Data Evaluation Report on the anaerobic biotransformation of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445 EPA MRID Number 46801712

Data Requirement:	PMRA Data Code:	8.2.3.4.4
	EPA DP Barcode:	D328639
	OECD Data Point:	IIA 7.2.4
	EPA Guideline:	162-2

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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Final Reviewer: Olga Braga
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Date: 24/01/2007

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EXECUTIVE SUMMARY

The biotransformation of [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone (pyrasulfotole, AE 0317309; radiochemical purities 100%) was studied in a loamy sand soil (pH 4.8-5.4, organic carbon 1.9%) from North Carolina for 120 days in darkness at 20 ± 1°C under anaerobic conditions (flooding, static nitrogen atmosphere) following 30 days of aerobic incubation. Soil moisture content prior to flooding was 50% of maximum water holding capacity. [^{14}C]Pyrasulfotole (both labels) was applied at a rate of 0.07 mg a.i./kg (equivalent to 0.05 kg a.i./ha). This study was conducted in accordance with OECD Guideline for the Testing of Chemicals No. 307, Aerobic and Anaerobic Transformation in Soil (2002), and in compliance with USEPA GLP Standards 40 CFR, Part 160. The test system consisted of 250-mL, Pyrex, Erlenmeyer flasks, each fitted with an air-permeable, solid-phase trap for the collection of CO_2 (soda lime) during the aerobic phase of the incubation. During anaerobic phase, the air-permeable, solid-phase traps were removed and the flasks incubated sealed. Duplicate flasks per test substance were taken for analysis at day 0 posttreatment, then after conversion to anaerobic conditions, duplicate water-soil systems were taken at 30, 32, 35, 38, 45, 63, 91, 120 and 150 days posttreatment (0, 2, 5, 8, 15, 33, 61, 90 and 120 days post-flooding). Upon collection, metabolism flasks were attached to a flow-through (nitrogen, flow rate not specified) system with traps for the collection of CO_2 (2M KOH) and volatile organics (ethylene glycol, 1M H_2SO_4). Water layers, when present, were decanted, filtered (0.45 µm), then concentrated via rotary evaporation for reverse-phase HPLC analysis. All soil samples, except 0-day pyrazole-label treated samples (not specified whether day 0 posttreatment or post-flood), were extracted using an Accelerated Solvent Extraction (ASE) system, which conducted two-phase ["ambient" (40°C, 1,500 psi) and "aggressive" (100°C, 1,500 psi) conditions], automated, multi-step extractions with acetonitrile:water (65:35, v:v) as the extraction solvent. The 0-day pyrazole-label treated samples were extracted ("ambient" and "aggressive") solely with acetonitrile; consequently, those samples were further extracted a third time using "aggressive" conditions and acetonitrile:water (65:35) extraction solvent. Subsequent "ambient" and "aggressive" extracts were separately concentrated via rotary evaporation (30-35°C, under vacuum) for HPLC analysis. One transformation product, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555), was identified via HPLC against reference standard. The identification was confirmed using LC/MS-ESI against reference standard.

The test conditions outlined in the study appear to have been maintained throughout the 150-day incubation. After flooding the soil at 30 days posttreatment, conditions in the water layers of untreated control systems incubated alongside the treated systems became increasingly anaerobic with measured redox potentials of +436.5 to +446.5 mV at day 0 post-flooding (30 days posttreatment) decreasing to +162.7 to +184.6 mV at 120 days post-flooding (150 days posttreatment). In the water layers, dissolved oxygen decreased from 3.0-4.1 mg/L at day 0 post-flooding to 0.1-0.2 mg/L at 120 days, while pH levels increased from 5.2-5.3 at day 0 to 6.3-6.4 at 90-120 days post-flooding.

For both labels, overall recovery of material balance averaged 96.7 ± 3.2% (range 90.6-102.4%) of the applied, with no consistent pattern of decline in recoveries for either label. [^{14}C]Residues partitioned between the soil and water layer with mean (n = 2) distribution ratios (water:soil) of 1:22-28 immediately after flooding (30 days posttreatment), decreasing to 1:5 after 33 days (63 days posttreatment) and were 1:7-11 at study termination (150 days posttreatment). The dissipation rate of [^{14}C]pyrasulfotole significantly slowed with the conversion to anaerobic conditions. [^{14}C]Pyrasulfotole comprised means of 93.5-97.3% of the applied in the soil at day 0 posttreatment, then at day 0 post-flooding (30 days posttreatment) was detected at 66.0-68.4% in the total system and was 62.2-64.1% at 120 days post-flooding (150 days posttreatment). In the water layer, [^{14}C]pyrasulfotole increased from means of 2.4-3.1% at day 0 post-flooding (30 days posttreatment) to 11.7-14.2% at 33 days (63 days posttreatment) and was 7.2-7.7% at study termination. In the soil, [^{14}C]pyrasulfotole decreased from means of 93.5-97.3% at day 0 posttreatment to 62.9-66.0% at day 0 post-flooding (30 days posttreatment) and was 53.3-56.5% at 90-120 days post-flooding (120-150 days posttreatment). In the water layer, [^{14}C]pyrasulfotole dissipated with a combined (both labels) **linear half-life** of 127 days and nonlinear **half-life** of 116 days. **Observed DT50** values for pyrasulfotole in the soil and total system were >120 days and *ca.* ≥120 days in the water layer. Calculated dissipation half-lives for [^{14}C]pyrasulfotole in the soil and total system could not be determined due to insufficient dissipation post-flooding. **Pyrasulfotole is therefore considered to be stable under anaerobic soil conditions.**

- 2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555)

was the sole major transformation product detected at maximum means of 5.1% (15 days post-flooding), 7.7% (day 0 post-flood) and 9.9% (15 and 61 days post-flood) of the applied in the water, soil and total system, respectively, of phenyl-label [^{14}C]pyrasulfotole treated soil and was 4.1%, 5.1% and 9.2%, respectively, at study termination. One minor unidentified transformation product, Unknown B, was detected at ≤2.6% in the total system of phenyl-label treated soil. No major or minor products were detected for pyrazole-label treated soil at any interval.

Phenyl-label extractable [^{14}C]residues decreased from a mean 99.2% of the applied at day 0 posttreatment to 59.4% at 120 days (90 days post-flooding) and were 62.8% at study termination, while nonextractable [^{14}C]residues increased from 0.8% at day 0 to 22.5% at study termination. Pyrazole-label extractable [^{14}C]residues decreased from a mean 98.0% of the applied at day 0 posttreatment to 53.4% at 120 days (90 days post-flooding) and were 55.0% at study termination, while nonextractable [^{14}C]residues increased from 2.0% at day 0 to 24.9% at study termination. At study termination, organic matter fractionation of nonextractable residues (both labels) found 51.8-54.5%, 27.9-35.4% and 12.8-17.6% of the recovered radioactivity associated with the humin, fulvic acids and humic acids, respectively. Maximum mean levels of volatilized $^{14}CO_2$ (identity not confirmed) detected were 2.6% and 6.6% of the applied for the phenyl- and pyrazole-label treated soils, respectively, while volatile [^{14}C]organic compounds were ≤0.1% (both labels) at all sampling intervals.

A transformation pathway was provided by the study author that was consistent with the products detected. Under aerobic conditions, transformation of pyrasulfotole involves hydrolytic cleavage of the phenyl and pyrazole moieties to yield the benzoic acid derivative, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) with gradual formation of bound soil residues and minimal levels of mineralization to CO_2. Under anaerobic conditions, the levels of pyrasulfotole, AE B197555 and bound residues all remained relatively constant.

In a supplementary experiment, pyrasulfotole and transformation product AE B197555 remained stable in a 120-day water layer sample after 126 days of frozen storage.

Results Synopsis:

Test system used: Loamy sand from North Carolina.
Half-life/DT50 values, post-flooding.

Linear half-life in water:	127.3 days ($r^2 = 0.7104$).
Linear half-life in soil:	ND (not determined).
Linear half-life in the total system:	ND.
Non-linear half-life in water:	115.5 days ($r^2 = 0.7100$).
Non-linear half-life in soil:	ND.
Non-linear half-life in total system:	ND.
Observed DT50 in water:	*ca.* ≥120 days.
Observed DT50 in soil:	>120 days.
Observed DT50 in total system:	>120 days.

Considered stable in anaerobic soil system.

Major transformation products
2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555, maximum mean 5.1%, 7.7% and 9.9% of applied in water, soil and total system, respectively).
Minor identified transformation products:
CO_2 (maximum means 2.6-6.6% 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 OECD Guideline for the Testing of Chemicals No. 307, Aerobic and Anaerobic Transformation in Soil (2002) and reported as in compliance with USEPA Subdivision N Guideline §162-2 (pp. 17, 36). 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, 17). Signed and dated Data Confidentiality, GLP, Quality Assurance and [study] Certification statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Materials [Phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]pyrasulfotole (p. 18; Figure 1, p. 47).

Chemical Structure: See DER Attachment 1.

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

Description: Technical; physical state not reported.

Purity:

Radiochemical purity:	100% (Figure 5, p. 52).
Batch No.	SEL/1006 (p. 18).
Analytical purity:	Not reported.
Specific activity:	28.6 µCi/µmol.
Location of the radiolabel:	Uniformly on phenyl ring.

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

Description: Technical; physical state, solid (p. 23).

Purity:

Radiochemical purity:	100% (Figure 5, p. 52).
Batch No.	SEL/1009 (p. 18).
Analytical purity:	Not reported.
Specific activity:	55.3 µCi/µmol.
Location of the radiolabel:	At 3-C position on pyrazole ring.

Storage conditions of test chemicals: Maintained in acetonitrile solution; additional storage conditions (temperature, light/darkness) were not specified (p. 18).

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. Soil Characteristics

Table 1: Description of soil collection and storage.

Description		Details
Geographic location		703 NOR-AM Road, Pikeville, North Carolina. Site planted to turf grass for previous 5 years.
Coordinates	Latitude:	N 35° 29.303'
	Longitude:	W 78° 02.421'
Collection date		March 22, 2004.
Pesticide use history at the collection site		No pesticide applications for previous 5 years.
Collection procedures		Soil collected with a spade into plastic buckets.
Sampling depth		0- to 8-inch depth.
Storage conditions		Soil transported at ambient temperature, then stored refrigerated (temperature not specified) upon receipt at test facility.
Storage length		25 days prior to use.
Soil preparation		Sieved (2-mm).

Data obtained from p. 20; Appendix 2, p. 77 of the study report.

Table 2: Properties of the soil.

Property		Details
Soil texture		Loamy sand.
% Sand (0.05-2.0 mm)		79
% Silt (0.002-0.05 mm)		14
% Clay (<0.002 mm)		7
pH	in water:	5.4
	in $CaCl_2$:	4.8
Organic carbon (%)[1]		1.9
Organic matter (%)		3.3
CEC (meq/100g)		6.2
Moisture (%)	at 1/3 bar:	9.8
	at 15 bar:	4.9
Maximum water holding capacity (MWHC, %)		31.3
Bulk density, disturbed (g/cm^3)		1.12
Microbial biomass (cells/g soil)[2]		1.2×10^8
Soil taxonomic classification (USDA)		Fine-loamy, siliceous, subactive, thermic aquic paleudults.
Soil series		Goldsboro.
Sol mapping unit		Not reported.

1 As presented in the study report, organic carbon (%) = organic matter (%)/1.724.
2 At study initiation.
Data obtained from Table 1, p. 37 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None reported.

2. Experimental conditions:

Table 3: Experimental design.

Parameter		Both labels
Duration of the test		150 days; 30 days of aerobic incubation followed by 120 days of anaerobic incubation.
Soil condition: (Air dried/fresh)		Fresh.
Soil (g/replicate)		50 g dry wt.
Application rates (mg a.i./kg & equiv. kg a.i./ha)	Nominal	0.07 mg a.i./kg (0.05 kg a.i./ha).
	Actual	0.067 mg a.i./kg for both labels (Reviewer's Comment No. 2).

Parameter		Both labels	
Control conditions, if used		Sterile controls were not prepared.	
No. of Replications	Controls, if used	Sterile controls were not prepared.	
	Treatment	Twenty-four treated, nonsterile soil samples were prepared for each label. This allowed for duplicate replicates at day 0 posttreatment and at each sampling interval post-flooding, plus reserves (Reviewer's Comment No. 3).	
Test apparatus	Type/material/volume	250-mL side-arm Pyrex Erlenmeyer flask. Aerobic phase: fitted with an air-permeable, solid-phase, volatiles trap. Anaerobic phase: solid-phase trap removed, flask closed with closeable, double-valve, glass stopper.	
	Details of traps for CO_2 and organic volatiles, if any	Aerobic phase: Soda lime to trap CO_2 (one 10-g layer).	
		Anaerobic phase: 2M potassium hydroxide (KOH) to trap CO_2 (two traps, each 30 mL). Ethylene glycol (one trap, 30 mL) and 1M sulfuric acid (one trap, 30 mL) to trap organic volatiles.	
If no traps were used, is the system closed/open?		Systems were incubated close and attached to a flow-through volatiles trapping system upon collection.	
Identity and concentration of co-solvent		Acetonitrile (ACN); final concentration <0.015% based on soil weight. [Phenyl-U-^{14}C]-label: 0.099 mL of water:ACN (97.8:2.2, v:v) test solution in 50 g dry wt. soil. [Pyrazole-3-^{14}C]-label: 0.094 mL of water:ACN (92.2:7.8, v:v) test solution in 50 g dry wt. soil.	
Test material	Volume of the test solution used/treatment:	[Phenyl-U-^{14}C]-label: 99 µL/50 g soil (dry wt). [Pyrazole-3-^{14}C]-label: 94 µL/50 g soil (dry wt.).	
	Application method (eg: mixed/not mixed):	Applied dropwise to soil surface using a 100-µL Hamilton Gastight syringe, after which sample was rotated to incorporate test material.	
	Is the co-solvent evaporated?	No.	
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.	
Microbial biomass/microbial population of controls (units)		Initial	Final
		Sterile controls were not prepared.	
Microbial biomass/microbial population of treated (units)		Initial	Final
		Treated soil samples were not analyzed for biomass.	

Parameter		Both labels
Experimental conditions:	Temperature (°C):	20 ± 1°C; maintained in an environmental chamber during aerobic phase or upright incubator during anaerobic phase.
	Continuous darkness (Yes/No):	Yes; soil flasks wrapped with aluminum foil and maintained in darkness in environmental chamber/incubator.
	Moisture content:	50% of MWHC during aerobic phase; 15.7% soil moisture.
	Moisture maintenance method:	Aerobic phase: Milli-Q purified water (1 mL) added to each treated soil sample at *ca.* 2 weeks posttreatment. Anaerobic phase: test soils flooded with Milli-Q purified water (50 mL) at 30 days posttreatment.
Other details, if any		The test systems were prepared and acclimatized to study conditions for 3 days prior to treatment.

Data obtained from pp. 15, 17, 21-24, 31; Tables 2-3, pp. 38-39; Figures 2-4, pp. 49-51 of the study report.

3. Aerobic/anaerobic conditions: Following treatment, the test soils were incubated aerobically under static conditions in a flask fitted with an air-permeable, solid-phase (soda lime, glass wool) volatiles trap that allowed for the passive exchange of air (pp. 21-22). The test systems were converted to anaerobic conditions at 30 days posttreatment by purging the flasks with nitrogen (*ca.* 15 minutes), flooding with Milli-Q purified water (50 mL, water layer depth *ca.* 1 cm), and the air-permeable volatiles trap was replaced with a closeable, double-valve glass stopper to seal the flask (pp. 20, 23; Figures 2-3, pp. 49-50). The converted test systems were then maintained in a nitrogen-filled incubator (p. 23). At day 0 post-flooding (30 days posttreatment) in untreated, control systems incubated alongside the treated systems, redox potentials and dissolved oxygen in the water layers were +436.5 to +446.5 mV and 3.0-4.1 mg/L, respectively; system parameters were not measured in the soil layers (Table 4, p. 40).

4. Supplementary experiments: Microbial biomass in untreated samples. Additional untreated, nonsterile soil samples were prepared and incubated under the same conditions as the treated samples to be used for biomass determinations (p. 21). Untreated soil or water-soil systems were taken for analysis at the beginning, mid-point and end of the study; sampling intervals were not specified (pp. 21, 31).

Metabolite identification (MID) samples. To facilitate identification of possible transformation products of pyrasulfotole, six additional soil samples per label were prepared and incubated as described above, but treated at 0.34 mg a.i./kg or five times the application rate (pp. 21-23).

5. Sampling:

Table 4: Sampling details.

Criteria		Both labels
Sampling intervals	Aerobic phase:	Day 0 posttreatment[1].
	Anaerobic phase:	0, 2, 5, 8, 15, 33, 61, 90 and 120 days post-flooding; (30, 32, 35, 38, 45, 63, 91, 120 and 150 days posttreatment).
Sampling method		Duplicate treated samples per label at each interval.
Method of collection of CO_2 and organic volatile compounds	Aerobic phase:	At 30 days posttreatment, solid-phase volatiles traps were purged with nitrogen to ensure headspace $^{14}CO_2$ was absorbed by soda lime, then traps were collected with respective soil flask.
	Anaerobic phase:	At each interval, the test flask was attached to a flow-through volatiles trapping system and purged with nitrogen (*ca.* 10-15 minutes, flow rate not specified).
Sampling intervals/times for:		
Sterility check, if sterile controls are used:		Sterile controls were not prepared.
Moisture content:		Not reported; Milli-Q purified water (1 mL) added to all treated soil sample at *ca.* 2 weeks posttreatment.
Redox potential, dissolved oxygen and pH:		Measured in water layer of untreated control systems at each sampling interval post-flooding.
Sample storage before analysis		**Soil samples** were extracted the day of collection. **Soil extracts and water samples** were reportedly analyzed within 30 days after collection, except for 61-day samples which were stored 126 days prior to analysis; however, specific extraction and analysis dates were not provided. Extracts were stored refrigerated or frozen (mean <5°C) when not in use.
Other details, if any		None reported.

1 Reviewer's Comment No. 3.
Data obtained from pp. 21-24; Table 3, p. 39; Figure 4, p. 51 of the study report.

C. ANALYTICAL METHODS:

Separation of the water and soil: The water layer, when present, was decanted and filtered (0.45 µm glass fiber), then triplicate aliquots (1 mL) were analyzed for total radioactivity by LSC (pp. 24-25; Figure 7, p. 54).

Extraction/clean up/concentration methods for water and soil samples: Prior to HPLC analysis, an aliquot (sufficient to characterize 1% of the applied radioactivity) of the water layer was concentrated using rotary evaporation (under vacuum, temperature not specified; p. 25).

Resulting residues were reconstituted to 1-5 mL with either 0.1% trifluoroacetic acid (TFA) or 30 mM triethylamine (TEA).

Soil samples were combined with diatomaceous earth (*ca.* 10 g, Hydromatrix sorbent) and transferred to a 100-g extraction cell of an Accelerated Solvent Extraction (ASE) system (Model ASE 300, Dionex; p. 25; Appendix 1, p. 76). Two-phase ("ambient" and "aggressive" conditions), automated, multi-step extractions were conducted using acetonitrile:water (65:35, v:v) as the extraction solvent. "Ambient" extraction conditions were as follows: 3 cycles, cell temperature 40°C, heating time 5 minutes, static time 5 minutes, flush volume 50%, purge time 180 seconds, pressure 1,500 psi. Subsequent "aggressive" conditions were as described above with the following changes: 2 cycles, cell temperature 100°C, static time 15 minutes. All soil samples were extracted as described, with the exception of the 0-day [pyrazole-3-^{14}C]-label treated samples (not specified whether day 0 posttreatment or post-flood samples) which were extracted ("ambient" and "aggressive") solely with acetonitrile; therefore, those samples were further extracted a third time using "aggressive" conditions and acetonitrile:water (65:35) as the extraction solvent (p. 26). Respective "ambient" and "aggressive" extracts were combined, then triplicate aliquots (1 mL) were analyzed for total radioactivity (Figure 7, p. 54). Prior to HPLC analysis, an aliquot (sufficient to characterize 1% of the applied radioactivity) was concentrated via rotary evaporation (30-35°C, under vacuum) to <2mL, with the resulting residues reconstituted to 2-5 mL using either 0.1% TFA or 30 mM TEA (p. 26).

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the water layers (when present), soil extracts, extracted soil and volatile trapping materials (p. 29).

Determination of nonextractable residues: Extracted soil was air-dried, then homogenized (method not reported, p. 26). Triplicate aliquots (*ca.* 0.25 g) were analyzed for total radioactivity by LSC following combustion (p. 26; Appendix 11, p. 87; Appendix 14, p. 91).

Organic matter fractionation. Aliquots (25 g) of 120-day post-flood extracted soil (both labels) were further extracted with 0.5N sodium hydroxide (NaOH, 50 mL) via shaking (30 minutes, mechanism, speed not specified), with the resulting extract separated from soil by centrifugation (1,300 *g*, 20 minutes; p. 26). The supernatant was decanted, analyzed for total radioactivity by LSC, then acidified to pH 1 with 5M hydrochloric acid with the resulting precipitate (humic acids) removed by centrifugation (4,075 *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 soil (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. 25).

To recover radioactivity (presumably, $^{14}CO_2$) from the soda lime, concentrated HCl (volume not reported) was applied dropwise to the soda lime with agitation via magnetic stirrer (p. 25; Figure

8, p. 55). Released $^{14}CO_2$ was purged (nitrogen, flow rate not specified) through ice-cooled Carbosorb/Permafluor (3:5, v:v, *ca.* 14 mL) scintillation cocktail and quantified by LSC.

Derivatization method, if used: None was reported.

Identification and quantification of parent compound: Concentrated water and soil extract samples through 33 days post-flooding were analyzed by reverse-phase HPLC under the following conditions: Phenomenex Prodigy C8 (4.6 x 150 mm, 5 µm) column, gradient mobile phase combining (A) 0.1% aqueous TFA and (B) acetonitrile [percent A:B at 0 min. 85:15 (v:v), 27 min. 5:95, 30 min. 5:95], injection volume 0.9-1.8 mL, flow rate 1.5 mL/minute, UV detector (wavelength not specified), and Ramona Classic radioactivity detector (pp. 26-27).

The 61-, 90- and 120-day post-flood water and soil extract samples were analyzed by reverse-phase HPLC under the following conditions: Phenomenex Luna C18(2) (10 x 250 mm, 5 µm) column, Phenomenex C18 (10 x 10 mm) guard column, gradient mobile phase combining (A) 30 mM TEA adjusted to pH 2.5-2.9 with phosphoric acid and (B) acetonitrile [percent A:B at 0-5 min. 90:10 (v:v), 5.1-30 min. 67:33], injection volume 4.5 mL, flow rate 4 mL/minute, UV and radioactivity detectors as described above (pp. 26-27).

Parent [^{14}C]pyrasulfotole was identified by co-chromatography with and comparison to the retention time of unlabeled reference standard (pp. 27-28; Figure 9, p. 56; Figures 12-13, pp. 59-62; Figures 15-16, pp. 64-67; Figure 18, p. 69). Column recoveries were monitored through the collection and LSC analysis of bulk column eluates, with "representative" average recoveries reported as 94.0% and 97.2% for [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-label treated soil extracts, respectively (pp. 27, 32).

To confirm identifications, [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-pyrasulfotole were isolated from 49-day post-flood MID soil extract and 15-day post-flood definitive study soil extract, respectively, via HPLC separation and fraction collection. Fractions were concentrated (method not specified), then analyzed by LC/MS under the following conditions: Zorbax Rx-C8 (4.6 x 75 mm, 3.5 µm) LC column, gradient mobile phase combining (A) 0.1% aqueous formic acid and (B) methanol [gradient conditions were not specified], flow rate 800 µL/minute, post-column split ratio 200:600 µL/min. (MS:RD), Ramona 5 (Raytest) radioactivity detector (RD), Quantum Ultra AM (Thermo Electron) triple quadrupole MS, electrospray ionization (ESI) in negative ion mode, scan range generally 100-600 amu, scan time 1 second (pp. 27-28). Identifications of [^{14}C]pyrasulfotole in sample extracts were made against labeled test substances (p. 28; Figure 6, p. 53; Figure 17, p. 68; Figure 19, p. 70).

Identification and quantification of transformation products: Transformation products were separated, quantified and identified using HPLC as described for the parent compound (pp. 26-28; Figure 9, p. 56; Figures 12-13, pp. 59-62; Figure 18, p. 69). To confirm identification, [^{14}C]AE B197555 was isolated from 49-day post-flood MID soil extract via HPLC separation

and fraction collection, then analyzed by LC/MS-ESI against reference standard (p. 27-28; Figure 20, p. 71).

Table 5: 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 1073910, K-1385, AE 0317309 N-desmethyl	(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 pp. 19-20; Figure 1, p. 48 of the study report.

Detection limits (LOD, LOQ) for the parent compound and transformation products: For HPLC analyses (both labels), limits of detection (LOD) and quantitation (LOQ) were reported as 1,000 dpm and ≤1.76% of the applied radioactivity, respectively (pp. 30, 32). HPLC detector response was linear from 929-182,125 dpm (r^2 = 0.9998; p. 32; Appendix 3, p. 78).

For LSC analyses of [phenyl-U-^{14}C]- and pyrazole-3-^{14}C]-label treated samples, minimum sensitivities (MSP) were reported as 0.10% and 0.05% of the applied, respectively, for aqueous samples, 1.25% and 0.63%, respectively, for soil extracts and 0.90% and 0.47%, respectively, for soil combustions (Appendices 4-7, pp. 79-82).

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: After flooding the soil at 30 days posttreatment, the conditions in the water layers of untreated control systems incubated alongside the treated systems became increasingly anaerobic decreasing from moderately oxidizing (+200 to +400 mV) at day 0 post-flooding (30 days posttreatment), with measured redox potentials of +436.5 to +446.5 mV to moderately reducing (-50 to +200 mV) at 120 days post-flooding (150 days posttreatment), with redox potentials of +162.7 to +184.6 mV (Table 4, p. 40). In the water layers, dissolved oxygen decreased from 3.0-4.1 mg/L at day 0 post-flooding to 0.1-0.2 mg/L at 120 days post-flooding, while pH levels increased from 5.2-5.3 at day 0 to 6.3-6.4 at 90-120 days post-flooding.

B. MATERIAL BALANCE: Overall recovery (both labels) of radiolabeled material averaged 96.7 ± 3.2% (range 90.6-102.4%, n = 39) of the applied, with no consistent pattern of decline in recoveries for either label (DER Attachment 2, Reviewer's Comment No. 1). For each label, recoveries averaged 98.8 ± 2.4% (range 92.3-102.4%, n = 20) of the applied in [phenyl-^{14}C]-label treated soil and 94.6 ± 2.4% (range 90.6-100.6%, n = 19) in [pyrazole-3-^{14}C]-label treated soil. [^{14}C]Residues (both labels) partitioned between the soil and water layer with mean (n = 2)

distribution ratios (water:soil) of 1:22-28 immediately after flooding (30 days posttreatment), decreased to 1:5 at 33 days post-flooding (63 days posttreatment) and were 1:7-11 at 120 days (150 days posttreatment, DER Attachment 2).

Table 6. Biotransformation of [phenyl-U-^{14}C]pyrasulfotole (AE 0317309), expressed as percentage of applied radioactivity (mean ± s.d., n = 2[1]), in North Carolina loamy sand soil under anaerobic conditions.

Compound		Sampling times (days)									
		Aerobic	Anaerobic								
		0	30	32	35	38	45	63	91	120	150
Pyrasulfotole	water	--	2.4 ± 0.7	5.0 ± 0.0	7.6 ± 1.0	9.7 ± 0.5	11.3 ± 0.5	11.7 ± 0.5	8.2 ± 0.2	8.2 ± 0.0	7.7 ± 0.8
	soil	97.3 ± 0.7	66.0 ± 1.3	63.4 ± 1.4	61.5 ± 2.4	60.9 ± 1.9	58.8 ± 0.0	57.1 ± 0.7	55.7 ± 0.4	53.3 ± 1.9	56.5 ± 1.3
	system	97.3 ± 0.7	68.4 ± 2.0	68.4 ± 1.4	69.1 ± 3.3	70.6 ± 1.3	70.0 ± 0.5	68.8 ± 1.3	63.9 ± 0.2	61.5 ± 1.9	64.1 ± 0.4
AE B197555[2]	water	--	1.7 ± 0.3	3.0 ± 0.3	3.9 ± 0.1	3.9 ± 0.3	5.1 ± 0.6	4.3 ± 0.2	4.8 ± 0.3	4.2 ± 0.2	4.1 ± 0.5
	soil	0.0 ± 0.0	7.7 ± 0.1	6.6 ± 1.0	5.8 ± 0.0	5.3 ± 1.5	4.8 ± 0.1	5.0 ± 0.0	5.1 ± 1.1	5.4 ± 0.8	5.1 ± 0.3
	system	0.0 ± 0.0	9.4 ± 0.3	9.6 ± 1.3	9.7 ± 0.0	9.1 ± 1.8	9.9 ± 0.7	9.2 ± 0.1	9.9 ± 0.8	9.5 ± 0.5	9.2 ± 0.1
Unknown B	water	0.0 ± 0.0	0.0, 0.7	0.7 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	1.3 ± 0.2	0.9 ± 0.5	1.1 ± 0.0	1.3 ± 0.1
	soil	0.0 ± 0.0	0.0, 1.5	0.0, 1.8	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	1.1 ± 0.1	1.5, 0.0	1.3 ± 0.0
	system	0.0 ± 0.0	0.0, 2.2	1.6 ± 0.9	0.0 ± 0.0	0.0 ± 0.0	0.0 ± 0.0	1.3 ± 0.2	2.0 ± 0.4	1.8 ± 0.8	2.6 ± 0.0
CO_2		0.0 ± 0.0	1.3 ± 0.2	1.8 ± 0.4	2.2 ± 0.3	2.4 ± 0.1	1.9 ± 0.0	2.6 ± 0.2	2.5 ± 0.0	2.3 ± 0.3	2.2 ± 0.2
Volatile organics		0.0 ± 0.0	0.0 ± 0.0	0.1 ± 0.0	0.1 ± 0.0	0.1 ± 0.0	0.1 ± 0.0	0.1 ± 0.0	0.1 ± 0.0	0.1 ± 0.0	0.1 ± 0.0
Extractable soil residues		99.3 ± 1.3	74.5 ± 0.5	70.9 ± 0.5	67.3 ± 2.4	66.1 ± 0.5	63.6 ± 0.0	62.0 ± 0.7	61.9 ± 0.6	59.4 ± 3.4	62.8 ± 1.7
Nonextractable soil residues		0.8 ± 0.2	18.1 ± 0.4	16.3 ± 0.4	16.6 ± 0.2	17.8 ± 0.0	18.6 ± 0.8	18.3 ± 0.2	19.4 ± 0.1	21.2 ± 0.7	22.5 ± 1.1
Total recovery	water	--	4.4 ± 0.6	8.7 ± 0.4	11.5 ± 0.9	13.6 ± 0.8	16.4 ± 1.1	17.3 ± 0.4	13.9 ± 0.4	13.4 ± 0.2	13.0 ± 1.5
	soil	100.0 ± 1.4	92.5 ± 0.9	87.2 ± 0.0	83.9 ± 2.3	83.9 ± 0.5	82.2 ± 0.8	80.3 ± 0.5	81.3 ± 0.4	80.6 ± 4.1	85.2 ± 0.6
	system	100.0 ± 1.4	98.2 ± 1.3	97.6 ± 0.1	97.6 ± 3.3	99.9 ± 0.4	100.4 ± 2.0	100.2 ± 0.8	97.7 ± 0.8	96.4 ± 4.1	100.6 ± 1.0

1 Reviewer's Comment No. 1.
2 2-Methylsulfonyl-4-trifluoromethylbenzoic acid (AE 0317309-benzoic acid; Figure 1, p. 48).
Data obtained from 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 North Carolina loamy sand soil under anaerobic conditions.

Compound		Sampling times (days)									
		Aerobic	Anaerobic								
		0	30	32	35	38	45	63	91	120	150
Pyrasulfotole	water	--	3.1 ± 0.0	7.0 ± 0.0	7.3 ± 0.5	7.9 ± 0.4	9.9 ± 0.4	14.2[2]	10.3 ± 1.1	8.8 ± 0.0	7.2 ± 0.1
	soil	93.5 ± 1.2	62.9 ± 0.6	61.2 ± 0.0	61.3 ± 0.3	59.6 ± 0.2	57.7 ± 0.5	54.2 ± 0.4	54.5 ± 0.5	53.4 ± 0.7	55.0 ± 0.0
	system	93.5 ± 1.2	66.0 ± 0.6	68.1 ± 0.0	68.6 ± 0.1	67.5 ± 0.6	67.6 ± 0.1	68.0[2]	64.7 ± 0.5	62.2 ± 0.7	62.2 ± 0.1
CO_2		0.0 ± 0.0	5.6 ± 0.1	6.0 ± 0.1	6.0 ± 0.2	6.1 ± 0.0	6.3 ± 0.2	5.9 ± 0.4	6.5 ± 0.2	5.3 ± 0.3	6.6 ± 0.0
Volatile organics		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	0.1, 0.0	0.0 ± 0.0	0.1 ± 0.0
Extractable soil residues		98.0 ± 0.8	62.9 ± 0.5	61.1 ± 0.1	61.3 ± 0.3	59.6 ± 0.2	57.7 ± 0.5	54.2 ± 0.4	54.5 ± 0.6	53.4 ± 0.8	55.1 ± 0.1
Nonextractable soil residues		2.0 ± 0.2	23.8 ± 0.4	19.8 ± 0.1	20.2 ± 0.1	18.4 ± 0.4	22.2 ± 0.5	21.9 ± 0.7	21.8 ± 0.6	24.2 ± 0.2	25.0 ± 1.1
Total recovery	water	--	3.1 ± 0.0	7.0 ± 0.1	7.3 ± 0.5	7.9 ± 0.4	9.9 ± 0.4	14.2[2]	10.3 ± 1.1	8.8 ± 0.0	7.2 ± 0.1
	soil	100.0 ± 0.6	86.7 ± 0.9	80.9 ± 0.1	81.5 ± 0.2	78.0 ± 0.6	79.9 ± 1.0	76.1 ± 1.1	76.3 ± 1.2	77.6 ± 1.0	80.0 ± 1.0
	system	100.0 ± 0.6	95.3 ± 0.8	93.9 ± 0.1	94.8 ± 0.5	92.1 ± 0.8	96.1 ± 0.8	95.6[2]	93.1 ± 0.1	91.7 ± 1.0	93.8 ± 0.9

1 Reviewer's Comment No. 1

2 Result represents 63-day replicate 1 water layer only as 63-day replicate 2 water layer was considered contaminated and not used (Appendix 12, p. 89).

Data obtained from DER Attachment 2.

C. TRANSFORMATION OF PARENT COMPOUND: In [phenyl-U-^{14}C]-pyrasulfotole treated soil, pyrasulfotole comprised 96.6-97.9% of the applied at day 0 posttreatment, then post-flooding, gradually decreased in the soil from 64.7-67.2% at 30 days (day 0 post-flooding) to 51.4-55.2% at 120 days (90 days post-flooding) and was 55.2-57.7% at 150 days (120 days post-flooding, DER Attachment 2). In the water layer, [^{14}C]pyrasulfotole increased from 1.7-3.1% at 30 days posttreatment (day 0 post-flooding) to 11.2-12.2% at 63 days (33 days post-flooding), then was 8.0-8.4% at 91-120 days (61-90 days post-flooding) and 6.8-8.5% at 150 days (120 days post-flooding).

In [pyrazole-3-^{14}C]-pyrasulfotole treated soil, pyrasulfotole comprised 92.3-94.7% of the applied at day 0 posttreatment, then post-flooding, gradually decreased in the soil from 62.3-63.4% at 30 days (day 0 post-flooding) to 52.7-54.1% at 120 days (90 days post-flooding) and was 54.9-55.0% at 150 days (120 days post-flooding, DER Attachment 2). In the water layer, [^{14}C]pyrasulfotole increased from 3.1% at 30 days posttreatment (day 0 post-flooding) to 14.2% at 63 days (33 days post-flooding), then decreased to 7.1-7.3% at 150 days (120 days post-flooding).

HALF-LIFE/DT50/DT90: For the soil and total system, calculated dissipation half-lives for [^{14}C]pyrasulfotole (both labels) could not be determined because of insufficient dissipation, with observed DT50 values of >120 days post-flooding.

For the water layers, using first order regression analysis (33- to 120-day post-flood intervals) the linear (Excel 2000) and nonlinear (SigmaPlot v 8) post-flooding half-life values were 157 and 139 days, respectively, for [phenyl-U-^{14}C]-labeled pyrasulfotole and 97 and 90 days, respectively, for the [pyrazole-3-^{14}C]-label (DER Attachment 2). Observed DT50 values were >120 and *ca.* ≥120 days for the [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labeled compounds, respectively.

For the total system, using first order regression nonlinear analysis (Excel, all post-flood intervals), the study author determined half-lives of >120 for both [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labeled pyrasulfotole (pp. 30, 35; Figures 21-22, pp. 72-73).

Half-lives/DT50/DT90

Phase	Half-life/DT50 [1] (days)	First order linear regression equation	r^2	DT50 (days)	DT90 (days)
[Phenyl-U-^{14}C]-pyrasulfotole					
Water layer (Milli-Q purified)					
Linear/natural log	157.0	y = -0.0044x + 2.5093	0.6461	--	--
Nonlinear/normal	138.6	--	0.6811	--	--
Observed DT50	>120	--	--	--	--
Loamy sand soil					
Linear/natural log	--[2]	--	--	--	--
Nonlinear/normal	--[2]	--	--	--	--
Observed DT50	>120	--	--	--	--
Total system					
Linear/natural log				--	--
Nonlinear/normal[3]	>120	$y = 69.455e^{(-0.0009x)}$	0.57	--	--
Observed DT50	>120	--	--	--	--
[Pyrazole-3-^{14}C]-pyrasulfotole					
Water layer (Milli-Q purified)					
Linear/natural log	97.1	y = -0.0071x + 2.8139	0.9039	--	--
Nonlinear/normal	90.0	--	0.9000	--	--
Observed DT50	*ca.* ≥120	--	--	--	--
Loamy sand soil					
Linear/natural log	--[2]	--	--	--	--
Nonlinear/normal	--[2]	--	--	--	--
Observed DT50	>120	--	--	--	--
Total system					
Linear/natural log	--[2]	--	--	--	--
Nonlinear/normal[3]	>120	$y = 67.659e^{(-0.0008x)}$	--	--	--
Observed DT50	>120	--	--	--	--
Both labels					
Water layer (Milli-Q purified)					
Linear/natural log	127.3	y = -0.0054x + 2.6283	0.7104	--	--
Nonlinear/normal	115.5	--	0.7100	--	--
Observed DT50	*ca.* ≥120	--	--	--	--
Loamy sand soil					
Linear/natural log	--[2]	--	--	--	--
Nonlinear/normal	--[2]	--	--	--	--

Phase	Half-life/DT50 [1] (days)	First order linear regression equation	r^2	DT50 (days)	DT90 (days)
Observed DT50	>120	--	--	--	--
Total system					
Linear/natural log	--[2]	--	--	--	--
Nonlinear/normal	--[2]	--	--	--	--
Observed DT50	>120	--	--	--	--

1 Determined by the primary reviewer using Excel 2000 (linear) and Sigmaplot v 8.0 (nonlinear) and individual sample data obtained from Appendix 8, p. 83; Appendix 12, p. 89 of the study report (DER Attachment 2).
2 Calculated half-life not determined due to insufficient dissipation of pyrasulfotole.
3 Determined by the study authors (p. 35; Figures 21 and 22)

TRANSFORMATION PRODUCTS: One major transformation product, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555), and one minor product (Unknown B) were detected in [phenyl-U-^{14}C]-label treated systems (p. 33). Identification of AE B197555 was confirmed via HPLC and LC/MS-ESI (p. 34; Figure 18, p. 69; Figure 20, p. 71). No major or minor products were detected in [pyrazole-3-^{14}C]-label treated systems (p. 33).

In [phenyl-U-^{14}C]-pyrasulfotole treated systems, AE B197555 was detected in the water, soil and total system at 1.4-1.9%, 7.6-7.8% and 9.0-9.7% of the applied, respectively, at 30 days posttreatment (day 0 post-flooding, DER Attachment 2). Maximum individual levels of AE B19755 detected in the water, soil and total system were 5.7% (45 days posttreatment/15 days post-flood), 7.8% (30 days posttreatment/0 days post-flood) and 10.9% (32 and 38 days posttreatment/2 and 8 days post-flood), respectively. At 150 days posttreatment (120 days post-flooding), AE B 197555 was detected at 3.6-4.6%, 4.7-5.4% and 9.0-9.3% in the water, soil and total system, respectively. One unidentified [^{14}C]component, Unknown B, was detected at maximums of 1.5%, 1.8% and 2.6% in the water, soil and total system, respectively.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: In [phenyl-U-^{14}C]-pyrasulfotole treated soil, extractable soil [^{14}C]residues decreased from 98.0-100.5% of the applied at day 0 posttreatment to 56.0-62.7% at 63-120 days posttreatment (33-90 days post-flooding) and were 61.1-64.4% at study termination (Table 5, p. 41). Nonextractable [^{14}C]residues increased from 0.6-0.9% of the applied at day 0 posttreatment to 17.7-18.4% at 30 days (day 0 post-flooding) and were 21.4-23.5% at 150 days (120 days post-flooding). At study termination, organic matter fractionation of nonextractable residues, comprising 22.5% of the applied, found 51.8%, 35.4% and 12.8% of the recovered radioactivity associated with the humin, fulvic acids and humic acids, respectively (p. 33).

In [pyrazole-3-^{14}C]-pyrasulfotole treated soil , extractable soil [^{14}C]residues decreased from 97.2-98.8% of the applied at day 0 posttreatment to 52.7-54.1% at 120 days (90 days post-flooding) and were 54.9-55.0% at study termination (Table 6, p. 42). Nonextractable [^{14}C]residues increased from 1.8-2.2% of the applied at day 0 posttreatment to 23.4-24.2% at 30 days (day 0 post-flooding) and were 23.9-26.0% at 150 days (120 days post-flooding). At study termination, organic matter

fractionation of nonextractable residues, comprising 24.9% of the applied, found 54.5%, 27.9% and 17.6% of the recovered radioactivity associated with the humin, fulvic acids and humic acids, respectively (p. 34).

VOLATILIZATION: Maximum levels of volatilized $^{14}CO_2$ (identity not confirmed) detected were 2.8% and 6.6% of the applied for the [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-label treated soils, respectively, while volatile [^{14}C]organic compounds were ≤0.1% (both labels) at all sampling intervals (Tables 5-6, pp. 41-42).

TRANSFORMATION PATHWAY: The study author provided a transformation pathway that was consistent with the products detected in this study (p. 35; Figure 23, p. 74). Under aerobic conditions, transformation of pyrasulfotole involves hydrolytic cleavage of the phenyl and pyrazole moieties to yield the benzoic acid derivative, 2-methylsulfonyl-4-trifluoromethylbenzoic acid (AE B197555) with gradual formation of bound soil residues and minimal levels of mineralization to CO_2. Under anaerobic conditions, the levels of pyrasulfotole, AE B197555 and bound residues all remained relatively constant.

Fig. 1. Proposed transformation pathway of [^{14}C] AE 0317309 in anaerobic soil.

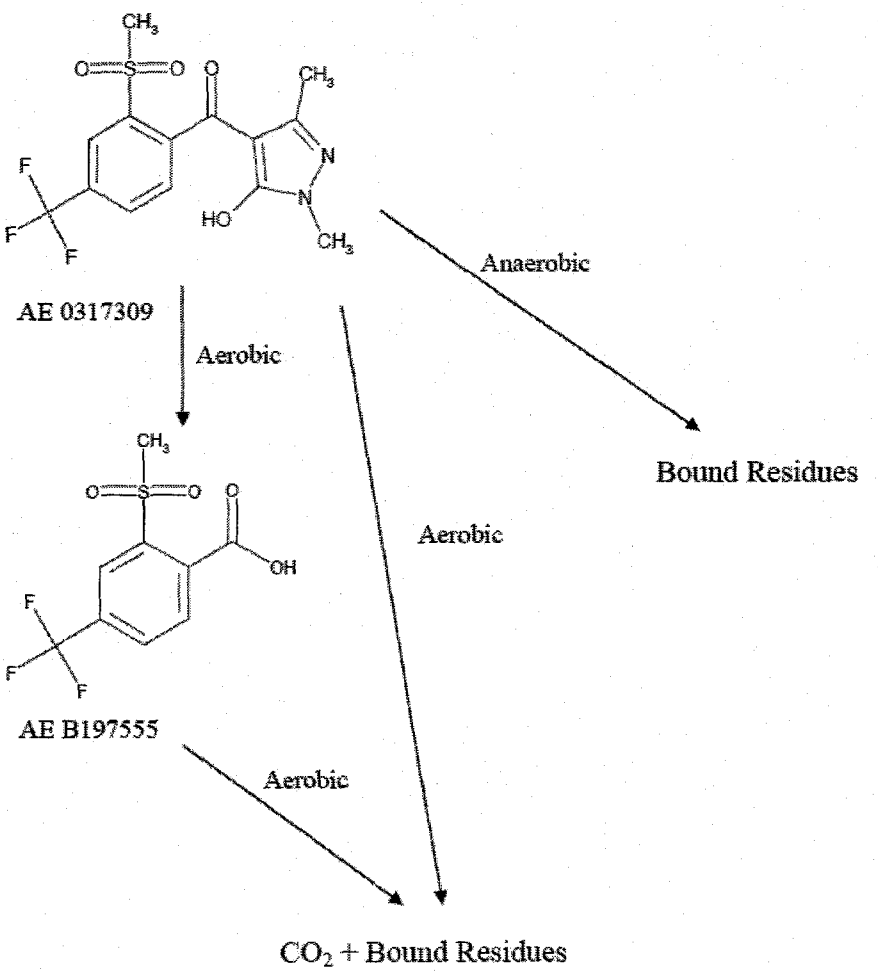


Table 8: Chemical names and CAS numbers for the transformation products of pyrasulfotole.[1]

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
AE B197555, K-1367	142994-06-07	CAS: 2-(Methylsulfonyl)-4-(trifluoromethyl)benzoic acid	--	268.21	CS(=O)(=O)c1cc(ccc1C(=O)O)C(F)(F)F

1 Identification confirmed using HPLC co-chromatography and LC/MS against reference standard (p. 34; Figure 18, p. 69; Figure 20, p. 71).
Data obtained from Figure 1, p. 48 of the study report.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Microbial biomass in untreated soil was 1.20 x 10^8 cells/g soil at study initiation (p. 31). At the study mid-point, microbial biomass was 7.8

x 10^7 cells/mL and 3.9 x 10^8 cells/g in the water and soil, respectively, and 6.2 x 10^7 cells/mL and 3.2 x 10^8 cells/g, respectively, at the study end; specific sampling intervals were not reported.

Storage stability. HPLC re-analysis found no significant quantitative differences in the chromatographic profile of a 120-day [phenyl-U-^{14}C]-label water layer sample after 126 days of frozen storage (p. 35; Figure 24, p. 75).

III. STUDY DEFICIENCIES

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

IV. REVIEWERS' COMMENTS

1. The reviewers agree with the conclusions made by the study author that AE 0317309 degraded to AE 197555 and bound residues during the aerobic phase, and that neither AE 0317309 nor AE 197555 degraded significantly during the anaerobic phase and that bound residues and volatiles did not change during the anaerobic phase.

2. 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 5-7, pp. 41-43; Table 9, p. 45) 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.

3. Actual test application rates were determined as follows:

   Phenyl-label:
   [(28.6 µCi/µmol)/(362.327 µg/µmol)] * 2.22 x 10^6 dpm/µCi = 175,234 dpm/µg (pp. 18, 22).
   (5,951,600 dpm/mL)/(175,234 dpm/µg) = 34.0 µg/mL.
   (34.0 µg/mL)*(0.099 mL) = 3.37 µg a.i.
   (3.37 µg a.i.)/50 g dry wt. soil = 0.067 µg a.i./g soil.

   Pyrazole-label:
   [(55.3 µCi/µmol)/(362.327 µg/µmol)] * 2.22 x 10^6 dpm/µCi = 338,827 dpm/µg.
   (12,037,400 dpm/mL)/(338,827 dpm/µg) = 35.5 µg/mL.
   (35.5 µg/mL)*(0.094 mL) = 3.34 µg a.i.

(3.34 µg a.i.)/50 g dry wt. soil = 0.067 µg a.i./g soil.

4. The study author reported that treated samples were taken for analysis after 0, 3, 9 and 30 days of aerobic incubation, then at 0, 2, 5, 8, 15, 33, 61, 90 and 120 days post-flooding during the anaerobic phase of the study (pp. 15, 24; Table 3, p. 39). No results were provided for the samples taken at 3, 9 and 30 days posttreatment (Tables 5-7, pp. 41-43; Table 9, p. 45; Appendix 8, p. 83; Appendix 12, p. 89).

5. The test application rate of 0.07 mg a.i./kg used in this study was based on a proposed maximum single use rate of 50 g a.i./ha (p. 17). Assuming a soil incorporation depth of 5 cm and bulk density of 1.5 g/cm3, the 50 g a.i./acre field rate converts to a test application rate of 0.07 mg a.i./kg.

6. Observed DT50 values for total residues (days post-flooding).

Phase	[Phenyl-U-^{14}C]-pyrasulfotole		[Pyrazole-3-^{14}C]-pyrasulfotole	
	Parent +nonvolatile [^{14}C]products[1]	Total [^{14}C]residues[2]	Parent +nonvolatile [^{14}C]products[1]	Total [^{14}C]residues[2]
Water	>120	>120	*ca.* ≥120	*ca.* ≥120
Soil	>120	>120	>120	>120
Total system	>120	>120	>120	>120

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.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-2, Anaerobic Soil 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.

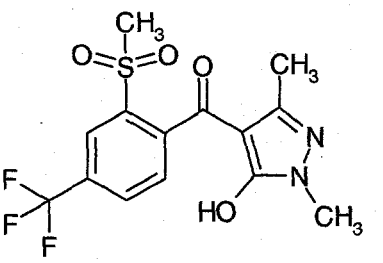
4. Wolfe, N., *et al.* 1990. Abiotic transformations in water, sediments and soil. *In* Pesticides in the Soil Environment, Soil Science Society of America, pp. 103-110.

Attachment 1: Structures of Parent Compound and Transformation Products

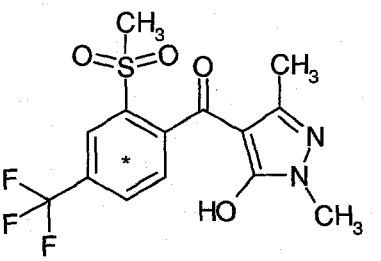
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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.

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

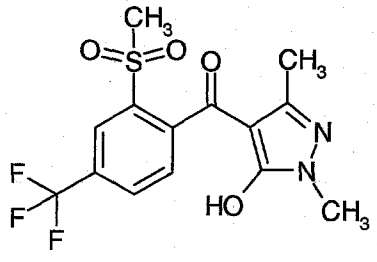
IUPAC Name: (5-Hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-*p*-tolyl)methanone.
(5-Hydroxy-1,3-dimethyl-1H-pyrazol-4-yl)(2-mesyl-4-trifluoromethylphenyl)methanone.

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].

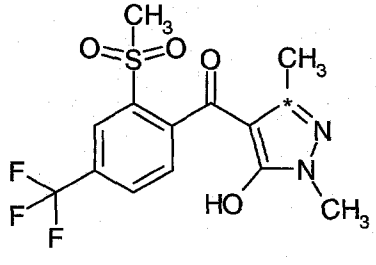
CAS Number: 365400-11-9.

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

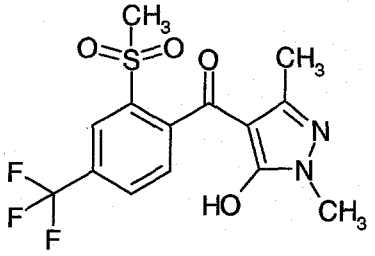


^{14}C = Position of radiolabel.

Identified Compounds

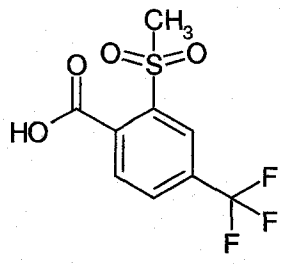
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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.



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.



Carbon Dioxide

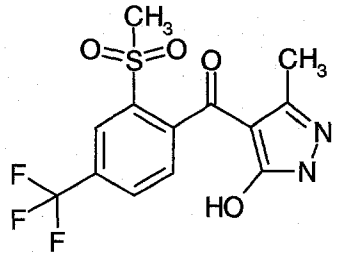
IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.

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: 46801712
Guideline: 162-2

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

North Carolina loamy sand

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

Phase	water	soil	system
Half-life (days)	138.6	ND[1]	ND
R squared	0.6811		

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

Phase	water	soil	system
Half-life (days)	90.0	ND	ND
R squared	0.9000		

Both labels

Phase	water	soil	system
Half-life (days)	115.5	ND	ND
R squared	0.7100		

[1]Calculated half-life not determined due to insufficient dissipation.

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Determination/confirmation of means/standard deviations of treated system parameters (pH, O_2 and redox potentials).

	Water layer		
Day[1]	pH	O_2 (mg/L)	Redox (mV)
30	5.2	4.1	436.5
	5.3	3.0	446.5
32	5.5	2.7	422.1
	5.5	2.3	415.6
35	5.6	1.0	374.6
	5.5	1.2	363.8
38	5.7	2.2	382.0
	5.6	2.0	383.0
45	5.5	1.1	337.5
	5.6	1.7	314.2
63	5.9	0.3	167.2
	5.8	0.2	143.9
91	5.8	0.5	187.6
	6.0	0.4	177.0
120	6.4	0.5	171.3
	6.3	0.4	199.2
150	6.3	0.1	184.6
	6.3	0.2	162.7
Mean	5.8	1.3	292.7
std.dev.	0.4	1.1	110.8
max.	6.4	4.1	446.5
min.	5.2	0.1	143.9
n =	18	18	18

Results from Table 4, p. 40 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: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.
[Phenyl-U-^{14}C]-label

	Water			Soil									CO_2			Volatile organics			Material Balance			Study Reported Material Balance		
				Amb	Aggr	Total extractable			Nonextractable															
Day[1]	% AR	Mean	s.d.	% AR	% AR	% 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				96.6	1.4	98.0			0.6									98.6			98.6		
		#####	#####	97.9	2.6	100.5	99.3	1.3	0.9	0.8	0.2		#####	#####		#####	#####	101.4	100.0	1.4	101.4	100.0	1.4
30	4.9			50.6	24.4	75.0			18.4			1.1			0.0			99.4			99.5		
	3.8	4.4	0.6	52.0	21.9	73.9	74.5	0.5	17.7	18.1	0.4	1.4	1.3	0.2	0.0	0.0	0.0	96.8	98.1	1.3	96.8	98.2	1.3
32	8.3			50.6	19.8	70.4			16.7			2.1			0.1			97.6			97.5		
	9.0	8.7	0.4	51.9	19.5	71.4	70.9	0.5	15.8	16.3	0.4	1.4	1.8	0.4	0.1	0.1	0.0	97.7	97.7	0.1	97.7	97.6	0.1
35	12.3			50.0	19.7	69.7			16.4			2.5			0.1			101.0			100.9		
	10.6	11.5	0.9	47.0	17.9	64.9	67.3	2.4	16.7	16.6	0.2	1.9	2.2	0.3	0.1	0.1	0.0	94.2	97.6	3.4	94.2	97.6	3.3
38	12.7			48.9	17.6	66.5			17.8			2.4			0.1			99.5			99.5		
	14.4	13.6	0.8	48.3	17.3	65.6	66.1	0.5	17.8	17.8	0.0	2.3	2.4	0.1	0.1	0.1	0.0	100.2	99.9	0.3	100.2	99.9	0.4
45	17.5			47.1	16.5	63.6			19.4			1.9			0.1			102.5			102.4		
	15.2	16.4	1.1	47.5	16.1	63.6	63.6	0.0	17.8	18.6	0.8	1.8	1.9	0.0	0.1	0.1	0.0	98.5	100.5	2.0	98.4	100.4	2.0
63	16.8			47.3	14.0	61.3			18.4			2.8			0.1			99.4			99.4		
	17.7	17.3	0.4	48.9	13.8	62.7	62.0	0.7	18.1	18.3	0.2	2.4	2.6	0.2	0.1	0.1	0.0	101.0	100.2	0.8	101.0	100.2	0.8
91	14.2			44.9	17.6	62.5			19.2			2.4			0.1			98.4			98.5		
	13.5	13.9	0.4	45.8	15.5	61.3	61.9	0.6	19.5	19.4	0.1	2.5	2.5	0.0	0.1	0.1	0.0	96.9	97.7	0.7	96.8	97.7	0.8
120	13.2			48.5	14.2	62.7			21.9			2.5			0.1			100.4			100.4		
	13.6	13.4	0.2	41.8	14.2	56.0	59.4	3.4	20.5	21.2	0.7	2.0	2.3	0.3	0.1	0.1	0.0	92.2	96.3	4.1	92.3	96.4	4.1
150	14.5			47.7	13.4	61.1			23.5			2.4			0.1			101.6			101.6		
	11.5	13.0	1.5	49.9	14.5	64.4	62.8	1.7	21.4	22.5	1.1	2.0	2.2	0.2	0.1	0.1	0.0	99.4	100.5	1.1	99.5	100.6	1.0
																	Overall:		98.8	2.4		98.8	2.4

[1]Days posttreatment; soil flooded at 30 days posttreatment.

Results from Table 5, p. 41 of the study report.

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

Both Phe + Pyr labels	
Mean	96.7
std. dev.	3.2
max =	102.4
min =	90.6
n =	39

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
[Phenyl-U-^{14}C]-label
Total [^{14}C]residues in soil.

Day[1]	Soil				
	Ext.	Nonext.	Total in Soil		
	% AR	% AR	% AR	Mean	s.d.
0	98.0	0.6	98.6		
	100.5	0.9	101.4	100.0	1.4
30	75.0	18.4	93.4		
	73.9	17.7	91.6	92.5	0.9
32	70.4	16.7	87.1		
	71.4	15.8	87.2	87.2	0.0
35	69.7	16.4	86.1		
	64.9	16.7	81.6	83.9	2.3
38	66.5	17.8	84.3		
	65.6	17.8	83.4	83.9	0.5
45	63.6	19.4	83.0		
	63.6	17.8	81.4	82.2	0.8
63	61.3	18.4	79.7		
	62.7	18.1	80.8	80.3	0.5
91	62.5	19.2	81.7		
	61.3	19.5	80.8	81.3	0.4
120	62.7	21.9	84.6		
	56.0	20.5	76.5	80.6	4.1
150	61.1	23.5	84.6		
	64.4	21.4	85.8	85.2	0.6

[14C]Residue water phase:soil ratios.

Day[1]	Water	Soil	Ratio	Ratio	W:S ratio		S:W ratio	
	% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
0		98.6						
		101.4						
30	4.9	93.4	0	19				
	3.8	91.6	0	24	0	0	22	3
32	8.3	87.1	0	10				
	9.0	87.2	0	10	0	0	10	0
35	12.3	86.1	0	7				
	10.6	81.6	0	8	0	0	7	0
38	12.7	84.3	0	7				
	14.4	83.4	0	6	0	0	6	0
45	17.5	83.0	0	5				
	15.2	81.4	0	5	0	0	5	0
63	16.8	79.7	0	5				
	17.7	80.8	0	5	0	0	5	0
91	14.2	81.7	0	6				
	13.5	80.8	0	6	0	0	6	0
120	13.2	84.6	0	6				
	13.6	76.5	0	6	0	0	6	0
150	14.5	84.6	0	6				
	11.5	85.8	0	7	0	0	7	1

[1]Days posttreatment; soil flooded at 30 days posttreatment.
Results imported from **Mat bal Phe** worksheet.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.
[Pyrazole-3-^{14}C]-label

	Water			Soil									CO_2			Volatile organics			Material Balance			Study Reported Material Balance		
				Amb	Aggr	Total extractable			Nonextractable															
Day[1]	% AR	Mean	s.d.	% AR	% AR	% 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				94.7	4.1	98.8			1.8									100.6			100.6		
		#####	#####	92.3	4.9	97.2	98.0	0.8	2.2	2.0	0.2		#####	#####		#####	#####	99.4	100.0	0.6	99.4	100.0	0.6
30	3.1			17.7	44.6	62.3			23.4			5.7			0.0			94.5			94.4		
	3.1	3.1	0.0	22.3	41.1	63.4	62.9	0.5	24.2	23.8	0.4	5.4	5.6	0.1	0.0	0.0	0.0	96.1	95.3	0.8	96.1	95.3	0.8
32	6.9			41.7	19.5	61.2			19.7			6.1			0.1			94.0			93.9		
	7.0	7.0	0.0	42.7	18.3	61.0	61.1	0.1	19.8	19.8	0.1	5.9	6.0	0.1	0.0	0.1	0.1	93.7	93.9	0.1	93.8	93.9	0.1
35	6.8			43.7	17.8	61.5			20.1			5.8			0.0			94.2			94.3		
	7.7	7.3	0.5	42.7	18.3	61.0	61.3	0.3	20.3	20.2	0.1	6.2	6.0	0.2	0.0	0.0	0.0	95.2	94.7	0.5	95.3	94.8	0.5
38	8.3			42.6	17.2	59.8			18.8			6.0			0.0			92.9			92.9		
	7.5	7.9	0.4	41.0	18.4	59.4	59.6	0.2	18.0	18.4	0.4	6.1	6.1	0.0	0.0	0.0	0.0	91.0	92.0	1.0	91.2	92.1	0.8
45	9.5			41.6	16.6	58.2			22.7			6.4			0.0			96.8			96.8		
	10.3	9.9	0.4	40.0	17.2	57.2	57.7	0.5	21.7	22.2	0.5	6.1	6.3	0.2	0.0	0.0	0.0	95.3	96.1	0.7	95.3	96.1	0.8
63	14.2			39.4	14.4	53.8			21.2			6.3			0.0			95.5			95.6		
		14.2	0.0	39.9	14.7	54.6	54.2	0.4	22.6	21.9	0.7	5.5	5.9	0.4	0.0	0.0	0.0		95.5	0.0		95.6	0.0
91	9.2			41.1	14.0	55.1			22.4			6.3			0.1			93.1			93.0		
	11.3	10.3	1.1	40.6	13.3	53.9	54.5	0.6	21.2	21.8	0.6	6.6	6.5	0.2	0.0	0.1	0.1	93.0	93.1	0.0	93.1	93.1	0.0
120	8.8			38.7	13.9	52.6			24.0			5.0			0.0			90.4			90.6		
	8.8	8.8	0.0	39.0	15.2	54.2	53.4	0.8	24.3	24.2	0.2	5.5	5.3	0.3	0.0	0.0	0.0	92.8	91.6	1.2	92.7	91.7	1.0
150	7.1			40.8	14.2	55.0			26.0			6.6			0.1			94.8			94.7		
	7.3	7.2	0.1	41.5	13.6	55.1	55.1	0.1	23.9	25.0	1.1	6.6	6.6	0.0	0.1	0.1	0.0	93.0	93.9	0.9	92.9	93.8	0.9
																	Overall:		94.5	2.4		94.6	2.4

[1]Days posttreatment; soil flooded at 30 days posttreatment.

Results from Table 6, p. 42 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: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
[Pyrazole-3-^{14}C]-label
Total [^{14}C]residues in soil.

Day[1]	Soil				
	Ext.	Nonext.	Total in Soil		
	% AR	% AR	% AR	Mean	s.d.
0	98.8	1.8	100.6		
	97.2	2.2	99.4	100.0	0.6
30	62.3	23.4	85.7		
	63.4	24.2	87.6	86.7	0.9
32	61.2	19.7	80.9		
	61.0	19.8	80.8	80.9	0.1
35	61.5	20.1	81.6		
	61.0	20.3	81.3	81.5	0.1
38	59.8	18.8	78.6		
	59.4	18.0	77.4	78.0	0.6
45	58.2	22.7	80.9		
	57.2	21.7	78.9	79.9	1.0
63	53.8	21.2	75.0		
	54.6	22.6	77.2	76.1	1.1
91	55.1	22.4	77.5		
	53.9	21.2	75.1	76.3	1.2
120	52.6	24.0	76.6		
	54.2	24.3	78.5	77.6	1.0
150	55.0	26.0	81.0		
	55.1	23.9	79.0	80.0	1.0

[14C]Residue water phase:soil ratios.

Day[1]	Water	Soil	Ratio	Ratio	W:S ratio		S:W ratio	
	% AR	% AR	W:S	S:W	Mean	s.d.	Mean	s.d.
0		100.6						
		99.4						
30	3.1	85.7	0	28				
	3.1	87.6	0	28	0	0	28	0
32	6.9	80.9	0	12				
	7.0	80.8	0	12	0	0	12	0
35	6.8	81.6	0	12				
	7.7	81.3	0	11	0	0	11	1
38	8.3	78.6	0	9				
	7.5	77.4	0	10	0	0	10	0
45	9.5	80.9	0	9				
	10.3	78.9	0	8	0	0	8	0
63	14.2	75.0	0	5				
					0	0	5	0
91	9.2	77.5	0	8				
	11.3	75.1	0	7	0	0	8	1
120	8.8	76.6	0	9				
	8.8	78.5	0	9	0	0	9	0
150	7.1	81.0	0	11				
	7.3	79.0	0	11	0	0	11	0

[1]Days posttreatment; soil flooded at 30 days posttreatment.
Results imported from **Mat bal Pyr** worksheet.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Confirmation/determination of means/std.dev. for pyrasulfotole and its transformation products.
[Phenyl-U-^{14}C]-label

	Pyrasulfotole									AE B197555									Unknown B								
	Water			Soil			Total system			Water			Soil			Total system			Water			Soil			Total system		
Day[1]	% 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.	% AR	mean	s.d.	% AR	mean	s.d.
0				96.6			96.6						0.0			0.0						0.0			0.0		
		#####	#####	97.9	97.3	0.7	97.9	97.3	0.7		#####	#####	0.0	0.0	0.0	0.0	0.0	0.0		#####	#####	0.0	0.0	0.0	0.0	0.0	0.0
30	3.1			67.2			70.3			1.9			7.8			9.7			0.0			0.0			0.0		
	1.7	2.4	0.7	64.7	66.0	1.3	66.4	68.4	2.0	1.4	1.7	0.3	7.6	7.7	0.1	9.0	9.4	0.3	0.7	0.4	0.4	1.5	0.8	0.8	2.2	1.1	1.1
32	5.0			64.8			69.8			2.7			5.6			8.3			0.7			0.0			0.7		
	5.0	5.0	0.0	62.0	63.4	1.4	67.0	68.4	1.4	3.3	3.0	0.3	7.6	6.6	1.0	10.9	9.6	1.3	0.7	0.7	0.0	1.8	0.9	0.9	2.5	1.6	0.9
35	8.5			63.9			72.4			3.8			5.8			9.6			0.0			0.0			0.0		
	6.6	7.6	1.0	59.1	61.5	2.4	65.7	69.1	3.3	4.0	3.9	0.1	5.7	5.8	0.0	9.7	9.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
38	9.2			62.7			71.9			3.5			3.8			7.3			0.0			0.0			0.0		
	10.2	9.7	0.5	59.0	60.9	1.9	69.2	70.6	1.3	4.2	3.9	0.3	6.7	5.3	1.5	10.9	9.1	1.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
45	11.8			58.7			70.5			5.7			4.9			10.6			0.0			0.0			0.0		
	10.7	11.3	0.5	58.8	58.8	0.0	69.5	70.0	0.5	4.5	5.1	0.6	4.7	4.8	0.1	9.2	9.9	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
63	11.2			56.3			67.5			4.1			5.0			9.1			1.5			0.0			1.5		
	12.2	11.7	0.5	57.8	57.1	0.7	70.0	68.8	1.3	4.4	4.3	0.2	4.9	5.0	0.0	9.3	9.2	0.1	1.1	1.3	0.2	0.0	0.0	0.0	1.1	1.3	0.2
91	8.4			55.3			63.7			4.5			6.2			10.7			1.3			1.0			2.3		
	8.0	8.2	0.2	56.0	55.7	0.4	64.0	63.9	0.2	5.1	4.8	0.3	4.0	5.1	1.1	9.1	9.9	0.8	0.4	0.9	0.5	1.2	1.1	0.1	1.6	2.0	0.4
120	8.2			55.2			63.4			3.9			6.1			10.0			1.1			1.5			2.6		
	8.2	8.2	0.0	51.4	53.3	1.9	59.6	61.5	1.9	4.4	4.2	0.2	4.6	5.4	0.8	9.0	9.5	0.5	1.0	1.1	0.0	0.0	0.8	0.8	1.0	1.8	0.8
150	8.5			55.2			63.7			4.6			4.7			9.3			1.4			1.2			2.6		
	6.8	7.7	0.8	57.7	56.5	1.3	64.5	64.1	0.4	3.6	4.1	0.5	5.4	5.1	0.3	9.0	9.2	0.1	1.2	1.3	0.1	1.3	1.3	0.0	2.5	2.6	0.0

[1]Days posttreatment; soil flooded at 30 days posttreatment.
Results from Appendix 8, p. 83 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: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Confirmation/determination of means/std.dev. for pyrasulfotole and its transformation products.
[Pyrazole-3-^{14}C]-label

	Pyrasulfotole								
	Water			Soil			Total system		
Day[1]	% AR	mean	s.d.	% AR	mean	s.d.	% AR	mean	s.d.
0				94.7			94.7		
		#####	#####	92.3	93.5	1.2	92.3	93.5	1.2
30	3.1			62.3			65.4		
	3.1	3.1	0.0	63.4	62.9	0.6	66.5	66.0	0.6
32	6.9			61.2			68.1		
	7.0	7.0	0.0	61.1	61.2	0.1	68.1	68.1	0.0
35	6.8			61.6			68.4		
	7.7	7.3	0.5	61.0	61.3	0.3	68.7	68.6	0.1
38	8.3			59.8			68.1		
	7.5	7.9	0.4	59.4	59.6	0.2	66.9	67.5	0.6
45	9.5			58.2			67.7		
	10.3	9.9	0.4	57.2	57.7	0.5	67.5	67.6	0.1
63	14.2			53.8			68.0		
		14.2	0.0	54.6	54.2	0.4		68.0	0.0
91	9.2			55.0			64.2		
	11.3	10.3	1.1	53.9	54.5	0.5	65.2	64.7	0.5
120	8.8			52.7			61.5		
	8.8	8.8	0.0	54.1	53.4	0.7	62.9	62.2	0.7
150	7.1			54.9			62.0		
	7.3	7.2	0.1	55.0	55.0	0.1	62.3	62.2	0.1

[1]Days posttreatment; soil flooded at 30 days posttreatment.
Results from Appendix 12, p. 89 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: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Determination of unidentified [^{14}C] following HPLC analyses.
[Phenyl-U-^{14}C]-label

	Water							Soil extract							Total system						
	Tot	Pyr	AE B197555	B	Unassigned [^{14}C]			Tot	Pyr	AE B197555	B	Unassigned [^{14}C]			Tot	Pyr	AE B197555	B	Unassigned [^{14}C]		
Day	% AR	% AR	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	% AR	% AR	mean	s.d.
0					0.0			98.0	96.6	0.0	0.0	1.4			98.0	96.6	0.0	0.0	1.4		
					0.0	0.0	0.0	100.5	97.9	0.0	0.0	2.6	2.0	0.6	100.5	97.9	0.0	0.0	2.6	2.0	0.6
30	4.9	3.1	1.9	0.0	-0.1			75.0	67.2	7.8	0.0	0.0			79.9	70.3	9.7	0.0	-0.1		
	3.8	1.7	1.4	0.7	0.0	0.0	0.0	73.9	64.7	7.6	1.5	0.1	0.1	0.1	77.7	66.4	9.0	2.2	0.1	0.0	0.1
32	8.3	5.0	2.7	0.7	-0.1			70.4	64.8	5.6	0.0	0.0			78.7	69.8	8.3	0.7	-0.1		
	9.0	5.0	3.3	0.7	0.0	0.0	0.0	71.4	62.0	7.6	1.8	0.0	0.0	0.0	80.4	67.0	10.9	2.5	0.0	0.0	0.1
35	12.3	8.5	3.8	0.0	0.0			69.7	63.9	5.8	0.0	0.0			82.0	72.4	9.6	0.0	0.0		
	10.6	6.6	4.0	0.0	0.0	0.0	0.0	64.9	59.1	5.7	0.0	0.1	0.1	0.0	75.5	65.7	9.7	0.0	0.1	0.0	0.1
38	12.7	9.2	3.5	0.0	0.0			66.5	62.7	3.8	0.0	0.0			79.2	71.9	7.3	0.0	0.0		
	14.4	10.2	4.2	0.0	0.0	0.0	0.0	65.6	59.0	6.7	0.0	-0.1	-0.1	0.1	80.0	69.2	10.9	0.0	-0.1	-0.1	0.1
45	17.5	11.8	5.7	0.0	0.0			63.6	58.7	4.9	0.0	0.0			81.1	70.5	10.6	0.0	0.0		
	15.2	10.7	4.5	0.0	0.0	0.0	0.0	63.6	58.8	4.7	0.0	0.1	0.1	0.1	78.8	69.5	9.2	0.0	0.1	0.0	0.1
63	16.8	11.2	4.1	1.5	0.0			61.3	56.3	5.0	0.0	0.0			78.1	67.5	9.1	1.5	0.0		
	17.7	12.2	4.4	1.1	0.0	0.0	0.0	62.7	57.8	4.9	0.0	0.0	0.0	0.0	80.4	70.0	9.3	1.1	0.0	0.0	0.0
91	14.2	8.4	4.5	1.3	0.0			62.5	55.3	6.2	1.0	0.0			76.7	63.7	10.7	2.3	0.0		
	13.5	8.0	5.1	0.4	0.0	0.0	0.0	61.3	56.0	4.0	1.2	0.1	0.0	0.0	74.8	64.0	9.1	1.6	0.1	0.0	0.0
120	13.2	8.2	3.9	1.1	0.0			62.7	55.2	6.1	1.5	-0.1			75.9	63.4	10.0	2.6	-0.1		
	13.6	8.2	4.4	1.0	0.0	0.0	0.0	56.0	51.4	4.6	0.0	0.0	0.0	0.1	69.6	59.6	9.0	1.0	0.0	-0.1	0.0
150	14.5	8.5	4.6	1.4	0.0			61.1	55.2	4.7	1.2	0.0			75.6	63.7	9.3	2.6	0.0		
	11.5	6.8	3.6	1.2	-0.1	0.0	0.0	64.4	57.7	5.4	1.3	0.0	0.0	0.0	75.9	64.5	9.0	2.5	-0.1	-0.1	0.0

Tot = total initial radioactivity associated with water layer or sediment extract.
Results imported from **Mat bal Phe** and **Profile Phe** worksheets.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Determination of unidentified [^{14}C] following HPLC analyses.
[Pyrazole-3-^{14}C]-label

	Water					Soil extract					Total system				
	Tot	Pyr	Unassigned [^{14}C]			Tot	Pyr	Unassigned [^{14}C]			Tot	Pyr	Unassigned [^{14}C]		
Day	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	mean	s.d.	% AR	% AR	% AR	mean	s.d.
0			0.0			98.8	94.7	4.1			98.8	94.7	4.1		
			0.0	0.0	0.0	97.2	92.3	4.9	4.5	0.4	97.2	92.3	4.9	4.5	0.4
30	3.1	3.1	0.0			62.3	62.3	0.0			65.4	65.4	0.0		
	3.1	3.1	0.0	0.0	0.0	63.4	63.4	0.0	0.0	0.0	66.5	66.5	0.0	0.0	0.0
32	6.9	6.9	0.0			61.2	61.2	0.0			68.1	68.1	0.0		
	7.0	7.0	0.0	0.0	0.0	61.0	61.1	-0.1	-0.1	0.1	68.0	68.1	-0.1	0.0	0.0
35	6.8	6.8	0.0			61.5	61.6	-0.1			68.3	68.4	-0.1		
	7.7	7.7	0.0	0.0	0.0	61.0	61.0	0.0	-0.1	0.1	68.7	68.7	0.0	-0.1	0.1
38	8.3	8.3	0.0			59.8	59.8	0.0			68.1	68.1	0.0		
	7.5	7.5	0.0	0.0	0.0	59.4	59.4	0.0	0.0	0.0	66.9	66.9	0.0	0.0	0.0
45	9.5	9.5	0.0			58.2	58.2	0.0			67.7	67.7	0.0		
	10.3	10.3	0.0	0.0	0.0	57.2	57.2	0.0	0.0	0.0	67.5	67.5	0.0	0.0	0.0
63	14.2	14.2	0.0			53.8	53.8	0.0			68.0	68.0	0.0		
			0.0	0.0	0.0	54.6	54.6	0.0	0.0	0.0	54.6	54.6	0.0	0.0	0.0
91	9.2	9.2	0.0			55.1	55.0	0.1			64.3	64.2	0.1		
	11.3	11.3	0.0	0.0	0.0	53.9	53.9	0.0	0.1	0.1	65.2	65.2	0.0	0.0	0.0
120	8.8	8.8	0.0			52.6	52.7	-0.1			61.4	61.5	-0.1		
	8.8	8.8	0.0	0.0	0.0	54.2	54.1	0.1	0.0	0.1	63.0	62.9	0.1	0.0	0.1
150	7.1	7.1	0.0			55.0	54.9	0.1			62.1	62.0	0.1		
	7.3	7.3	0.0	0.0	0.0	55.1	55.0	0.1	0.1	0.0	62.4	62.3	0.1	0.1	0.0

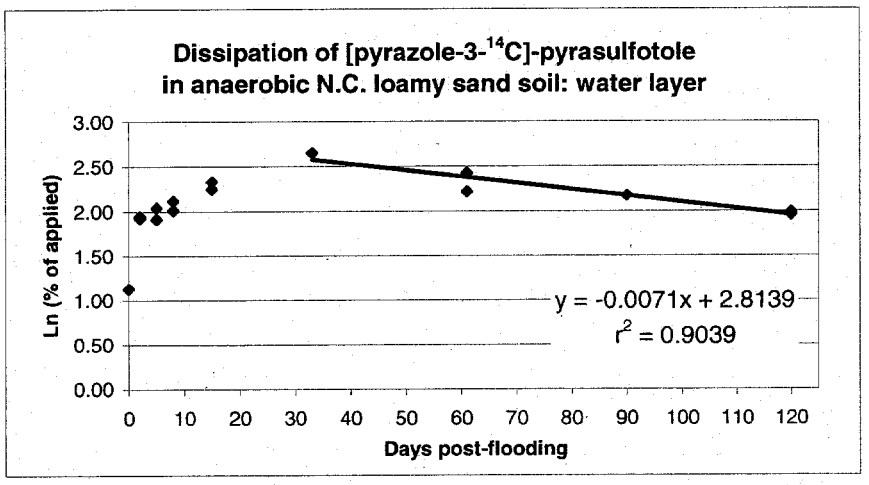
Tot = total initial radioactivity associated with water layer or sediment extract.
Results imported from **Mat bal Pyr** and **Profile Pyr** worksheets.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Half-life determination
[Pyrazole-3-^{14}C]-label/water layer
Half-life (days) 97.1 (33- to 120-day data)

Days Post-flooding	Pyrasolfotole (% of Applied)	Ln (% applied)
0	3.1	1.131402111
0	3.1	1.131402111
2	6.9	1.931521412
2	7.0	1.945910149
5	6.8	1.916922612
5	7.7	2.041220329
8	8.3	2.116255515
8	7.5	2.014903021
15	9.5	2.251291799
15	10.3	2.332143895
33	14.2	2.653241965
61	9.2	2.219203484
61	11.3	2.424802726
90	8.8	2.174751721
90	8.8	2.174751721
120	7.1	1.960094784
120	7.3	1.987874348

Results from Appendix 12, p. 89 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.950744489
R Square	0.903915084
Adjusted R Square	0.884698101
Standard Error	0.082565728
Observations	7

ANOVA

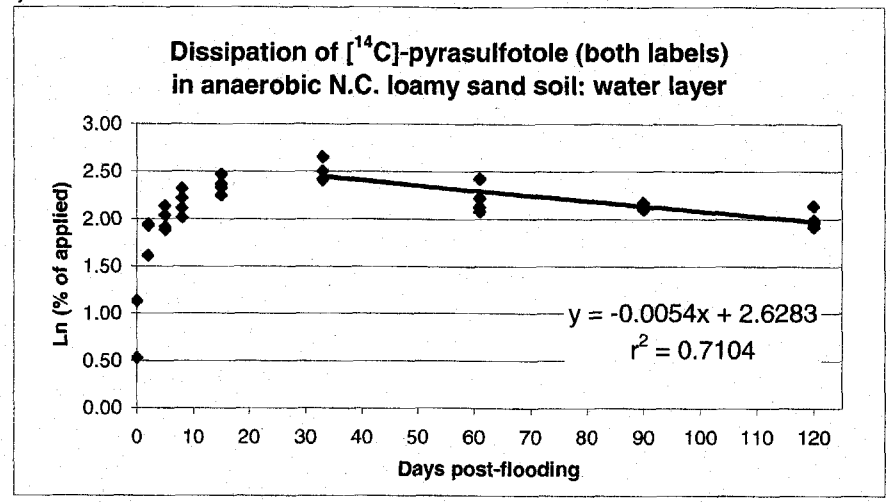
	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.320657981	0.32066	47.03730409	0.001007
Residual	5	0.034085497	0.00682		
Total	6	0.354743478			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.813901367	0.090975111	30.9305	6.63011E-07	2.5800428	3.04776	2.58004278	3.04775995
X Variable 1	-0.007134937	0.001040325	-6.8584	0.00100701	-0.009809	-0.0044607	-0.0098092	-0.0044607

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Half-life determination
[Phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labels/water layer
Half-life (days) 127.3 (33- to 120-day data)

	Pyrasulfotole		
Days Post.	Label	(% of Applied)	Ln (% applied)
0	phe	3.1	1.131402111
0	phe	1.7	0.530628251
0	pyr	3.1	1.131402111
0	pyr	3.1	1.131402111
2	phe	5.0	1.609437912
2	phe	5.0	1.609437912
2	pyr	6.9	1.931521412
2	pyr	7.0	1.945910149
5	phe	8.5	2.140066163
5	phe	6.6	1.887069649
5	pyr	6.8	1.916922612
5	pyr	7.7	2.041220329
8	phe	9.2	2.219203484
8	phe	10.2	2.32238772
8	pyr	8.3	2.116255515
8	pyr	7.5	2.014903021
15	phe	11.8	2.468099531
15	phe	10.7	2.370243741
15	pyr	9.5	2.251291799
15	pyr	10.3	2.332143895
33	phe	11.2	2.415913778
33	phe	12.2	2.501435952
33	pyr	14.2	2.653241965
61	phe	8.4	2.128231706
61	phe	8.0	2.079441542
61	pyr	9.2	2.219203484
61	pyr	11.3	2.424802726
90	phe	8.2	2.104134154
90	phe	8.2	2.104134154
90	pyr	8.8	2.174751721
90	pyr	8.8	2.174751721
120	phe	8.5	2.140066163
120	phe	6.8	1.916922612
120	pyr	7.1	1.960094784
120	pyr	7.3	1.987874348



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.84284854
R Square	0.710393661
Adjusted R Square	0.68811625
Standard Error	0.117469259
Observations	15

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.440030543	0.44003	31.88852017	7.97E-05
Residual	13	0.179387348	0.0138		
Total	14	0.619417891			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.628285659	0.081847477	32.112	9.06927E-14	2.451465	2.8051063	2.45146497	2.80510635
X Variable 1	-0.00544318	0.000963908	-5.647	7.96986E-05	-0.007526	-0.0033608	-0.0075256	-0.0033608

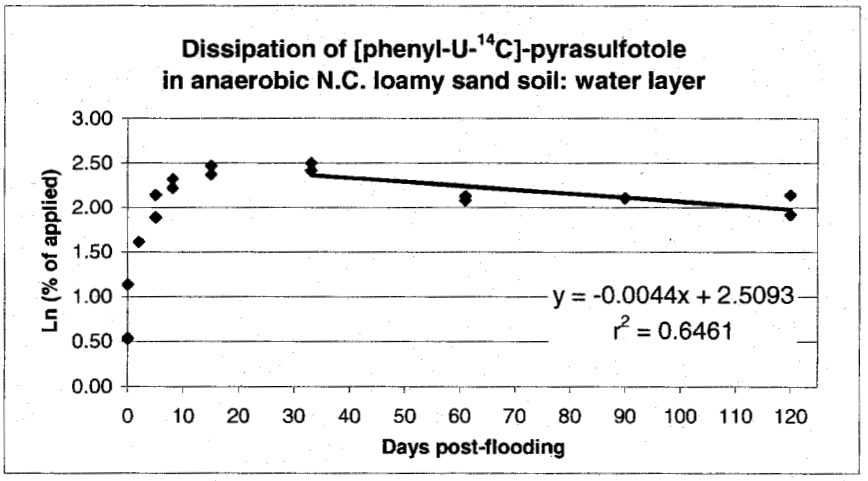
Results from Appendix 8, p. 83; Appendix 12, p. 89 of the study report.

Chemical: Pyrasulfotole (AE 0317309)
PC: 000692
MRID: 46801712
Guideline: 162-2

Anaerobic metabolism of [^{14}C]pyrasulfotole in a North Carolina loamy sand soil.
Half-life determination
[Phenyl-U-^{14}C]-label/water layer
Half-life (days) 157.0 (33- to 120-day data)

	Pyrasolfotole	
Days Post-flooding	(% of Applied)	Ln (% applied)
0	3.1	1.131402111
0	1.7	0.530628251
2	5.0	1.609437912
2	5.0	1.609437912
5	8.5	2.140066163
5	6.6	1.887069649
8	9.2	2.219203484
8	10.2	2.32238772
15	11.8	2.468099531
15	10.7	2.370243741
33	11.2	2.415913778
33	12.2	2.501435952
61	8.4	2.128231706
61	8.0	2.079441542
90	8.2	2.104134154
90	8.2	2.104134154
120	8.5	2.140066163
120	6.8	1.916922612

Results from Appendix 8, p. 83 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.803790721
R Square	0.646079522
Adjusted R Square	0.587092776
Standard Error	0.122349344
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.163958837	0.16396	10.95296085	0.0162143
Residual	6	0.089816172	0.01497		
Total	7	0.253775009			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	2.509315021	0.110225701	22.7652	4.70485E-07	2.2396023	2.7790278	2.23960225	2.77902779
X Variable 1	-0.004414869	0.001333988	-3.3095	0.016214311	-0.007679	-0.0011507	-0.007679	-0.00115071