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

PMRA Submission Number 2006-2445 EPA MRID Number 46801715

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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EXECUTIVE SUMMARY

The biotransformation of [pyrazole-3-^{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 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 14 days prior to treatment. Following treatment, duplicate flasks were collected after 0, 3, 14, 17, 28, 63, 91, 106, 120, 184, 275 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 primarily moderately reducing with mean redox potentials of -32.5 to +46.8 mV and -108.3 to +54.1 mV in the water layer and sediment, respectively. In the water layer, mean dissolved oxygen and pH levels were <0.3 mg/L and 6.6-7.2, respectively.

Overall recovery of radiolabeled material averaged 94.1 ± 3.6% (range 85.4-102.2%) 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, 1:1 at 14-184 days and were 1:2 thereafter. [^{14}C]Pyrasulfotole dissipated slowly in the total system decreasing from a mean 100.0% of the applied at day 0 to 54.9% at 275 days and was 59.7% at 365 days. In the water layer, [^{14}C]pyrasulfotole decreased from a mean 100.0% at day 0 to 49.9% at 17 days and was 37.3% at study termination. In the sediment, [^{14}C]pyrasulfotole increased to a mean 22.7% at 63 days and was 19.1-22.9% thereafter. Calculated linear and nonlinear 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 = <0.45), and the half-lives for pyrasulfotole in the total system were extrapolated significantly beyond the final sampling interval. Since concentrations of [^{14}C]pyrasulfotole in the sediment remained at steady levels from 63 days posttreatment through study termination, calculated half-lives could not be determined. **Observed DT50** values of pyrasulfotole were 14-28 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 722 and 4745 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 two [^{14}C]components, were detected in sediment extracts only at a maximum total of 1.6% of the applied, with neither individual component detected at >0.9% of applied. Extractable sediment [^{14}C]residues increased to a maximum mean 22.9% of applied at 120 days and were 22.4% at 365 days. Nonextractable sediment [^{14}C]residues increased to a maximum mean 36.4% at study termination. Acidic (0.1% formic acid) extraction of nonextractable [^{14}C]residues only recovered a mean 1.0% of the applied. At study termination, organic matter fractionation of the nonextractable residues (36.4% of applied) found 34.4%, 64.5% and 1.2% of the recovered radioactivity associated with the humin, fulvic acids and humic acids, respectively. Volatilized $^{14}CO_2$ totaled a mean 1.9% of the applied at study termination, with volatile [^{14}C]organic compounds ≤0.1% at any interval.

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 120-day water layer and sediment extract samples after 404 days of frozen storage.

Results Synopsis:

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

Linear half-life in water:	397 days ($r^2 = 0.4445$).
Linear half-life in sediment:	ND (not determined).
Linear half-life in the total system:	725 days ($r^2 = 0.4217$).

Non-linear half-life in water:	257 days ($r^2 = 0.4120$).
Non-linear half-life in sediment:	ND.
Non-linear half-life in total system:	578 days ($r^2 = 0.4053$).

Observed DT50 in water:	14-28 days.
Observed DT50 in sediment:	>365 days.
Observed DT50 in total system:	>365 days.

Non-linear DT50 in total system:	722 days ($r^2 = 0.947$)
Non-linear DT90 in total system:	4745 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 1.9% 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). 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, 31). Signed and dated Data Confidentiality, GLP, Quality Assurance and [study] Certification statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Material [Pyrazole-3-^{14}C]pyrasulfotole (p. 16; Figure 1, p. 40).

Chemical Structure: See DER Attachment 1.

Description: Technical; white solid (p. 16).

Purity:	Radiochemical purity:	>97% (p. 16; Figure 5A, p. 44); supporting quantitative data were not provided.
	Lot/Batch No.	SEL/1009.
	Analytical purity:	Not reported.
	Specific activity:	331,961 dpm/µg (54.2 mCi/mmol, 5.51 MBq/mg).
	Location of the radiolabel:	At 3-C position on pyrazole 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 14 days prior to treatment, with the date of application March 3, 2003.
Preparation	Water:	None.
	Sediment:	Sieved (2-mm).

Data obtained from pp. 4, 18-19; Table 1, p. 33; Appendix 2, p. 57 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
	-7.9	+7.6
Oxygen concentration (mg/L)[1]	Initial[2]	Final
	0.28	0.13
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	5.45×10^6

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	7.0	
Organic carbon (%)	1.1	
Organic matter (%)	2.0	
CEC (meq/100 g)	35.7	
Redox potential (mV)[1]	Initial[2]	Final
	-13.4	-4.8
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	1.44 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.).

Parameter		**Details**	
Application rates (mg a.i./L)	Nominal:	0.004 mg a.i./L	
	Actual:	0.00416 mg a.i./L	
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 0.08% based on water volume (120 µL ACN in 150 mL water).	
Test material application method	Volume of the test solution used/treatment:	120 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 (pp. 18-20).	
	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, 18-21, 27; Table 2, p. 35; Figures 2-4, pp. 41-43; Appendix 2, p. 57 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.* 14 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 -7.9 mV and 0.28 mg/L, respectively, with a mean redox potential of -13.4 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 0.051 mg a.i./L or *ca.* thirteen times the nominal application rate (pp. 19-20).

5. Sampling:

Table 5: Sampling details.

Criteria	**Details**
Sampling intervals	0, 3, 14, 17, 28, 63, 91, 106, 120, 184, 275 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 93 days prior to analysis, with the majority of samples reportedly analyzed within 30 days. However, specific extraction and analysis dates were not provided for review.
Other details, if any	None reported.

Data obtained from pp. 21, 30; Table 3, p. 36; Figure 4, p. 43 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. 66-67).

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. 45). 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. 56) 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. 66-67).

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, 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.

Acid extraction. Extracted sediment (sampling interval not reported) was further extracted with 0.1% formic acid using the ASE system under "harsh" conditions (p. 28); no additional information was provided.

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 2.9 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 4 mL/minute, Ramona radioactivity detector (Method II, pp. 23-24).

Parent [^{14}C]pyrasulfotole was identified by co-chromatography with and comparison to the retention time of unlabeled reference standard (pp. 24, 29; Figure 7, p. 46; Figure 11, p. 50; Figures 13-14, pp. 52-53). Column recoveries were monitored through the collection and LSC analysis of selected bulk column eluates, with the average recovery reported as 100.5% (pp. 24, 28).

To confirm identification, [^{14}C]pyrasulfotole was isolated from a 135-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 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. 44; Figure 12, p. 51).

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, 29, 31; Figure 7, p. 46; Figure 11, p. 50; Figures 13-14, pp. 52-53).

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

Applicant codes	Chemical Name	Purity[1]
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, p. 40 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. 60).

For LSC analyses, minimum sensitivities (MSP) were reported as 1.37% of the applied for water layer samples, 3.54% for sediment extracts and 2.11% for sediment combustions (Appendices 3-4, pp. 58-59).

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: Conditions in untreated, control water-sediment systems incubated alongside the treated systems were primarily moderately reducing (-50 to +200 mV) throughout the 1-year incubation with mean (n = 2) redox potentials of -32.5 to +46.8 mV and -108.3 to +54.1 mV in the water layer and sediment, respectively (Table 4, p. 37). In the water layer, mean dissolved oxygen and pH levels were <0.3 mg/L and 6.6-7.2, respectively.

B. MATERIAL BALANCE: Overall recovery of radiolabeled material averaged 94.1 ± 3.6% (range 85.4-102.2%, 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, 1:1 at 14-184 days and were 1:2 at 275-365 days (DER Attachment 2).

Table 7. Biotransformation of [pyrazole-3-^{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	14	17	28	63	91	106	120	184	275	365
Pyrasulfotole	Water	100.0 ± 2.2	72.2 ± 2.6	52.4 ± 1.4	49.9 ± 3.2	46.1 ± 2.2	43.3 ± 1.0	41.6 ± 1.8	42.4 ± 0.7	40.8 ± 0.7	38.4 ± 0.3	35.3 ± 3.0	37.3 ± 0.3
	Sed.[2]	0.0 ± 0.0	12.4 ± 0.3	17.2 ± 0.6	18.7 ± 0.8	17.2 ± 0.5	22.7 ± 1.3	20.3 ± 1.8	19.1 ± 0.5	22.9 ± 1.7	19.4 ± 0.5	19.6 ± 0.5	22.4 ± 1.1
	System	100.0 ± 2.2	84.6 ± 2.3	69.6 ± 1.9	68.6 ± 3.9	63.3 ± 2.6	66.0 ± 0.3	61.9 ± 0.1	61.5 ± 1.2	63.8 ± 1.0	57.8 ± 0.3	54.9 ± 2.5	59.7 ± 0.7
Unidentified [^{14}C]residues[3]	Sed.	0.0 ± 0.0	0.0 ± 0.0	0.0, 0.8	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0, 1.6	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0
CO_2		0.0 ± 0.0	1.5 ± 0.1	1.3 ± 0.2	1.2 ± 0.0	1.5 ± 0.0	1.4 ± 0.0	1.3 ± 0.1	1.2 ± 0.1	1.4 ± 0.0	1.4 ± 0.0	1.6 ± 0.0	1.9 ± 0.0
Volatile organics		0.0 ± 0.0	0.0 ± 0.00	0.0 ± 0.0	0.0 ± 0.0	0.0, 0.1	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	12.4 ± 0.3	17.6 ± 1.0	18.7 ± 0.8	17.2 ± 0.5	22.7 ± 1.3	20.3 ± 1.8	19.9 ± 1.3	22.9 ± 1.7	19.4 ± 0.5	19.6 ± 0.5	22.4 ± 1.1
Nonextractable sediment residues		0.0 ± 0.0	7.5 ± 0.4	20.9 ± 2.4	22.1 ± 0.8	28.0 ± 0.8	26.5 ± 1.0	29.4 ± 2.4	30.8 ± 0.2	32.1 ± 1.0	33.9 ± 2.5	34.1 ± 2.7	36.4 ± 1.4
Total recovery	Water	100.0 ± 2.2	72.2 ± 2.6	52.4 ± 1.4	49.9 ± 3.2	46.1 ± 2.2	43.3 ± 1.0	41.6 ± 1.8	42.4 ± 0.7	40.8 ± 0.7	38.4± 0.3	35.3 ± 3.0	37.3 ± 0.3
	Sed.	0.0 ± 0.0	19.9 ± 0.1	38.5 ± 1.4	40.8 ± 0.0	45.2 ± 0.4	49.2 ± 2.3	49.7 ± 0.7	50.7 ± 1.1	55.0 ± 0.7	53.3 ± 1.9	53.6 ± 2.1	58.8 ± 0.3
	System	100.0 ± 2.2	93.5 ± 2.8	92.2 ± 0.1	91.8 ± 3.1	92.9 ± 1.9	93.9 ± 1.3	92.5 ± 2.4	94.3 ± 1.7	97.2 ± 0.1	93.0 ± 2.2	90.5 ± 5.1	97.9 ± 0.7

1 Reviewer's Comment No. 1.

2 Sediment.

3 Consisting of two [^{14}C]components (Unknowns 1and 2) detected only in sediment extracts, each at ≤0.9% of the applied (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 97.8-102.2% of the applied at day 0 to 52.4-57.3% at 275 days and was 58.9-60.4% at 365 days (DER Attachment 2). In the water layer, [^{14}C]pyrasulfotole decreased from 97.8-102.2% at day 0 to 46.7-53.0% at 17 days and was 32.3-38.3% at 275-365 days. In the sediment, [^{14}C]pyrasulfotole increased to 21.2-24.6% at 120 days and was 21.3-23.5% at 365 days.

HALF-LIFE/DT50/DT90: Observed DT50 values of pyrasulfotole were 14-28 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 397 days in the water layer and 725 days in the total system (DER Attachment 2). Based on nonlinear analysis (SigmaPlot v 8), half-lives were 257 and 578 days in the water and total system, respectively. However, the calculated half-lives are of limited use given the low correlation coefficient values ($r^2 = <0.45$), and the half-lives for pyrasulfotole in the total system were extrapolated significantly beyond the final sampling interval. Concentrations of [^{14}C]pyrasulfotole in the sediment remained at steady levels (18.5-24.6% of applied) from 63 days posttreatment through 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 75 days ($r^2 = 0.5628$) in the water layer and 227 days ($r^2 = 0.4601$) in the total system (pp. 25-26, 30; Appendices 10-11, pp. 69-70). 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 4.2 days ($r^2 = 0.95$) and a secondary half-life of >1 year (pp. 26, 30; Appendix 12, p. 71).

Half-lives/DT50/DT90

Phase	Half-life/DT50 [1] (days)	First order linear regression equation	r^2	DT50 (days)	DT90[2] (days)
Pond water					
Linear/natural log	397	y = -0.0017x + 4.0470	0.4445	--	--
Nonlinear/normal	257	--	0.4120	--	249
Observed DT50	14-28	--	--	--	--
Silty clay sediment					
Linear/natural log	--[3]	--	--	--	--
Nonlinear/normal	--[3]	--	--	--	--
Observed DT50	>365	--	--	--	--
Total system					
Linear/natural log	725	y = -0.0010x + 4.3002	0.4217	--	--
Nonlinear/normal[4]	578	--	0.4053	--	754
		y = 34.7281*exp(-0.1613*x)+66.7369*exp(-0.0004*x)	0.947	722	4745
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. 62-63 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. 69-70).
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 two [^{14}C]components, Unknowns 1 and 2, were detected only in sediment extracts at maximums of 0.8% and 0.9% of the applied, respectively (DER Attachment 2).

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: Extractable sediment [^{14}C]residues increased from <MSP (minimum sensitivity, 3.54% of applied) at day 0 posttreatment to 21.4-24.0% at 63 days and were 21.3-23.5% at 365 days (DER Attachment 2). Nonextractable sediment [^{14}C]residues increased from <MSP (2.11% of applied) at day 0 to 35.0-37.8% at 365 days. Further acidic (0.1% formic acid) extraction of the nonextractable [^{14}C]residues (sampling interval not reported) only recovered an average 1.0% of the applied (p. 28). At study termination, organic matter fractionation of nonextractable [^{14}C]residues, comprising a mean 36.4% of the applied, found 34.4%, 64.5% and 1.2% of the recovered radioactivity associated with the humin, fulvic acids and humic acids, respectively (p. 28, DER Attachment 2).

VOLATILIZATION: At study termination (365 days), volatilized $^{14}CO_2$ (identity not confirmed) totaled 1.8-1.9% of the applied, with volatile [^{14}C]organic compounds ≤0.1% at any interval (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 two 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 x 10^7 cells/mL water and 2.89 x 10^8 cells/g sediment, respectively, at study initiation, 6.93 x 10^6 cells/mL and 3.09 x 10^8 cells/g, respectively, at the study mid-point, and 5.45 x 10^6 cells/mL and 1.44 x 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 120-day water layer and sediment extract samples after 404 days of frozen storage (pp. 30-31; Figure 15, pp. 54-55).

III. STUDY DEFICIENCIES

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

IV. REVIEWERS' 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	**[Pyrazole-3-^{14}C]-pyrasulfotole**	
	Parent +nonvolatile [^{14}C]products[1]	**Total [^{14}C]residues**[2]
Water	14-28	14-28
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 = 34.7281*exp(-0.1613*x)+66.7369*exp(-0.0004*x); r2 = 0.95. This model is nearly identical to the non-linear model proposed by the study authors. The DT50 and DT90 estimates were 722 and 4745 days, respectively (Sigma Plot, equation solver module).

6. DEH conducted a brief examination using the Timme-Frehse model and for water dissipation a half life of 325 days was obtained (square root time versus reciprocal concentration, r^2 = 0.8123).

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.

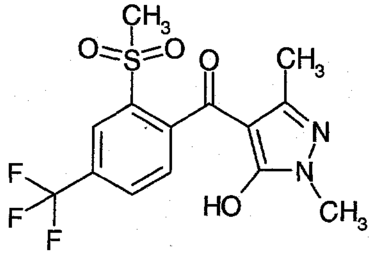
4. Wolfe, N., *et al.* 1990. Abiotic transformations in water, sediments and soil. *In* Pesticides in the Soil Environment, Soil Science Society of America, pp. 103-110.

Attachment 1: Structures of Parent Compound and Transformation Products

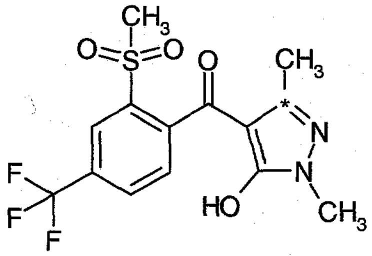
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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



[Pyrazole-3-^{14}C]pyrasulfotole

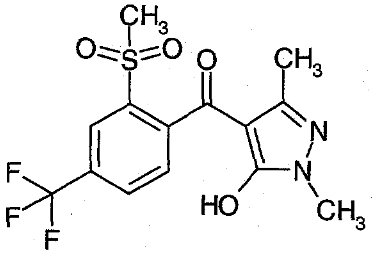


^{14}C = Position of radiolabel.

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

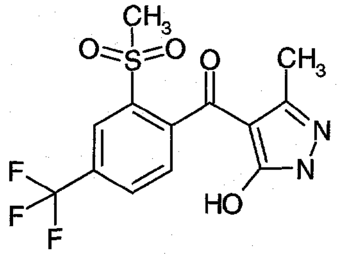
IUPAC Name:	Not reported.
CAS Name:	Not reported.
CAS Number:	Not reported.

O=C=O

Unidentified Reference Compounds

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: 46801715
Guideline: 162-3

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

Kansas silty clay
[Pyrazole-3-14C]-label

Phase	water	sediment	system
Half-life (days)	256.7	ND[1]	577.6
R squared	0.4120		0.4053

[1] Calculated half-life not determined.

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801715
Guideline: 162-3

Anaerobic metabolism of [pyrazole-3-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.

				Sediment																	
	Water			Extracts			Nonextractable			CO_2			Volatile organics			Material Balance			Study Reported Material Balance		
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.	% AR	Mean	s.d.
0	97.8			0.0			0.0			0.0			0.0			97.8			97.8		
	102.2	100.0	2.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	102.2	100.0	2.2	102.2	100.0	2.2
3	69.6			12.7			7.0			1.4			0.0			90.7			90.7		
	74.8	72.2	2.6	12.1	12.4	0.3	7.9	7.5	0.4	1.6	1.5	0.1	0.0	0.0	0.0	96.4	93.6	2.8	96.3	93.5	2.8
14	51.0			16.6			23.3			1.1			0.0			92.0			92.1		
	53.8	52.4	1.4	18.5	17.6	1.0	18.5	20.9	2.4	1.4	1.3	0.2	0.0	0.0	0.0	92.2	92.1	0.1	92.2	92.2	0.1
17	46.7			17.9			22.9			1.2			0.0			88.7			88.7		
	53.0	49.9	3.2	19.4	18.7	0.8	21.3	22.1	0.8	1.2	1.2	0.0	0.0	0.0	0.0	94.9	91.8	3.1	94.9	91.8	3.1
28	43.9			16.7			28.8			1.4			0.0			90.8			91.0		
	48.3	46.1	2.2	17.6	17.2	0.5	27.2	28.0	0.8	1.5	1.5	0.0	0.1	0.1	0.1	94.7	92.8	1.9	94.7	92.9	1.9
63	42.2			24.0			27.5			1.4			0.0			95.1			95.1		
	44.3	43.3	1.0	21.4	22.7	1.3	25.5	26.5	1.0	1.4	1.4	0.0	0.0	0.0	0.0	92.6	93.9	1.3	92.6	93.9	1.3
91	39.8			22.1			26.9			1.4			0.0			90.2			90.1		
	43.3	41.6	1.8	18.5	20.3	1.8	31.8	29.4	2.4	1.2	1.3	0.1	0.0	0.0	0.0	94.8	92.5	2.3	94.9	92.5	2.4
106	41.7			18.6			31.0			1.3			0.0			92.6			92.6		
	43.1	42.4	0.7	21.2	19.9	1.3	30.6	30.8	0.2	1.1	1.2	0.1	0.0	0.0	0.0	96.0	94.3	1.7	96.0	94.3	1.7
120	40.1			24.6			31.1			1.4			0.0			97.2			97.3		
	41.5	40.8	0.7	21.2	22.9	1.7	33.1	32.1	1.0	1.3	1.4	0.0	0.0	0.0	0.0	97.1	97.2	0.1	97.1	97.2	0.1
184	38.6			18.9			36.3			1.4			0.0			95.2			95.2		
	38.1	38.4	0.3	19.9	19.4	0.5	31.4	33.9	2.5	1.4	1.4	0.0	0.0	0.0	0.0	90.8	93.0	2.2	90.7	93.0	2.2
275	38.3			19.0			36.7			1.6			0.0			95.6			95.6		
	32.3	35.3	3.0	20.1	19.6	0.5	31.4	34.1	2.7	1.6	1.6	0.0	0.0	0.0	0.0	85.4	90.5	5.1	85.4	90.5	5.1
365	37.6			21.3			37.8			1.9			0.0			98.6			98.6		
	36.9	37.3	0.3	23.5	22.4	1.1	35.0	36.4	1.4	1.8	1.9	0.0	0.0	0.0	0.0	97.2	97.9	0.7	97.1	97.9	0.7
																Overall	94.1	3.6		94.1	3.6
																maximum	102.2			102.2	
																minimum	85.4			85.4	
																n =	24			24	

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).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801715
Guideline: 162-3

Anaerobic metabolism of [pyrazole-3-^{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	12.7	7.0	19.7		
	12.1	7.9	20.0	19.9	0.1
14	16.6	23.3	39.9		
	18.5	18.5	37.0	38.5	1.4
17	17.9	22.9	40.8		
	19.4	21.3	40.7	40.8	0.0
28	16.7	28.8	45.5		
	17.6	27.2	44.8	45.2	0.4
63	24.0	27.5	51.5		
	21.4	25.5	46.9	49.2	2.3
91	22.1	26.9	49.0		
	18.5	31.8	50.3	49.7	0.7
106	18.6	31.0	49.6		
	21.2	30.6	51.8	50.7	1.1
120	24.6	31.1	55.7		
	21.2	33.1	54.3	55.0	0.7
184	18.9	36.3	55.2		
	19.9	31.4	51.3	53.3	1.9
275	19.0	36.7	55.7		
	20.1	31.4	51.5	53.6	2.1
365	21.3	37.8	59.1		
	23.5	35.0	58.5	58.8	0.3

[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	97.8	0.0						
	102.2	0.0						
3	69.6	19.7	4	0				
	74.8	20.0	4	0	4	0	0	0
14	51.0	39.9	1	1				
	53.8	37.0	1	1	1	0	1	0
17	46.7	40.8	1	1				
	53.0	40.7	1	1	1	0	1	0
28	43.9	45.5	1	1				
	48.3	44.8	1	1	1	0	1	0
63	42.2	51.5	1	1				
	44.3	46.9	1	1	1	0	1	0
91	39.8	49.0	1	1				
	43.3	50.3	1	1	1	0	1	0
106	41.7	49.6	1	1				
	43.1	51.8	1	1	1	0	1	0
120	40.1	55.7	1	1				
	41.5	54.3	1	1	1	0	1	0
184	38.6	55.2	1	1				
	38.1	51.3	1	1	1	0	1	0
275	38.3	55.7	1	1				
	32.3	51.5	1	2	1	0	2	0
365	37.6	59.1	1	2				
	36.9	58.5	1	2	1	0	2	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: 46801715
Guideline: 162-3

Anaerobic metabolism of [pyrazole-3-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment. Confirmation/determination of means/std.dev. for pyrasulfotole.

	Pyrasulfotole								
	Water			**Sediment**			**Total system**		
Day	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0	97.8			0.0			97.8		
	102.2	100.0	2.2	0.0	0.0	0.0	102.2	100.0	2.2
3	69.6			12.7			82.3		
	74.8	72.2	2.6	12.1	12.4	0.3	86.8	84.6	2.3
14	51.0			16.6			67.6		
	53.8	52.4	1.4	17.7	17.2	0.6	71.5	69.6	1.9
17	46.7			17.9			64.7		
	53.0	49.9	3.2	19.4	18.7	0.8	72.5	68.6	3.9
28	43.9			16.7			60.7		
	48.3	46.1	2.2	17.6	17.2	0.5	65.9	63.3	2.6
63	42.2			24.0			66.2		
	44.3	43.3	1.0	21.4	22.7	1.3	65.7	66.0	0.3
91	39.8			22.1			61.8		
	43.3	41.6	1.8	18.5	20.3	1.8	61.9	61.9	0.1
106	41.7			18.6			60.3		
	43.1	42.4	0.7	19.6	19.1	0.5	62.7	61.5	1.2
120	40.1			24.6			64.8		
	41.5	40.8	0.7	21.2	22.9	1.7	62.7	63.8	1.0
184	38.6			18.9			57.5		
	38.1	38.4	0.3	19.9	19.4	0.5	58.0	57.8	0.3
275	38.3			19.0			57.3		
	32.3	35.3	3.0	20.1	19.6	0.5	52.4	54.9	2.5
365	37.6			21.3			58.9		
	36.9	37.3	0.3	23.5	22.4	1.1	60.4	59.7	0.7

Results from Appendix 7, pp. 62-63 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: 46801715
Guideline: 162-3

Anaerobic metabolism of [pyrazole-3-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment. Determination of total unidentified [^{14}C] following HPLC analyses.

	Unknown 1		Unknown 2		Total Uknowns								
	Water	Sed	Water	Sed	Water			Sediment			Total system		
Day	% 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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
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	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
14	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	0.8	0.0	0.0	0.0	0.0	0.0	0.8	0.4	0.4	0.8	0.4	0.4
17	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
28	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
63	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
91	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
106	0.0	0.0	0.0	0.0	0.0			0.0			0.0		
	0.0	0.7	0.0	0.9	0.0	0.0	0.0	1.6	0.8	0.8	1.6	0.8	0.8
120	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
184	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
275	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
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

Results from Appendix 7, pp. 62-63 of the study report.

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

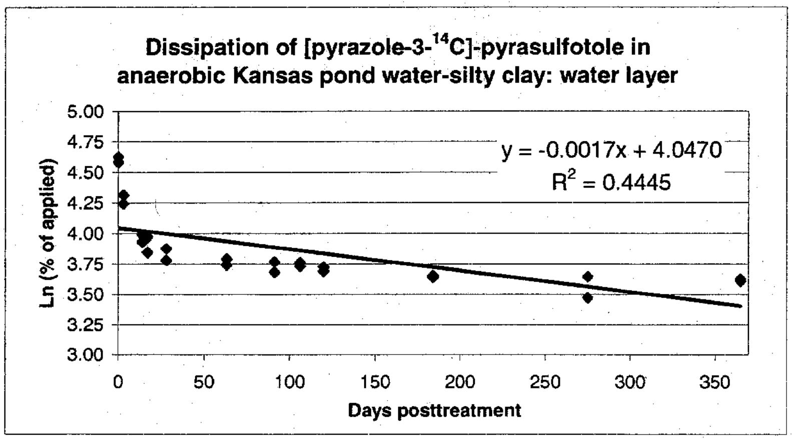
Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801715
Guideline: 162-3

Anaerobic metabolism of [pyrazole-3-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Half-life determination/water layer

Half-life (days) 396.7 (0- to 365-day data)

	Pyrasolfotole	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	97.8	4.582924577
0	102.2	4.626931678
3	69.6	4.242764567
3	74.8	4.314817885
14	51.0	3.931825633
14	53.8	3.985273467
17	46.7	3.843744165
17	53.0	3.970291914
28	43.9	3.78191432
28	48.3	3.877431561
63	42.2	3.742420221
63	44.3	3.790984677
91	39.8	3.683866912
91	43.3	3.768152635
106	41.7	3.730501129
106	43.1	3.763522997
120	40.1	3.691376334
120	41.5	3.725693427
184	38.6	3.653252276
184	38.1	3.640214282
275	38.3	3.645449896
275	32.3	3.47506723
365	37.6	3.62700405
365	36.9	3.608211551

Results from Appendix 7, pp. 62-63 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.666721821
R Square	0.444517987
Adjusted R Square	0.419268805
Standard Error	0.22679991
Observations	24

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.905581988	0.90558	17.60524282	0.000374
Residual	22	1.131640384	0.05144		
Total	23	2.037222372			

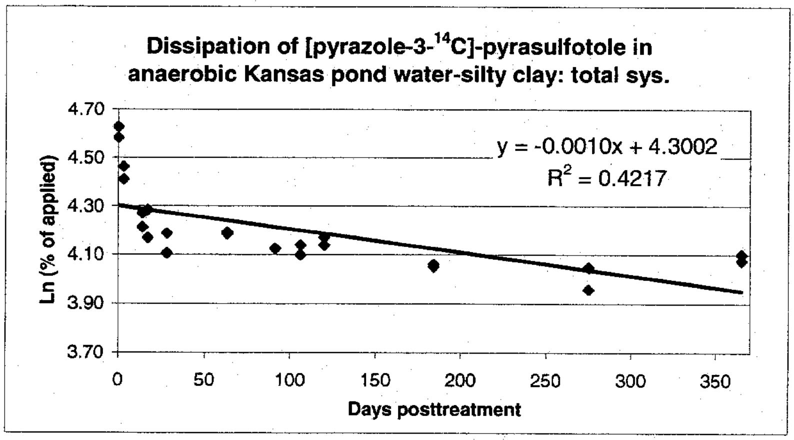
	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.046991957	0.063823536	63.4091	2.08992E-26	3.9146299	4.179354	3.9146299	4.17935401
X Variable 1	-0.001747302	0.000416435	-4.1959	0.000373962	-0.002611	-0.0008837	-0.0026109	-0.0008837

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801715
Guideline: 162-3

Anaerobic metabolism of [pyrazole-3-^{14}C]pyrasulfotole in Kansas pond water-silty clay sediment.
Half-life determination/total system
Half-life (days) **725.2** **(0- to 365-day data)**

	Pyrasolfotole	
Days Posttreatment	(% of Applied)	Ln (% applied)
0	97.8	4.582924577
0	102.2	4.626931678
3	82.3	4.410371108
3	86.8	4.463606622
14	67.6	4.213607983
14	71.5	4.26969745
17	64.7	4.169761202
17	72.5	4.283586562
28	60.7	4.105943698
28	65.9	4.188138442
63	66.2	4.192680463
63	65.7	4.185098925
91	61.8	4.123903364
91	61.9	4.12552018
106	60.3	4.099332104
106	62.7	4.138361448
120	64.8	4.171305603
120	62.7	4.138361448
184	57.5	4.051784948
184	58.0	4.060443011
275	57.3	4.048300624
275	52.4	3.958906591
365	58.9	4.075841091
365	60.4	4.100989105

Results from Appendix 7, pp. 62-63 of the study report.



Dissipation of [pyrazole-3-^{14}C]-pyrasulfotole in anaerobic Kansas pond water-silty clay: total sys.

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.649397012
R Square	0.42171648
Adjusted R Square	0.395430865
Standard Error	0.129959786
Observations	24

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.2709695	0.27097	16.0436226	0.0005952
Residual	22	0.371570009	0.01689		
Total	23	0.642539509			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.300227879	0.036571853	117.583	2.73897E-32	4.2243824	4.3760733	4.22438242	4.37607334
X Variable 1	-0.000955794	0.000238623	-4.0054	0.000595186	-0.001451	-0.0004609	-0.0014507	-0.0004609