64.6	4.168214411
63	61.0	4.110873864
63	63.1	4.14472077
92	65.4	4.180522258
92	65.7	4.185098925
120	63.3	4.147885329
120	60.5	4.102643365
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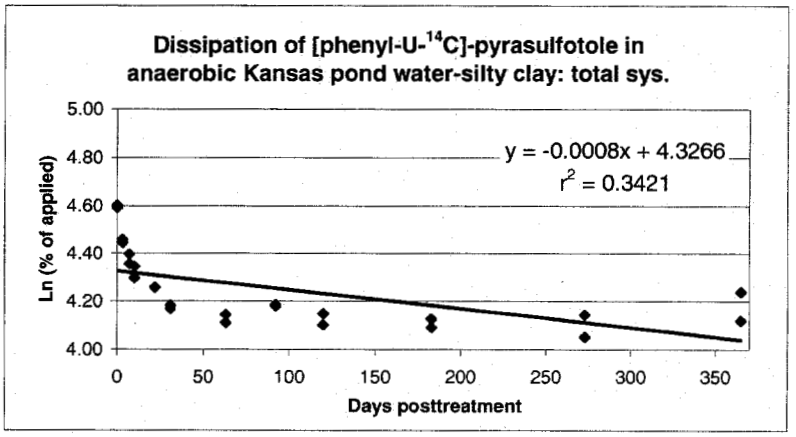

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.584857689
R Square	0.342058517
Adjusted R Square	0.312152086
Standard Error	0.12899717
Observations	24

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.190325152	0.19033	11.43762411	0.0026844
Residual	22	0.366085938	0.01664		
Total	23	0.55641109			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.326628174	0.034643033	124.892	7.28201E-33	4.2547828	4.3984735	4.25478284	4.3984735
X Variable 1	-0.000781539	0.000231091	-3.382	0.0026844	-0.001261	-0.0003023	-0.0012608	-0.0003023

[Phenyl-U-^{14}C]pyrasulfotole in anaerobic Kansas pond water-silty clay: total system, nonlinear regression (MRID 46801714)