Data Evaluation Report on the adsorption-desorption of pyrasulfotole (AE 0317309) in soil

PMRA Submission Number 2006-2445 EPA MRID Number 46801703

Data Requirement: PMRA Data Code: 8.2.4.2
EPA DP Barcode: D328639
OECD Data Point: IIA 7.4.1
EPA Guideline: §163-1

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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CITATION: Maurer, T., U. Eyrich, and R. Fliege. 2003. Adsorption/desorption of AE 0317309 on five soils and one sediment. Unpublished study performed by Bayer CropScience GmbH, Franfurt am Main, Germany; sponsored and submitted by Bayer CropScience, USA. Laboratory Project ID CP 02/014. Study start date July 09, 2002, and completion date October 31, 2002 (p. 6). Final report issued September 26, 2003.

EXECUTIVE SUMMARY

The adsorption/desorption characteristics of [pyrazole-3-^{14}C]-labeled (5-hydroxy-1,3-dimethylpyrazol-4-yl)(α,α,α-trifluoro-2-mesyl-ρ-tolyl)methanone. (pyrasulfotole; AE 0317309) were studied in definitive experiments using three US soils: a silt loam [HCB, pH 7.7, organic carbon 4.7%], a loamy sand [Pikeville, pH 6.4, organic carbon 1.2%], and a silt loam [Carlyle, pH 5.2, organic carbon 1.5%]; two German soils: a clay loam [CL6S, pH 7.5, organic carbon 1.7%] and a sandy loam [SL2.3, pH 6.7, organic carbon 1.1%]; and a German sandy loam sediment [Nidda, pH 5.8, organic carbon 4.6%], in a batch equilibrium experiment. The experiment was conducted in accordance with the USEPA Guidelines for Pesticides Registration, Subdivision N §163-1, and in compliance with OECD Good Laboratory Practices. The adsorption phase of the study was carried out by equilibrating air-dried soils with [pyrazole-3-^{14}C]pyrasulfotole at actual test concentrations of *ca.* 0.0057, 0.0124, 0.0418, 0.1235, and 0.4275 mg a.i./kg soil for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam soils; *ca.* 0.0285, 0.0618, 0.209, 0.6175, and 2.1375 mg a.i./kg soil for the Carlyle silt loam soil; and *ca.* 0.114, 0.247, 0.836, 2.47, and 8.55 mg a.i./kg soil for the Nidda sandy loam sediment. The samples were shaken in the dark at ambient temperature for 24 hours. The equilibrating solution used was 0.01M $CaCl_2$ solution, with soil/solution ratios ranging from 1:1 to 20 (w:v) for all test soils. The desorption phase of the study was carried out by replacing the adsorption solution with an equivalent volume of pesticide-free 0.01M $CaCl_2$ solution and equilibrating in the dark at ambient temperature for 24 hours. For all test soils, two desorption cycles were conducted for the desorption phase.

The supernatant after adsorption and desorption was separated by centrifugation, and aliquots were analyzed for total radioactivity using LSC. Following the second desorption cycle, the soils were homogenized and analyzed for total radioactivity using LSC following combustion. Samples were not analyzed for pyrasulfotole or its transformation products.

The incubation temperature during the study was maintained at ambient temperature; no supporting information was provided. The pH values of the supernatant solutions during the adsorption and desorption phases were not reported. LSC analysis of application control samples without soil (three samples per soil type and test concentration), concurrently run with each definitive test series, verified application accuracy and lack of test material adsorption to the glass test containers; >98% of the applied radioactivity was recovered in the application control solutions.

Mass balances at the end of the adsorption phase were not reported. Mean mass balances at the end of the desorption phase averaged 95.3% (range 93.3-97.3%), 96.6% (range 93.9-99.3%), 95.0% (range 93.6-96.3%), 98.5% (range 98.3-98.7%), 98.8% (range 98.7-99.0%), and 100.6% (range 100.4-100.7%) of the applied for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively.

After 24 hours of equilibration, 55.7-63.3%, 60.3-71.0%, 26.4-32.3%, 30.1-35.2%, 43.9-52.2%, and 50.4-73.5% of the applied [^{14}C]pyrasulfotole was adsorbed to the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively (reviewer-calculated). Registrant-calculated adsorption K_d values averaged 1.32, 1.77, 0.367, 0.47, 4.25, and 32.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding adsorption K_{oc} values averaged 28.1, 148, 21.6, 42.7, 283, and 715. Registrant-calculated Freundlich adsorption K_F values were 0.980, 1.20, 0.341, 0.386, 3.20, and 15.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding Freundlich adsorption K_{Foc} values were 20.8, 100, 20.0, 35.1, 213, and 345. At the end of the desorption phase, 55.0%, 49.7%, 70.4% 69.0% 65.6%, and 61.1% of the applied [pyrazole-3-^{14}C]pyrasulfotole desorbed from the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively (reviewer-calculated). Registrant-calculated desorption K_d values averaged 2.26, 3.67, 0.923, 1.51, 10.4, and 56.6 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding adsorption K_{oc} values averaged 48.2, 306, 54.3, 137, 696, and 1230. Registrant-calculated Freundlich desorption K_F values were 1.37, 2.30, 0.678, 1.13, 8.46, and 30.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding Freundlich desorption K_{Foc} values were 29.2, 192, 40, 103, 564, and 672.

Adsorption coefficients were re-calculated by the secondary reviewer using slopes of adsorption isotherms rather than mean coefficients. $K_{d\text{-}ads}$ values were 1.12, 1.37, 0.37, 0.42, 3.46 and 18.2 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding $K_{OC\text{-}ads}$ values were 24, 114, 22, 38, 231 and 395, respectively. Freundlich regressions gave $K_{F\text{-}ads}$ values of 0.98, 1.20, 0.34, 0.39, 3.20 and 15.9 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding $K_{FOC\text{-}ads}$ values were 21, 100, 20, 35, 214 and 346, respectively. Based on the $K_{OC\text{-}ads}$ values and the mobility classification of McCall *et al.* (1981), pyrasulfotole is expected to exhibit moderate to very high mobility in the range of soils studied. Pyrasulfotole mobility tended to increase with increasing pH, with pyrasulfotole showing the greatest mobility at neutral soil pH levels

Desorption coefficients were similarly re-calculated by the secondary reviewer using slopes of desorption isotherms. Desorption isotherms were based on consecutive desorption through two cycles from the highest test concentration only. Consecutive desorption $K_{d\text{-}des}$ values were 0.76, 0.75, 0.15, 0.25, 2.40 and 12.7 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding $K_{OC\text{-}des}$ values were 16, 63, 9, 23, 160 and 276, respectively. Freundlich regressions gave $K_{F\text{-}des}$ values of 0.55, 0.51, 0.17, 0.20, 1.76 and 9.21 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the

Nidda sandy loam sediment, respectively; corresponding $K_{FOC\text{-}des}$ values were 12, 42, 10, 18, 117 and 200, respectively. After two desorption cycles, $K_{OC\text{-}des}$ values remained very similar to $K_{OC\text{-}ads}$ values, indicating that pyrasulfotole remains relatively strongly bound to soils after initial adsorption.

Results Synopsis:

Soil type: **HCB Silt loam**

Amount adsorbed:	55.7-63.3% of the applied.
Adsorption K_d:	1.32
Adsorption K_{oc}:	28.1
Freundlich adsorption K_F:	0.980
Freundlich adsorption K_{Foc}:	20.8
Amount desorbed:	55.0% of the adsorbed (high-dose soils only).
Desorption K_d:	2.26
Desorption K_{oc}:	48.2
Freundlich desorption K_F:	1.37
Freundlich desorption K_{Foc}:	29.2

Soil type: **Pikeville Loamy sand**

Amount adsorbed:	60.3-71.0% of the applied.
Adsorption K_d:	1.77
Adsorption K_{oc}:	148
Freundlich adsorption K_F:	1.20
Freundlich adsorption K_{Foc}:	100
Amount desorbed:	49.7% of the adsorbed (high-dose soils only).
Desorption K_d:	3.67
Desorption K_{oc}:	306
Freundlich desorption K_F:	2.30
Freundlich desorption K_{Foc}:	192

Soil type: **CL6S Clay loam**

Amount adsorbed:	26.4-32.3% of the applied.
Adsorption K_d:	0.367
Adsorption K_{oc}:	21.6
Freundlich adsorption K_F:	0.341
Freundlich adsorption K_{Foc}:	20.0
Amount desorbed:	70.4% of the adsorbed (high-dose soils only).
Desorption K_d:	0.923
Desorption K_{oc}:	54.3
Freundlich desorption K_F:	0.678
Freundlich desorption K_{Foc}:	40

Soil type: **SL2.3 Sandy loam**

Amount adsorbed:	30.1-35.2% of the applied.
Adsorption K_d:	0.47
Adsorption K_{oc}:	42.7
Freundlich adsorption K_F:	0.386
Freundlich adsorption K_{Foc}:	35.1
Amount desorbed:	69.0% of the adsorbed (high-dose soils only).
Desorption K_d:	1.51
Desorption K_{oc}:	137
Freundlich desorption K_F:	1.13
Freundlich desorption K_{Foc}:	103

Soil type: **Carlyle Silt loam**

Amount adsorbed:	43.9-52.2% of the applied.
Adsorption K_d:	4.25
Adsorption K_{oc}:	283
Freundlich adsorption K_F:	3.20
Freundlich adsorption K_{Foc}:	213
Amount desorbed:	65.6% of the adsorbed (high-dose soils only).
Desorption K_d:	10.4
Desorption K_{oc}:	696
Freundlich desorption K_F:	8.46
Freundlich desorption K_{Foc}:	564

Soil type: **Nidda Sandy loam**

Amount adsorbed:	50.4-73.5% of the applied.
Adsorption K_d:	32.86
Adsorption K_{oc}:	715
Freundlich adsorption K_F:	15.9
Freundlich adsorption K_{Foc}:	345
Amount desorbed:	61.1% of the adsorbed (high-dose soils only).
Desorption K_d:	56.59
Desorption K_{oc}:	1230
Freundlich desorption K_F:	30.9
Freundlich desorption K_{Foc}:	672

PMRA Results Synopsis:

Soil type: **HCB Silt loam**

Amount adsorbed:	55.7-63.3% of the applied.
Adsorption K_d:	1.12
Adsorption K_{oc}:	24
Freundlich adsorption K_F:	0.98
Freundlich adsorption K_{Foc}:	21
Mobility classification:	Very high

Amount desorbed: 55.0% of the adsorbed (high-dose soils only).
Desorption K_d: 0.76
Desorption K_{oc}: 16
Freundlich desorption K_F: 0.55
Freundlich desorption K_{Foc}: 12

Soil type: **Pikeville Loamy sand**
Amount adsorbed: 60.3-71.0% of the applied.
Adsorption K_d: 1.37
Adsorption K_{oc}: 114
Freundlich adsorption K_F: 1.20
Freundlich adsorption K_{Foc}: 100
Mobility classification: High
Amount desorbed: 49.7% of the adsorbed (high-dose soils only).
Desorption K_d: 0.75
Desorption K_{oc}: 63
Freundlich desorption K_F: 0.51
Freundlich desorption K_{Foc}: 42

Soil type: **CL6S Clay loam**
Amount adsorbed: 26.4-32.3% of the applied.
Adsorption K_d: 0.37
Adsorption K_{oc}: 22
Freundlich adsorption K_F: 0.34
Freundlich adsorption K_{Foc}: 20
Mobility classification: Very high
Amount desorbed: 70.4% of the adsorbed (high-dose soils only).
Desorption K_d: 0.15
Desorption K_{oc}: 9
Freundlich desorption K_F: 0.17
Freundlich desorption K_{Foc}: 10

Soil type: **SL2.3 Sandy loam**
Amount adsorbed: 30.1-35.2% of the applied.
Adsorption K_d: 0.42
Adsorption K_{oc}: 38
Freundlich adsorption K_F: 0.39
Freundlich adsorption K_{Foc}: 35
Mobility classification: Very high
Amount desorbed: 69.0% of the adsorbed (high-dose soils only).
Desorption K_d: 0.25
Desorption K_{oc}: 23
Freundlich desorption K_F: 0.2
Freundlich desorption K_{Foc}: 18

Soil type: **Carlyle Silt loam**

Amount adsorbed:	43.9-52.2% of the applied.
Adsorption K_d:	3.46
Adsorption K_{oc}:	231
Freundlich adsorption K_F:	3.20
Freundlich adsorption K_{Foc}:	214
Mobility classification:	Moderate
Amount desorbed:	65.6% of the adsorbed (high-dose soils only).
Desorption K_d:	2.40
Desorption K_{oc}:	160
Freundlich desorption K_F:	1.76
Freundlich desorption K_{Foc}:	117

Soil type: **Nidda Sandy loam**

Amount adsorbed:	50.4-73.5% of the applied.
Adsorption K_d:	18.2
Adsorption K_{oc}:	395
Freundlich adsorption K_F:	15.9
Freundlich adsorption K_{Foc}:	346
Mobility classification:	Moderate
Amount desorbed:	61.1% of the adsorbed (high-dose soils only).
Desorption K_d:	12.7
Desorption K_{oc}:	276
Freundlich desorption K_F:	9.21
Freundlich desorption K_{Foc}:	200

Study Acceptability: This study is classified as **acceptable**. No significant deviations from good scientific practices were noted. It could not be determined if the foreign soils used in the study were typical of the pesticide use area in the U.S. Also, material balances were determined for high-dose soils only.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with the USEPA Guidelines for Pesticides Registration, Subdivision N §163-1 (1982) and the OECD Guideline for Testing of Chemicals No. 106 "Adsorption/-Desorption" (2000; pp. 6, 16). Significant deviations from the objectives of Subdivision N guidelines were:

It could not be determined if the foreign soils that were used in the study were typical of the pesticide use area in the U.S.

Material balances were determined for high-dose soils only.

COMPLIANCE: This study was conducted in compliance with OECD Good Laboratory Practices (p. 3; Appendix 3, p. 84). Signed and dated No Data Confidentiality, GLP, Quality Assurance, and Certificate of Authenticity statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Material [Pyrazole-3-^{14}C]pyrasulfotole (p. 18).
[Phenyl-U-^{14}C]pyrasulfotole (p. 18; preliminary experiments only).

Chemical Structure: See DER Attachment 1.
Description: Technical grade.

Purity:

[Pyrazole-U-^{14}C]-label
Radiochemical purity: 100% (p. 18).
Batch No.: SEL/1009.
Specific activity: 5510 MBq/g (330600 dpm/μg).
Location of the label: 3 carbon of the pyrazole ring.

[Phenyl-U-^{14}C]-label
Radiochemical purity: 99.12% (p. 18; preliminary experiments only).
Batch No.: SEL/1006.
Specific activity: 3190 MBq/g (191400 dpm/μg).
Location of the label: Uniformly labeled in the phenyl ring.

Storage conditions of test chemicals: Not reported.

Physico-chemical properties of pyrasulfotole (AE 0317309):

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	HCB Silt loam	Pikeville Loamy sand	CL6S Clay loam	SL2.3 Sandy loam	Carlyle Silt loam	Nidda Sandy loam
Geographic location	Grand Forks, North Dakota.	Pikeville, North Carolina.	Rheinland-Pfalz, Germany.	Rheinland-Pfalz, Germany.	Carlyle, Illinois.	Frankfurt am Main, Germany.
Pesticide use history at the collection site	None for previous 5 years.					
Collection procedures	Sampled from the A horizon; no further details were provided.					
Sampling depth	0-15.2 cm.	0-15.2 cm.	0/5-20 cm.	0/5-20 cm.	0-15.2 cm.	Sediment sampled from 40 cm water depth.
Storage conditions	Not reported.					
Storage length [1]	*ca.* 3 months.	*ca.* 2 months.	*ca.* 4 months.	*ca.* 1 month.	*ca.* 12 months.	*ca.* 3 months.
Soil preparation	Partially air-dried at ambient temperature, sieved (≤2 mm), and mixed thoroughly.					

Data were obtained from pp. 19-20 of the study report.

1 Storage length was determined by the reviewer as the interval between the field sampling date (July 2001 for the Illinois silt loam, March 2002 for the German clay loam, April 2002 for the North Dakota silt loam and German sandy loam sediment, May 2002 for the North Carolina loamy sand, and June 2002 for the German sandy loam) and the experimental study initiation (July 2002; Table 2, p. 41 of the study report).

Table 2: Properties of the soils.

Property	HCB	Pikeville	CL6S	SL2.3	Carlyle	Nidda
Soil texture (USDA)	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
% Sand	29	77	37	65	29	49
% Silt	54	22	32	28	56	44
% Clay	17	1	31	7	15	7
pH water (1:1) 0.01M $CaCl_2$ (1:1)	 7.7 7.3	 6.4 5.7	 7.5 7.1	 6.7 6.1	 5.2 4.9	 5.8 5.5
Organic carbon (%)	4.7	1.2	1.7	1.1	1.5	4.6
Organic matter (%) [1]	8.0	2.0	2.9	1.9	2.6	7.8
CEC (meq/100g)	26.0	5.8	25.4	9.7	15.1	18.7
Moisture at 1/3 bar (%)	Not reported.					
Soil moisture (g/100 g soil DM)	10.08	1.25	4.91	7.59	4.10	4.52
Bulk density (g/cm^2)	0.86	1.40	1.29	1.33	1.12	0.87
Biomass (mg microbial C/100 g or CFU or other)	Not reported.					
Soil taxonomic classification	Not reported.					
Sol mapping unit (for EPA)	Not reported.					

Data were obtained from Table 2, p. 41 of the study report.
1 Reviewer-calculated as % organic carbon × 1.7.

C. STUDY DESIGN:

1. Preliminary study: Preliminary experiments were conducted to determine the adsorption of the test material to the test vessels, and to determine the appropriate soil:solution ratio and equilibrium time to be used in the definitive study (pp. 23, 25-26).

Prior to study initiation, application solutions were prepared by diluting a stock solution of [phenyl-U-^{14}C]pyrasulfotole, at a nominal concentration of *ca.* 4.6 mg/mL, and a stock solution of [pyrazole-3-^{14}C]pyrasulfotole, at a nominal concentration of *ca.* 4.0 mg/mL, with 0.01M $CaCl_2$ solution (pp. 19, 23).

To determine the stability of the test material and adsorption of the test material to the glass centrifuge jars, aliquots (1 × 10 µL) of the [pyrazole-3-^{14}C]pyrasulfotole application solution were diluted to 50 mL with 0.01M $CaCl_2$ solution (pp. 20, 25). The samples were incubated in the dark at room temperature. After 0, 1, and 3 days, aliquots were analyzed using LSC. Additional aliquots were analyzed using HPLC. HPLC analysis was performed under the following conditions (p. 22): Waters symmetry C18 column (4.6 × 250 mm; 5-µm particle size), mobile combining (Solvent System A) ammonium formate 0.02M adjusted to pH 2 with formic acid and (Solvent System B) acetonitrile [percent A:B (v:v) at 0-5 min., 90:10; 10 min., 75:25;

30 min., 40:60; 40-45 min., 5:95; 50-60 min., 90:10], and flow rate of 1 mL/minute. [^{14}C]Pyrasulfotole was identified by comparison to the retention time of an unlabeled reference standard (Rt = *ca.* 18-19 min.). Based on HPLC analysis, it was determined that there was no significant degradation of [pyrazole-3-^{14}C]pyrasulfotole after 3 days of shaking (p. 33). In addition, no significant adsorption of [pyrazole-3-^{14}C]pyrasulfotole to the glass centrifuge jars was observed (Table 8, p. 49).

To determine the adsorption kinetics, aliquots (6 × *ca.* 20 g, per soil type) of each test soil were placed into glass centrifuge jars (p. 25). Each sample was mixed with *ca.* 19 mL of 0.01M $CaCl_2$ solution, sealed with screw caps, and shaken on a gyro wheel mixer for *ca.* 24 hours. Following pre-equilibration, the Carlyle silt loam, HCB silt loam, CL6S clay loam, and Pikeville loamy sand soils were treated with a 1.0-mL aliquot of a [phenyl-U-^{14}C]pyrasulfotole test solution at a nominal test concentration of *ca.* 1.1 mg/L (Table A, p. 24). The Nidda sandy loam sediment and SL2.3 sandy loam soil were treated with a 1.0-mL aliquot of a [pyrazole-3-^{14}C] pyrasulfotole test solution at a nominal test concentration of *ca.* 1.1 mg/L. The samples were shaken for 2, 4, 6, 16, 24, and 48 hours. Following each sampling interval, duplicate samples were centrifuged and aliquots of the supernatants were analyzed for total radioactivity using LSC. An additional experiment, Accelerated Solvent Extraction (ASE), was conducted on selected soil samples following 24 hours of adsorption exposure to [^{14}C]pyrasulfotole at *ca.* 1.1 Φg/mL (p. 34). described. The 24-hour soil samples were mixed with 20 g of diatomaceous earth and extracted using acetonitrile:water (2:1, v:v; Figure 3, p. 70). A primary "mild" extraction phase (40EC) and a consecutive "aggravated" extraction phase (i.e. 100EC, elevated temperature) were each analyzed using LSC, then concentrated *in vacuo* using a rotary evaporator and analyzed using HPLC as previously described (p. 26). The extracted soils were ground to a powder and analyzed using LSC following combustion. It was determined that 40.2-68.0% and 2.4-28.2% of the applied radioactivity was released from the test soils under "mild" and "aggravated" extraction conditions, respectively (Table 6, p. 47). Most of the recovered radioactivity was unchanged pyrasulfotole, based on HPLC analysis (Figures 4-5, pp. 71-72). Mass balances ranged from 98.2-100.6% of the applied for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, with [^{14}C] pyrasulfotole accounting for 89.5-95.1% of the applied (pp. 34-35; Table 6, p. 47). For the Nidda sandy loam sediment, a mass balance of 97.3% of the applied was observed, with [phenyl-U-^{14}C] pyrasulfotole accounting for 82.5% of the applied. The low recovery of parent compound from the Nidda sandy loam sediment was due to an incomplete test material extraction, according to the study authors.

To determine the desorption kinetics, aliquots (6 × *ca.* 20 g, per soil type) of each test soil were prepared, pre-equilibrated, and treated with test material as previously described (p. 26). Following 24 hours of adsorption, the samples were centrifuged, the supernatants were decanted, and *ca.* 20 mL of fresh 0.01M $CaCl_2$ solution were added to each sample. The samples were shaken for 2, 4, 6, 16, 24, and 48 hours. Following each sampling interval, duplicate samples were centrifuged and aliquots of the supernatants were analyzed for total radioactivity using LSC. Additional samples were analyzed using HPLC as previously described.

To check for levels of background radioactivity, blank samples were included in the preliminary adsorption and desorption kinetics tests (p. 26). Aliquots (2 × *ca.* 20 g, per soil type) were treated with *ca.* 20 mL of 0.01M $CaCl_2$ solution and pre-equilibrated for *ca.* 24 hours. Following pre-equilibration, the samples were shaken on a gyro wheel mixer for 96 hours and centrifuged. Aliquots of the supernatants were analyzed using LSC. For all test soils, an insignificant amount of background radioactivity was released into the supernatants (p. 35).

Based on the results of these preliminary experiments, an equilibration time of 24 hours and soil:solution ratios of 1:5 (w:v) for the Carlyle silt loam soil, 1:20 (w:v) for the Nidda sandy loam sediment, and 1:1 (w:v) for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, and SL2.3 sandy loam soils were selected for use in the definitive study (pp. 33-34; Figures 6-7, pp. 73-74).

2. Definitive study experimental conditions:

Table 3: Study design for the adsorption phase.

Parameters		**HCB Silt loam**	**Pikeville Loamy sand**	**CL6S Clay loam**	**SL2.3 Sandy loam**	**Carlyle Silt loam**	**Nidda Sandy loam**
Condition of soil (air dried/fresh) [1]		Air-dried.					
Have these soils been used for other laboratory studies? (specify which)		No.					
Soil (g/replicate)		20				5	3
Equilibrium solution used (eg: 0.01N $CaCl_2$)		0.01M $CaCl_2$ solution.					
Control used (with salt solution only) (Yes/No)		Yes.					
Test material concentrations [2]	Nominal application rates (mg a.i./kg soil)	Not reported.					
	Analytically measured concentrations (mg a.i./kg soil)	*ca.* 0.0057, 0.0124, 0.0418, 0.1235, 0.4275				*ca.* 0.0285, 0.0618, 0.209, 0.6175, 2.1375	*ca.* 0.114, 0.247, 0.836, 2.47, 8.55
Identity and concentration of co-solvent, if any		0.01M $CaCl_2$ (<0.05%).					
Soil:solution ratio (w:v)		1:1				1:5	1:20
Initial pH of the equilibration solution, if provided		Not reported.					
No. of replications	Controls	Triplicate samples without soil. Duplicate samples without test material.					
	Treatments	Duplicate.					
Equilibration	Time (hours)	24					
	Temperature (°C)	Ambient.					

	Darkness (Yes/No)	Yes
	Shaking method	Gyro wheel overhead shaker.
	Shaking time (hours)	24
Method of separation of supernatant (eg., centrifugation)		Centrifugation
Centrifugation	Speed (G)	*ca.* 6000
	Duration (min)	10
	Method of separation of soil and solution	Decanted.

Data were obtained from pp. 20, 23-24, 26-27 and Table 3, p. 42 of the study report.
1 Prior to use, aliquots of each test soil were pre-equilibrated by rotation on a gyro wheel mixer for *ca.* 24 hours with 0.01M $CaCl_2$ solution.
2 Test material concentrations were calculated by the reviewer by converting mg/L to mg a.i./kg using the following equation: [test concentration (mg/L) × total volume of test material (mL)] ÷ amount of soil (g); eg. for the Carlyle silt loam soil [0.006 mg/L × 23.75 mL] ÷ 5.0 g = 0.0285 mg a.i./kg soil.

Table 4: Study design for the desorption phase.

Parameters		HCB Silt loam	Pikeville Loamy sand	CL6S Clay loam	SL2.3 Sandy loam	Carlyle Silt loam	Nidda Sandy loam
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption Table		Yes.					
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.0057/0.0285/0.114	0.0034	0.0038	0.0016	0.0020	0.0137	0.0757
	0.0124/0.0618/0.247	0.0079	0.0088	0.0035	0.0040	0.0323	0.1817
	0.0418/0.209/0.836	0.0259	0.0294	0.0119	0.0147	0.1045	0.5740
	0.1235/0.6175/2.47	0.0744	0.0839	0.0326	0.0390	0.2709	1.4668
	0.4275/2.1375/8.55	0.2382	0.2578	0.1204	0.1287	0.9487	4.3058
No. of desorption cycles		2					
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M $CaCl_2$)		0.01M $CaCl_2$ solution; *ca.* 20 mL.				0.01M $CaCl_2$ solution; *ca.* 25 mL.	0.01M $CaCl_2$ solution; *ca.* 60 mL.
Soil:solution ratio		1:1				1:5	1:20
Replications	Controls	Triplicate samples without soil. Duplicate samples without test material.					
	Treatments	Duplicate.					
Desorption equilibration	Time (hours)	24					
	Temperature (°C)	Ambient.					
	Darkness	Yes					
	Shaking method	Gyro wheel overhead shaker.					
	Shaking time (hours)	24					
Centrifugation	Speed (G)	6000					
	Duration (min)	10					
	Method of separation of soil and solution	Decanted.					
Second desorption cycle		Followed same procedure as first desorption cycle.					

Data were obtained from pp. 26-27; Table 3, p. 42; Table 9, p. 50; Table 12, p. 53; Table 15, p. 56; Table 18, p. 59; Table 21, p. 62; and Table 24, p. 65 of the study report.

3. Description of analytical procedures:

Extraction/clean up/concentration methods: No extraction/clean up/concentration methods were employed in this study.

Total ^{14}C measurement: Following adsorption and each desorption cycle, aliquots (*ca.* 3 × 0.5-2.0 mL) of the supernatants were analyzed for total radioactivity using LSC (pp. 21-22, 27). Mass balances were determined for high-dose soils by summing the radioactivity recovered in the adsorption solutions, two desorption solutions, and unextracted radiocarbon (p. 32).

Non-extractable residues, if any: Following the second desorption cycle, the soils were homogenized and analyzed for total radioactivity using LSC following combustion; combustion efficiency ranged from 98.4-100.3% (p. 22).

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

Identification and quantification of parent compound: Samples were not analyzed for pyrasulfotole.

Identification and quantification of transformation products, if appropriate: Samples were not analyzed for transformation products of pyrasulfotole.

Detection limits (LOD, LOQ) for the parent compound: The Limit of Quantification (LOQ) for LSC analysis was 30 dpm; the Limit of Detection (LOD) was not reported (p. 21).

Detection limits (LOD, LOQ) for the transformation products, if appropriate: For LSC analysis, the LOQ was 30 dpm; the LOD was not reported (p. 21).

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The incubation temperature during the study was maintained at ambient temperature; no supporting information was provided (Table 3, p. 42). The pH values of the supernatants solutions during the adsorption and desorption phases were not reported. The test samples were not analyzed for parent or its transformation products. LSC analysis of application control samples without soil (three samples per soil type and test concentration), concurrently run with each definitive test series, verified the application accuracy and lack of test material adsorption to the glass test containers; >98% of the applied radioactivity was recovered in the application control solutions (p. 37; Table 8, p. 49).

B. MASS BALANCE: Mass balances at the end of the adsorption phase were not reported. Mean mass balances at the end of the desorption phase averaged 95.3% (range 93.3-97.3%), 96.6% (range 93.9-99.3%), 95.0% (range 93.6-96.3%), 98.5% (range 98.3-98.7%), 98.8% (range 98.7-99.0%), and 100.6% (range 100.4-100.7%) of the applied for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively (p. 37; Table 7, p. 48).

Table 5: Recovery of [pyrazole-3-^{14}C]pyrasulfotole, expressed as percentage of applied radioactivity, in high-dose soil after adsorption/desorption (mean ± s.d.; n = 2).

Matrices	**HCB Silt loam**	**Pikeville Loamy sand**	**CL6S Clay loam**	**SL2.3 Sandy loam**	**Carlyle Silt loam**	**Nidda Sandy loam**
At the end of the adsorption phase						
Supernatant solution [1]	22.4 ± 0.6	29.7 ± 0.6	41.8 ± 1.4	44.1 ± 1.0	53.9 ± 0.6	51.7 ± 0.7
Solid phase (extracted)	Not determined.					
Non-extractable residues in soil, if measured	Not determined.					
Total recovery	Not determined.					
At the end of the desorption phase						
Supernatant solution [2] (Desorption 1)	25.4 ± 0.1	21.4 ± 0.4	23.7 ± 6.0	26.9 ± 0.2	20.8 ± 0.3	20.3 ± 0.1
Supernatant solution [2] (Desorption 2)	14.7 ± 0.3	11.9 ± 0.1	13.8 ± 2.7	10.6 ± 0.0	8.7 ± 0.1	9.6 ± 0.1
Solid phase (extracted)	Not determined.					
Non-extractable residues in soil, if measured [3,4]	32.9 ± 2.5	33.6 ± 3.9	15.6 ± 2.9	16.8 ± 0.9	15.5 ± 0.2	19.1 ± 0.5
Total recovery [5]	95.3 ± 2.9	96.6 ± 3.8	95.0 ± 1.9	98.5 ± 0.2	98.8 ± 0.2	100.6 ± 0.2

Data were obtained from Table 7, p. 48 of the study report. Means and standard deviations were determined by the reviewer using Excel.

1 Determined by the reviewer by dividing the mass of test item in supernatant after adsorption (dpm) by the total mass of test item before adsorption (dpm); e.g. for the HCB silt loam soil $[6.77 \times 10^5 \div 2.97 \times 10^6] \times 100 = 22.79\%$.

2 Determined by the reviewer by dividing the mass of test item in supernatant after desorption (dpm) by the total mass of test item before adsorption (dpm); e.g. for the HCB silt loam soil, first desorption $[7.56 \times 10^5 \div 2.97 \times 10^6] \times 100 = 25.45\%$.

3 All soils were combusted following desorption.

4 Determined by dividing the total mass of test item in soil after the last desorption (dpm) by the total mass of test item before adsorption (dpm); e.g. for the HCB silt loam soil $[1.03 \times 10^6 \div 2.97 \times 10^6] \times 100 = 34.68\%$.

5 Determined by dividing the amount recovered (dpm) by the total mass of test item before adsorption (dpm); e.g. for the HCB silt loam soil $[2.89 \times 10^6 \div 2.97 \times 10^6] \times 100 = 97.31\%$.

Table 6: Concentration of [pyrazole-3-^{14}C]pyrasulfotole in the solid and liquid phases at the end of adsorption equilibration period (mean ± s.d.; n = 2).

Concentration (mg a.i./kg soil)	HCB Silt loam			Pikeville Loamy sand			CL6S Clay loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.0057	0.0034 ± 0.0	0.0022 ± 0.0	59.7 ± 0.0	0.0038 ± 0.0	0.0018 ± 0.0	66.7 ± 0.0	0.0016 ± 0.0	0.0038 ± 0.0	27.2 ± 1.2
0.0124	0.0079 ± 0.0	0.0056 ± 0.0	63.3 ± 1.7	0.0088 ± 0.0	0.0046 ± 0.0	71.0 ± 2.3	0.0035 ± 0.0	0.0096 ± 0.0	27.8 ± 0.6
0.0418	0.0259 ± 0.0	0.0193 ± 0.0	62.0 ± 0.0	0.0294 ± 0.0	0.0157 ± 0.0	70.2 ± 0.2	0.0119 ± 0.0	0.0319 ± 0.0	28.4 ± 0.2
0.1235	0.0744 ± 0.0	0.0637 ± 0.0	60.2 ± 1.8	0.0839 ± 0.0	0.0521 ± 0.0	67.9 ± 0.5	0.0326 ± 0.0	0.1013 ± 0.0	26.4 ± 0.0
0.4275	0.2382 ± 0.0	0.2132 ± 0.0	55.7 ± 2.2	0.2578 ± 0.0	0.1907 ± 0.0	60.3 ± 0.2	0.1204 ± 0.0	0.3189 ± 0.0	28.2 ± 3.6

Concentration (mg a.i./kg soil)	SL2.3 Sandy loam			Carlyle Silt loam			Nidda Sandy loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed[1]
0.0057/0.0285/0.114	0.0020 ± 0.0	0.0035 ± 0.0	34.2 ± 1.2	0.0137 ± 0.0	0.0028 ± 0.0	48.1 ± 1.0	0.0757 ± 0.0	0.0019 ± 0.0	66.4 ± 1.2
0.0124/0.0618/0.247	0.0040 ± 0.0	0.0090 ± 0.0	32.3 ± 2.3	0.0323 ± 0.0	0.0071 ± 0.0	52.2 ± 2.0	0.1817 ± 0.0	0.0046 ± 0.0	73.5 ± 0.9
0.0418/0.209/0.836	0.0147 ± 0.0	0.0290 ± 0.0	35.2 ± 0.3	0.1045 ± 0.0	0.0240 ± 0.0	50.0 ± 0.2	0.5740 ± 0.0	0.0161 ± 0.0	68.7 ± 0.4
0.1235/0.6175/2.47	0.0390 ± 0.0	0.0934 ± 0.0	31.5 ± 1.7	0.2709 ± 0.0	0.0676 ± 0.0	43.9 ± 0.1	1.4668 ± 0.0	0.0491 ± 0.0	59.4 ± 0.3
0.4275/2.1375/8.55	0.1287 ± 0.0	0.3058 ± 0.0	30.1 ± 1.1	0.9487 ± 0.0	0.2770 ± 0.0	44.4 ± 0.2	4.3058 ± 0.0	0.2445 ± 0.0	50.4 ± 0.1

Data were obtained from Table 9, p. 50; Table 12, p. 53; Table 15, p. 56; Table 18, p. 59; Table 21, p. 62; and Table 24, p. 65 of the study report. Means and standard deviations were determined by the reviewer using Excel.

1 Percent adsorbed was calculated by the reviewer using the following equation: [concentration on soil (mg a.i./kg) ÷ nominal test concentration (mg a.i./kg)] × 100; e.g. for the HCB silt loam soil at 0.0057 mg a.i./kg, [0.0034 mg a.i./kg ÷ 0.0057 mg a.i./kg soil] × 100 = 59.65%.

Table 7: Concentration of [pyrazole-3-^{14}C]pyrasulfotole in the solid and liquid phases at the end of the second desorption cycle (mean ± s.d.; n = 2).

Concentration (mg a.i./kg soil)	HCB Silt loam			Pikeville Loamy sand			CL6S Clay loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]
0.0057	0.0022 ± 0.0	0.0008 ± 0.0	ND	0.0026 ± 0.0	0.0006 ± 0.0	ND	0.0008 ± 0.0	0.0007 ± 0.0	ND
0.0124	0.0048 ± 0.0	0.0019 ± 0.0	ND	0.0058 ± 0.0	0.0015 ± 0.0	ND	0.0015 ± 0.0	0.0017 ± 0.0	ND
0.0418	0.0153 ± 0.0	0.0067 ± 0.0	ND	0.0191 ± 0.0	0.0049 ± 0.0	ND	0.0057 ± 0.0	0.0056 ± 0.0	ND
0.1235	0.0411 ± 0.0	0.0214 ± 0.0	ND	0.0517 ± 0.0	0.0157 ± 0.0	ND	0.0113 ± 0.0	0.0169 ± 0.0	ND
0.4275	0.1283 ± 0.0	0.0700 ± 0.0	55.0 ± 2.0	0.1517 ± 0.0	0.0524 ± 0.0	49.7 ± 2.5	0.0600 ± 0.0	0.0658 ± 0.0	70.4 ± 5.5

Concentration (mg a.i./kg soil)	SL2.3 Sandy loam			Carlyle Silt loam			Nidda Sandy loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed[1]
0.0057/0.0285/0.114	0.0010 ± 0.0	0.0005 ± 0.0	ND	0.0062 ± 0.0	0.0006 ± 0.0	ND	0.0419 ± 0.0	0.0007 ± 0.0	ND
0.0124/0.0618/0.247	0.0019 ± 0.0	0.013 ± 0.0	ND	0.0141 ± 0.0	0.0014 ± 0.0	ND	0.1000 ± 0.0	0.0016 ± 0.0	ND
0.0418/0.209/0.836	0.0072 ± 0.0	0.0043 ± 0.0	ND	0.0455 ± 0.0	0.0042 ± 0.0	ND	0.3015 ± 0.0	0.0050 ± 0.0	ND
0.1235/0.6175/2.47	0.0195 ± 0.0	0.0135 ± 0.0	ND	0.1167 ± 0.0	0.0606 ± 0.1	ND	0.7345 ± 0.0	0.013 ± 0.0	ND
0.4275/2.1375/8.55	0.0629 ± 0.0	0.0491 ± 0.0	69.0 ± 1.2	0.3690 ± 0.0	0.0401 ± 0.0	65.6 ± 0.1	1.6901 ± 0.0	0.0434 ± 0.0	61.1 ± 0.7

Data were obtained from Table 11, p. 52; Table 14, p. 55; Table 17, p. 58; Table 20, p. 61; Table 23, p. 64; and Table 26, p. 67 of the study report. Means and standard deviations were determined by the reviewer using Excel.

1 Percent desorbed as percent of the adsorbed was calculated by the reviewer using data obtained from Table 7, p. 48 and the following equation: [% Desorbed (Desorption cycles 1 + 2) ÷ (% Total Recovery - % Adsorbed)] × 100; e.g. for the HCB silt loam soil at 0.4275 mg a.i./kg soil [(25.45% + 14.48%) ÷ (97.31% - 22.79%] × 100 = 53.58%.

ND = Not determined.

Table 8: Adsorption and desorption constants of [pyrazole-3-^{14}C]pyrasulfotole in the soils. [1]

Soil	Adsorption						Second Desorption					
	K_d	K_F	1/N	R^2	K_{oc}	K_{Foc}	K_d	K_F	1/N	R^2	K_{oc}	K_{Foc}
HCB Silt loam	1.32	0.980	0.926	0.9998	28.1	20.8	2.26	1.374	0.902	0.9996	48.2	29.2
Pikeville Loamy sand	1.77	1.204	0.908	0.9995	148	100	3.67	2.298	0.913	0.9995	305.6	192
CL6S Clay loam	0.367	0.341	0.979	0.9981	21.6	20.0	0.923	0.678	0.943	0.9914	54.3	40
SL2.3 Sandy loam	0.47	0.386	0.946	0.9978	42.7	35.1	1.51	1.133	0.948	0.9969	137.1	103
Carlyle Silt loam	4.25	3.196	0.925	0.9997	283	213	10.44	8.461	0.962	0.9993	696	564
Nidda Sandy loam	32.86	15.866	0.831	0.9944	715	345	56.59	30.899	0.889	0.9958	1230	672

Data were obtained from pp. 35-36, Table 1, p. 40, Tables 9-26, pp. 50-67, and Figures 8-13, pp. 75-80 of the study report.
K_d - Adsorption and desorption coefficients; K - Freundlich adsorption and desorption coefficients; 1/N - Slope of Freundlich adsorption/desorption isotherms.
K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).
R^2 - Regression coefficient of Freundlich equation.
1 Freundlich K_F values were calculated by the study author using the following equation (p. 30):

$\log C_s = 1/n \times \log C_{aq} + \log K_F$, where

C_s = soil concentration after adsorption or desorption (Φg/g);
C_{aq} = concentration of supernatant after adsorption or desorption (Φg/g);
1/n = Freundlich exponent; and
K_F = Freundlich coefficient.

Table 8b: Adsorption and desorption constants of [pyrazole-3-^{14}C]pyrasulfotole in the soils, as determined by the PMRA. [1]

	Adsorption							Consecutive desorption (after two cycles)						
Soil	K_d	R^2	K_{oc}	K_F	1/N	R^2	K_{Foc}	K_d	R^2	K_{oc}	K_F	1/N	R^2	K_{Foc}
HCB Silt loam	1.12	0.995	24	0.980	0.925	0.999	21	0.76	0.975	16	0.55	0.554	0.981	12
Pikeville Loamy sand	1.37	0.995	114	1.204	0.908	0.9995	100	0.75	0.991	63	0.51	0.411	0.998	42
CL6S Clay loam	0.37	0.975	22	0.341	0.976	0.997	20	0.15	0.221*	9	0.17	0.323	0.337	10
SL2.3 Sandy loam	0.42	0.998	38	0.39	0.945	0.997	35	0.25	0.987	23	0.20	0.393	0.984	18
Carlyle Silt loam	3.46	0.997	231	3.20	0.926	0.9995	214	2.40	0.995	160	1.76	0.490	0.996	117
Nidda Sandy loam	18.17	0.964	395	15.90	0.832	0.994	346	12.692	0.992	276	9.21	0.541	0.999	200

Data were obtained from pp. 35-36, Table 1, p. 40, Tables 9-26, pp. 50-67, and Figures 8-13, pp. 75-80 of the study report.
K_d - Adsorption and desorption coefficients; K_F - Freundlich adsorption and desorption coefficients; 1/N - Slope of Freundlich adsorption/desorption isotherms.
K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).
R^2 - Regression coefficient.
* - Low R^2 predominantly driven by one outlier.

C. ADSORPTION: After 24 hours of equilibration, 55.7-63.3%, 60.3-71.0%, 26.4-32.3%, 30.1-35.2%, 43.9-52.2%, and 50.4-73.5% of the applied [pyrazole-3-^{14}C]pyrasulfotole was adsorbed to the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively (reviewer-calculated; Table 9, p. 50; Table 12, p. 53; Table 15, p. 56; Table 18, p. 59; Table 21, p. 62; Table 24, p. 65). Registrant-calculated adsorption K_d values averaged 1.32, 1.77, 0.367, 0.47, 4.25, and 32.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding adsorption K_{oc} values averaged 28.1, 148, 21.6, 42.7, 283, and 715. Registrant-calculated Freundlich adsorption K_F values were 0.980, 1.20, 0.341, 0.386, 3.20, and 15.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding Freundlich adsorption K_{Foc} values were 20.8, 100, 20.0, 35.1, 213, and 345.

Adsorption coefficients were re-calculated by the secondary reviewer using slopes of adsorption isotherms rather than mean coefficients. $K_{d\text{-}ads}$ values were 1.12, 1.37, 0.37, 0.42, 3.46 and 18.2 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding $K_{OC\text{-}ads}$ values were 24, 114, 22, 38, 231 and 395, respectively. Freundlich regressions gave $K_{F\text{-}ads}$ values of 0.98, 1.20, 0.34, 0.39, 3.20 and 15.9 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding $K_{FOC\text{-}ads}$ values were 21, 100, 20, 35, 214 and 346, respectively. The slopes (1/n) of the Freundlich adsorption regressions were all within the range of 0.9-1.1, with the exception of Nidda sediment (Table 8b).

The registrant demonstrated that adsorption of pyrasulfotole is influenced by pH. Registrant-calculated K_{FOC} values tended to decrease with increasing pH, with pyrasulfotole showing the greatest mobility at neutral soil pH levels (Fig 1).

Figure 1. pH dependency of AE 0317309 (pyrasulfotole) soil adsorption*.

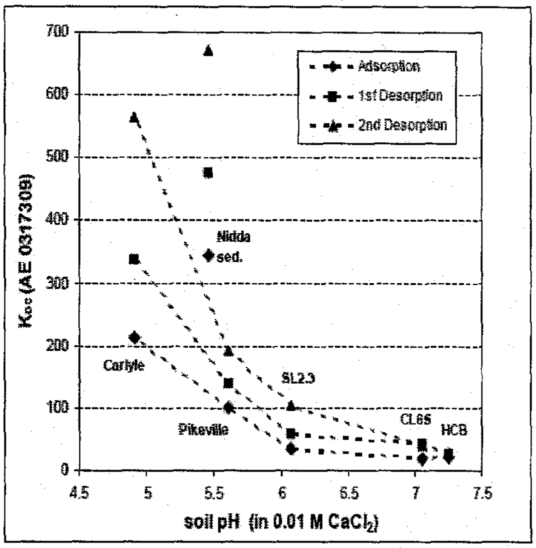


*Figure 14 from original study report (UKID # 1190145; p 81).

D. DESORPTION: At the end of the desorption phase, 55.0%, 49.7%, 70.4% 69.0% 65.6%, and 61.1% of the applied [pyrazole-3-^{14}C]pyrasulfotole desorbed from the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively (reviewer-calculated; Table 7, p. 48). Registrant-calculated desorption K_d values averaged 2.26, 3.67, 0.923, 1.51, 10.4, and 56.6 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding adsorption K_{oc} values averaged 48.2, 306, 54.3, 137, 696, and 1230 (Table 11, p. 52; Table 14, p. 55; Table 17, p. 58; Table 20, p. 61; Table 23, p. 64; Table 26, p. 67). Registrant-calculated Freundlich desorption K_F values were 1.37, 2.30, 0.678, 1.13, 8.46, and 30.9 for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils, and the Nidda sandy loam sediment, respectively; corresponding Freundlich desorption K_{Foc} values were 29.2, 192, 40, 103, 564, and 672.

Desorption coefficients were similarly re-calculated by the secondary reviewer using slopes of desorption isotherms. Desorption isotherms were based on consecutive desorption through two cycles from the highest test concentration only. Consecutive desorption $K_{d\text{-}des}$ values were 0.76, 0.75, 0.15, 0.25, 2.40 and 12.7 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding $K_{OC\text{-}des}$ values were 16, 63, 9, 23, 160 and 276, respectively. Freundlich regressions gave $K_{F\text{-}des}$ values of 0.55, 0.51, 0.17, 0.20, 1.76 and 9.21 for HCB silt loam, Pikeville loamy sand, CL6S clay loam, SL2.3 sandy loam, and Carlyle silt loam soils and the Nidda sandy loam sediment, respectively; corresponding $K_{FOC\text{-}des}$ values were 12, 42, 10, 18, 117 and 200, respectively. The slopes (1/n) of the Freundlich desorption regressions were all within the range of 0.32 – 0.55 (Table 8b).

III. STUDY DEFICIENCIES

1. It was not established that the foreign soils used in this study were comparable to soils that would be found at the intended use sites in the United States. The foreign test soils were from Germany, and the FAO classifications were not provided.

2. Material balances were determined for high-dose soils only. Mass balances should have been determined for all test concentrations/test soil groups following adsorption and desorption.

IV. REVIEWERS' COMMENTS

1. To confirm adsorption constant data reported in the study report, the reviewer calculated adsorption K_d values using the following EPA-approved equation:

   $K_d = [(C_0V_0 - C_{eq}V_0) \div m] \div C_{eq}$ where

   S = the sorbed phase concentration with units of mass of sorbate per solid sorbent mass;
   C_0 = the concentration in the water before sorption;
   V_0 = the total water volume in the batch system;
   C_{eq} = the aqueous-phase equilibrium concentration; and
   m = the dry mass of sorbent.

   Adsorption K_d values determined by the reviewer are tabulated below:

Table 9: Reviewer-calculated adsorption constants of [pyrazole-3-^{14}C]pyrasulfotole in the soils.

Soil	K_d
HCB Silt loam	1.24
Pikeville Loamy sand	1.68
CL6S Clay loam	0.38
SL2.3 Sandy loam	0.48
Carlyle Silt loam	4.14
Nidda Sandy loam	31.63

K_d values were reviewer-calculated using data obtained from Table 9, p. 50; Table 12, p. 53; Table 15, p. 56; Table 18, p. 59; Table 21, p. 62; and Table 24, p. 65 of the study report.

The reviewer-calculated adsorption K_d values were similar to those reported by the study authors The reviewer-calculated r^2 value for the relationship of K_d vs. % organic carbon is 0.3581, for K_d vs. pH is 0.2226, and for K_d vs. % clay is 0.0868.

2. Based on the adsorption phase study results and the Briggs classification, pyrasulfotole is classified as mobile, intermediately mobile or having low mobility in soil, mainly depending on soil pH (pp. 36, 38; Figure 14, p. 81).

3. None of the test soils had an organic matter content ≤1%, as recommended by Subdivision N guidelines.

4. The study authors reported the following information following the first desorption cycle:

Table 10: Desorption constants of [pyrazole-3-^{14}C]pyrasulfotole in the soils.

Soil	First desorption					
	K_d	K_F	1/N	R^2	K_{oc}	K_{Foc}
HCB Silt loam	1.73	1.131	0.907	0.9996	36.9	24.1
Pikeville Loamy sand	2.70	1.665	0.902	0.993	225	139
CL6S Clay loam	0.665	0.707	0.975	0.9621	39.1	42
SL2.3 Sandy loam	0.83	0.635	0.941	0.9979	75.6	57.7
Carlyle Silt loam	6.95	5.056	0.933	0.9993	463	337
Nidda Sandy loam	44.81	21.864	0.855	0.9953	974	475

Data were obtained from Table 10, p. 51; Table 13, p. 54; Table 16, p. 57; Table 19, p. 60; Table 22, p. 63; and Table 25, p. 66 of the study report.

5. An alternative mathematical evaluation of the desorption behaviour of pyrasulfotole was performed in accordance with the Canadian Guideline (p. 30). Freundlich desorption isotherms were plotted through soil and supernatant concentration data pairs from the adsorption phase and each of the two consecutive cycles of the desorption phase, using the following actual test concentrations: for the HCB silt loam, Pikeville loamy sand, CL6S clay loam, and SL2.3 sandy loam soils, 0.0418 mg a.i./kg soil; for the Carlyle silt loam soil, 0.209 mg a.i./kg soil; and for the Nidda sandy loam sediment, 0.836 mg a.i./kg soil. These actual test concentrations were converted into mole fractions (mol/mol water phase) or molar concentrations (mol/g soil dry weight) prior to setting up the desorption isotherms (p. 31). Calculations and graphical plots of the desorption isotherms are presented in Appendices 1-2, pp. 82-83, respectively, of the study report.

6. The average radiopurities of the [phenyl-U-^{14}C]- and [pyrazole-3-^{14}C]-labeled pyrasulfotole stock solutions were confirmed to be 97.26% and 97.12%, respectively, using HPLC analysis (Figures 1-2, pp. 68-69).

7. The Freundlich 1/n values for the adsorption and desorption phases for the Nidda sandy loam sediment were below 0.9. Subdivision N guidelines specify that 1/n values should be in the range of 0.9 to 1.1.

8. The maximum field application rate for pyrasulfotole was not reported. Subdivision N guidelines specify that one test concentration should be roughly equivalent to the maximum proposed or registered field application rate of the parent compound.

9. The secondary reviewer re-calculated K_d and K_F values for both adsorption and desorption phases based on current PMRA practices (Table 8b). PMRA-calculated K_d values were very similar to those reported by the study author, but differ slightly as they represent the slope of the adsorption coefficients across all test concentrations, rather than an average of the individual K_d values from all concentrations. With the exception of the Nidda sediment results, this does not result in a difference in interpretation of pyrasulfotole's adsorptive capabilities. To determine the desorptive capabilities of the active ingredient following absorption, the PMRA models the consecutive desorption of the highest test concentration through two desorption cycles, and therefore $K_{d\text{-}des}$ values in Table 8b differ significantly than those presented by the study authors. As the 1/n values for all sediments (with the exception of Nidda sediments) fall between 0.9-1.1, the PMRA recommends using the non-Freundlich K_{OC} values to classify pyrasultatole's mobility potential and for subsequent water modelling.

10. DEH does not agree with the study author's comment "the analyte sorption to soils increases at low concentration" because the provided sorption isotherm does not support the claim (it is linear over the tested concentration). A linear sorption isotherm is the one in which the affinity of the sorbate for the sorbent remains the same over the observed concentration range. If sorption increases at low concentrations (as claimed by the study author), it can mean that analyte sorbs to specific sites. Such a case involves an adsorbent (e.g., soot, clay mineral) exhibiting a limited number of sites with a high affinity for the sorbate that dominate the overall sorption at low concentration, plus a partitioning process (e.g., into natural organic matter; linear isotherm) predominating at higher concentration. If this is pyrasulfotole sorption behaviour, a mixed and not a linear isotherm should be observed.

11. There is some indication that pyrasulfotole could have combined sorption behaviour due to the value of n (1.02-1.2). When $n > 1$ it means that more sorbate present in the sorbent enhances the further sorption (isotherm is concave upward). While, when $n = 1$ it means that there is constant sorption free energy at all sorbate concentration (meaning the isotherm is linear). However, to see this combined sorption behaviour further experiments are needed as the provided data doesn't support this claim.

12. DEH does not agree with the study author's interpretation that "the Koc for the adsorption and the two corresponding consecutive desorption cycles revealed significant increase in adsorption". We do not consider the increase significant (increase by a factor of 1.4 to 2.9) especially when compared to the increased factor observed with the benzoic acid metabolite of up to a factor of 12.

13. DEH does not agree with the study author's interpretation "once pyrasulfotole is adsorbed, the compound is not readily released back into aqueous environment" because the Koc values in the two consecutive desorptions are still classified as mobile in most soil.

V. REFERENCES

1. McCall, J.P., D.A. Laskowski, R.L. Swann and H.J. Dishburger. 1981. Measurement of sorption coefficients of organic chemicals and their use in environmental fate analysis. Pages 89-109 *in* Test protocols for environmental fate and movement of toxicants. Proceedings of a symposium. Assoc. of Official Analytical Chemists. 94th Annual Meeting, October 21-22, 1980. Washington, D.C.

2. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 163-1. Mobility studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

3. 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.

4. 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.

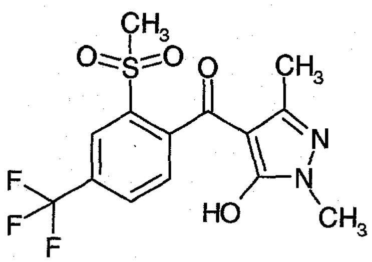
5. U.S. Environmental Protection Agency. 2003. Guidance for Calculating Sorption Coefficients in Batch Equilibrium Studies.

Attachment 1: Structures of Parent Compound and Transformation Products

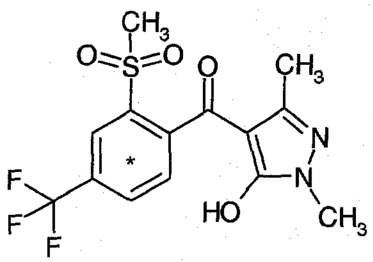
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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

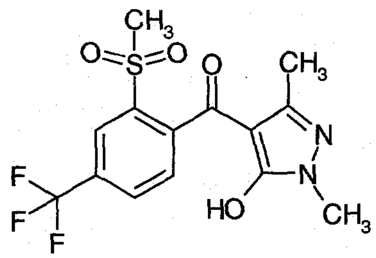


^{14}C = Position of radiolabel.

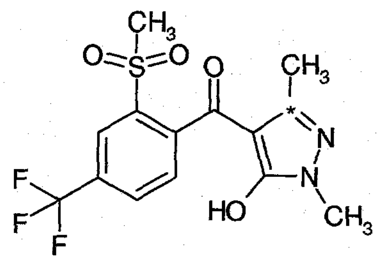
Pyrasulfotole [AE 0317309; K-1196; K-1267]

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.

Chemical: Pyrasulfotole
PC Code: 000692
MRID: 46801703
Guideline No: 163-1

Table 4/6 Adsorption on soil

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	0.2315	0.2573	0.1311	0.1321	0.9452	4.2996
0.45	0.2448	0.2583	0.1096	0.1253	0.9522	4.3120
AVG	0.2382	0.2578	0.1204	0.1287	0.9487	4.3058
STDEV	0.01	0.00	0.02	0.00	0.00	0.01
0.13	0.0728	0.0843	0.0326	0.0404	0.2706	1.4713
0.13	0.0760	0.0834	0.0326	0.0375	0.2712	1.4623
AVG	0.0744	0.0839	0.0326	0.0390	0.2709	1.4668
STDEV	0.00	0.00	0.00	0.00	0.00	0.01
0.044	0.0259	0.0293	0.0118	0.0148	0.1042	0.5760
0.044	0.0259	0.0294	0.0119	0.0146	0.1048	0.5719
AVG	0.0259	0.0294	0.0119	0.0147	0.1045	0.5740
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.013	0.0077	0.0086	0.0034	0.0038	0.0331	0.1800
0.013	0.0080	0.0090	0.0035	0.0042	0.0314	0.1833
AVG	0.0079	0.0088	0.0035	0.0040	0.0323	0.1817
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.006	0.0034	0.0038	0.0015	0.0020	0.0135	0.0747
0.006	0.0034	0.0038	0.0016	0.0019	0.0139	0.0766
AVG	0.0034	0.0038	0.0016	0.0020	0.0137	0.0757
STDEV	0.00	0.00	0.00	0.00	0.00	0.00

Data were obtained from Table 9, p. 50, Table 12, p. 53, Table 15, p. 56, Table 18, p. 59, Table 21, p. 62, and Table 24, p. 65 of the study report.

Table 5 High-dose adsorption solution

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	22.79	30.13	40.74	43.43	53.51	52.16
0.45	21.92	29.29	42.76	44.78	54.29	51.16
AVG	22.36	29.71	41.75	44.11	53.90	51.66
STDEV	0.6	0.6	1.4	1.0	0.6	0.7

Data were obtained from Table 7, p. 48 of the study report.

Chemical: Pyrasulfotole
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Guideline No: 163-1

Table 5 High-dose desorption 1 solution

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	25.45	21.04	19.43	27.10	21.06	20.38
0.45	25.32	21.65	27.95	26.77	20.57	20.27
AVG	25.39	21.35	23.69	26.94	20.82	20.33
STDEV	0.1	0.4	6.0	0.2	0.3	0.1

Table 5 High-dose desorption 2 solution

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	14.48	11.82	15.69	10.54	8.73	9.50
0.45	14.95	11.95	11.82	10.61	8.62	9.59
AVG	14.72	11.89	13.76	10.58	8.68	9.55
STDEV	0.3	0.1	2.7	0.0	0.1	0.1

Table 5 Combusted

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	34.68	30.91	17.68	17.37	15.64	18.72
0.45	31.11	36.36	13.54	16.16	15.40	19.38
AVG	32.90	33.64	15.61	16.77	15.52	19.05
STDEV	2.5	3.9	2.9	0.9	0.2	0.5

Table 5 Recovery

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	97.31	93.94	93.60	98.65	98.96	100.66
0.45	93.27	99.33	96.30	98.32	98.70	100.44
AVG	95.29	96.64	94.95	98.49	98.83	100.55
STDEV	2.9	3.8	1.9	0.2	0.2	0.2

Data were obtained from Table 7, p. 48 of the study report.

Chemical: Pyrasulfotole
PC Code: 000692
MRID: 46801703
Guideline No: 163-1

Table 6 Adsorption solution

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	0.2189	0.1918	0.3077	0.3043	0.2757	0.2463
0.45	0.2075	0.1895	0.3300	0.3072	0.2783	0.2426
AVG	0.2132	0.1907	0.3189	0.3058	0.2770	0.2445
STDEV	0.01	0.00	0.02	0.00	0.00	0.00
0.13	0.0637	0.0529	0.1014	0.0924	0.0673	0.0495
0.13	0.0636	0.0512	0.1012	0.0944	0.0679	0.0487
AVG	0.0637	0.0521	0.1013	0.0934	0.0676	0.0491
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.044	0.0193	0.0156	0.0319	0.0290	0.0241	0.0161
0.044	0.0193	0.0158	0.0319	0.0289	0.0238	0.0161
AVG	0.0193	0.0157	0.0319	0.0290	0.0240	0.0161
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.013	0.0055	0.0045	0.0096	0.0091	0.0069	0.0045
0.013	0.0057	0.0046	0.0096	0.0088	0.0073	0.0046
AVG	0.0056	0.0046	0.0096	0.0090	0.0071	0.0046
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.006	0.0022	0.0018	0.0038	0.0035	0.0028	0.0019
0.006	0.0021	0.0018	0.0038	0.0035	0.0028	0.0018
AVG	0.0022	0.0018	0.0038	0.0035	0.0028	0.0019
STDEV	0.00	0.00	0.00	0.00	0.00	0.00

Data were obtained from Table 9, p. 50, Table 12, p. 53, Table 15, p. 56, Table 18, p. 59, Table 21, p. 62, and Table 24, p. 65 of the study report.

Chemical: Pyrasulfotole
PC Code: 000692
MRID: 46801703
Guideline No: 163-1

Table 6 % Adsorbed

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	54.15	60.19	30.67	30.90	44.22	50.29
0.45	57.26	60.42	25.64	29.31	44.55	50.43
AVG	55.71	60.30	28.15	30.11	44.38	50.36
STDEV	2.20	0.17	3.56	1.12	0.23	0.10
0.13	58.95	68.26	26.40	32.71	43.82	59.57
0.13	61.54	67.53	26.40	30.36	43.92	59.20
AVG	60.24	67.89	26.40	31.54	43.87	59.38
STDEV	1.83	0.52	0.00	1.66	0.07	0.26
0.044	61.96	70.10	28.23	35.41	49.86	68.90
0.044	61.96	70.33	28.47	34.93	50.14	68.41
AVG	61.96	70.22	28.35	35.17	50.00	68.65
STDEV	0.00	0.17	0.17	0.34	0.20	0.35
0.013	62.10	69.35	27.42	30.65	53.56	72.87
0.013	64.52	72.58	28.23	33.87	50.81	74.21
AVG	63.31	70.97	27.82	32.26	52.18	73.54
STDEV	1.71	2.28	0.57	2.28	1.95	0.94
0.006	59.65	66.67	26.32	35.09	47.37	65.53
0.006	59.65	66.67	28.07	33.33	48.77	67.19
AVG	59.65	66.67	27.19	34.21	48.07	66.36
STDEV	0.00	0.00	1.24	1.24	0.99	1.18

Data were obtained from Table 9, p. 50, Table 12, p. 53, Table 15, p. 56, Table 18, p. 59, Table 21, p. 62, and Table 24, p. 65 of the study report.

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Table 7 Desorption 2 on soil

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	0.1248	0.1505	0.0679	0.0650	0.3644	1.6621
0.45	0.1317	0.1528	0.0520	0.0607	0.3736	1.7180
AVG	0.1283	0.1517	0.0600	0.0629	0.3690	1.6901
STDEV	0.00	0.00	0.01	0.00	0.01	0.04
0.13	0.0403	0.0516	0.0083	0.0234	0.1180	0.7305
0.13	0.0418	0.0518	0.0142	0.0155	0.1154	0.7384
AVG	0.0411	0.0517	0.0113	0.0195	0.1167	0.7345
STDEV	0.00	0.00	0.00	0.01	0.00	0.01
0.044	0.0153	0.0191	0.0053	0.0078	0.0447	0.2993
0.044	0.0153	0.0190	0.0060	0.0066	0.0462	0.3037
AVG	0.0153	0.0191	0.0057	0.0072	0.0455	0.3015
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.013	0.0047	0.0057	0.0015	0.0015	0.0146	0.0985
0.013	0.0048	0.0059	0.0015	0.0022	0.0136	0.1014
AVG	0.0048	0.0058	0.0015	0.0019	0.0141	0.1000
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.006	0.0022	0.0026	0.0007	0.0012	0.0061	0.0408
0.006	0.0022	0.0026	0.0008	0.0007	0.0063	0.0429
AVG	0.0022	0.0026	0.0008	0.0010	0.0062	0.0419
STDEV	0.00	0.00	0.00	0.00	0.00	0.00

Data were obtained from Table 11, p. 52, Table 14, p. 55, Table 17, p. 58, Table 20, p. 61, Table 23, p. 64, and Table 26, p. 67 of the study report.

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Table 7 Desorption 2 in solution

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	0.0706	0.0525	0.0782	0.0493	0.0405	0.0432
0.45	0.0694	0.0523	0.0534	0.0489	0.0397	0.0435
AVG	0.0700	0.0524	0.0658	0.0491	0.0401	0.0434
STDEV	0.00	0.00	0.02	0.00	0.00	0.00
0.13	0.0215	0.0159	0.0168	0.0136	0.0112	0.0133
0.13	0.0212	0.0155	0.0169	0.0134	0.0110	0.0133
AVG	0.0214	0.0157	0.0169	0.0135	0.0111	0.0133
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.044	0.0067	0.0049	0.0058	0.0043	0.0042	0.0050
0.044	0.0067	0.0049	0.0054	0.0043	0.0042	0.0050
AVG	0.0067	0.0049	0.0056	0.0043	0.0042	0.0050
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.013	0.0019	0.0015	0.0017	0.0013	0.0014	0.0016
0.013	0.0019	0.0015	0.0016	0.0013	0.0014	0.0016
AVG	0.0019	0.0015	0.0017	0.0013	0.0014	0.0016
STDEV	0.00	0.00	0.00	0.00	0.00	0.00
0.006	0.0008	0.0006	0.0007	0.0005	0.0005	0.0007
0.006	0.0008	0.0006	0.0007	0.0005	0.0006	0.0006
AVG	0.0008	0.0006	0.0007	0.0005	0.0006	0.0007
STDEV	0.00	0.00	0.00	0.00	0.00	0.00

Data were obtained from Table 11, p. 52, Table 14, p. 55, Table 17, p. 58, Table 20, p. 61, Table 23, p. 64, and Table 26, p. 67 of the study report.

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Table 7 % Desorbed as % of the adsorbed

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
0.45	53.58	51.50	66.44	68.16	65.54	61.61
0.45	56.44	47.97	74.28	69.82	65.73	60.59
AVG	55.01	49.73	70.36	68.99	65.64	61.10
STDEV	2.02	2.49	5.54	1.17	0.13	0.72

Data were obtained from Table 7, p. 48 of the study report.

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Table 8 Adsorption Kd

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
	1.12	1.35	0.377	0.42	3.42	17.61
	1.17	1.61	0.322	0.42	4.01	29.87
	1.34	1.87	0.373	0.51	4.37	35.72
	1.40	1.92	0.358	0.45	4.53	39.78
	1.57	2.12	0.404	0.56	4.94	41.34
AVG	1.32	1.77	0.367	0.47	4.25	32.86

Table 8 Adsorption Koc

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
	23.8	113	22.2	38.3	228	383
	24.9	134	18.9	37.9	267	649
	28.6	156	21.9	46.1	291	777
	29.8	160	21.0	40.6	302	865
	33.5	176	23.8	50.5	329	899
AVG	28.1	148	21.6	42.7	283	715

Data were obtained from Table 9, p. 50; Table 12, p. 53; Table 15, p. 56; Table 18, p. 59; Table 21, p. 62; and Table 24, p. 65 of the study report.

Table 8 Desorption 1 Kd

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
	1.41	2.04	1.023	0.71	5.61	27.27
	1.49	2.39	0.380	0.77	6.78	42.30
	1.76	2.85	0.639	0.90	7.24	47.26
	1.86	2.96	0.587	0.79	7.42	53.15
	2.15	3.24	0.695	0.98	7.69	54.05
AVG	1.73	2.70	0.665	0.83	6.95	44.81

Table 8 Desorption 1 Koc

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
	29.9	170	60.2	64.5	374	593
	31.6	199	22.4	70.1	452	920
	37.5	238	37.6	82.2	483	1027
	39.5	246	34.6	71.9	494	1155
	45.8	270	40.9	89.5	513	1175
AVG	36.9	225	39.1	75.6	463	974

Data were obtained from Table 10, p. 51; Table 13, p. 54; Table 16, p. 57; Table 19, p. 60; Table 22, p. 63; and Table 25, p. 66 of the study report.

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Table 8 Desorption 2 Kd

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
	1.83	2.89	0.911	1.28	9.19	38.99
	1.92	3.29	0.668	1.44	10.52	55.25
	2.28	3.89	1.015	1.68	10.81	60.62
	2.45	3.98	0.917	1.38	10.36	63.37
	2.84	4.30	1.106	1.76	11.32	64.72
AVG	2.26	3.67	0.923	1.51	10.44	56.59

Table 8 Desorption 2 Koc

	Silt loam	Loamy sand	Clay loam	Sandy loam	Silt loam	Sandy loam
	39.0	241	53.6	116.3	613	848
	40.9	274	39.3	130.7	702	1201
	48.5	324	59.7	152.6	720	1318
	52.1	331	54.0	125.8	691	1378
	60.4	358	65.0	159.9	755	1407
AVG	48.2	306	54.3	137.1	696	1230

Data were obtained from Table 11, p. 52; Table 14, p. 55; Table 17, p. 58; Table 20, p. 61; Table 23, p. 64; and Table 26, p. 67 of the study report.

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HCB Silt loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.45	19	0.2189	19	20	0.2195	1.00	
0.45	19	0.2075	19	20	0.2304	1.11	
0.13	19	0.0637	19	20	0.0630	0.99	
0.13	19	0.0636	19	20	0.0631	0.99	
0.044	19	0.0193	19	20	0.0235	1.22	
0.044	19	0.0193	19	20	0.0235	1.22	
0.013	19	0.0055	19	20	0.0071	1.30	
0.013	19	0.0057	19	20	0.0069	1.22	
0.006	19	0.0022	19	20	0.0036	1.64	
0.006	19	0.0021	19	20	0.0037	1.76	
						1.24	AVG

Pikeville Loamy sand- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_{o)}-(C_{eq}V_{o)}]$/soil mass	Kd	
0.45	19	0.1918	19	20	0.2453	1.28	
0.45	19	0.1895	19	20	0.2475	1.31	
0.13	19	0.0529	19	20	0.0732	1.38	
0.13	19	0.0512	19	20	0.0749	1.46	
0.044	19	0.0156	19	20	0.0270	1.73	
0.044	19	0.0158	19	20	0.0268	1.70	
0.013	19	0.0045	19	20	0.0081	1.79	
0.013	19	0.0046	19	20	0.0080	1.73	
0.006	19	0.0018	19	20	0.0040	2.22	
0.006	19	0.0018	19	20	0.0040	2.22	
						1.68	AVG

CL6S Clay loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_{o)}-(C_{eq}V_{o)}]$/soil mass	Kd	
0.45	19	0.3077	19	20	0.1352	0.44	
0.45	19	0.33	19	20	0.1140	0.35	
0.13	19	0.1014	19	20	0.0272	0.27	
0.13	19	0.1012	19	20	0.0274	0.27	
0.044	19	0.0319	19	20	0.0115	0.36	
0.044	19	0.0319	19	20	0.0115	0.36	
0.013	19	0.0096	19	20	0.0032	0.34	
0.013	19	0.0096	19	20	0.0032	0.34	
0.006	19	0.0038	19	20	0.0021	0.55	
0.006	19	0.0038	19	20	0.0021	0.55	
						0.38	AVG

Data were obtained from Table 9, p. 50, Table 12, p. 53, Table 15, p. 56, Table 18, p. 59, Table 21, p. 62, and Table 24, p. 65 of the study report.

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SL2.3 Sandy loam- Adsorption

Initial soln concen (C_o) (ug/mL)	Volume of soln (V_o) (mL)	Concen in soln after equil (C_{eq}) (ug/mL)	Volume of soln (V_o) (mL)	Dry mass of sorbent (m) (g)	$[(C_oV_o)-(C_{eq}V_o)]$/soil mass	Kd	
0.45	19	0.3043	19	20	0.1384	0.45	
0.45	19	0.3072	19	20	0.1357	0.44	
0.13	19	0.0924	19	20	0.0357	0.39	
0.13	19	0.0944	19	20	0.0338	0.36	
0.044	19	0.029	19	20	0.0143	0.49	
0.044	19	0.0289	19	20	0.0143	0.50	
0.013	19	0.0091	19	20	0.0037	0.41	
0.013	19	0.0088	19	20	0.0040	0.45	
0.006	19	0.0035	19	20	0.0024	0.68	
0.006	19	0.0035	19	20	0.0024	0.68	
						0.48	AVG

Carlyle Silt loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil	Kd	
0.45	23.75	0.2757	23.75	5	0.8279	3.00	
0.45	23.75	0.2783	23.75	5	0.8156	2.93	
0.13	23.75	0.0673	23.75	5	0.2978	4.43	
0.13	23.75	0.0679	23.75	5	0.2950	4.34	
0.044	23.75	0.0241	23.75	5	0.0945	3.92	
0.044	23.75	0.0238	23.75	5	0.0960	4.03	
0.013	23.75	0.0069	23.75	5	0.0290	4.20	
0.013	23.75	0.0073	23.75	5	0.0271	3.71	
0.006	23.75	0.0028	23.75	5	0.0152	5.43	
0.006	23.75	0.0028	23.75	5	0.0152	5.43	
						4.14	AVG

Nidda Sandy loam- Adsorption

Initial soln concen (C_o)	Volume of soln (V_o)	Concen in soln after equil (C_{eq})	Volume of soln (V_o)	Dry mass of sorbent (m)	$[(C_oV_o)-(C_{eq}V_o)]$/soil	Kd	
0.45	57	0.2463	57	3	3.8703	15.71	
0.45	57	0.2426	57	3	3.9406	16.24	
0.13	57	0.0495	57	3	1.5295	30.90	
0.13	57	0.0487	57	3	1.5447	31.72	
0.044	57	0.0161	57	3	0.5301	32.93	
0.044	57	0.0161	57	3	0.5301	32.93	
0.013	57	0.0045	57	3	0.1615	35.89	
0.013	57	0.0046	57	3	0.1596	34.70	
0.006	57	0.0019	57	3	0.0779	41.00	
0.006	57	0.0018	57	3	0.0798	44.33	
						31.63	AVG

Data were obtained from Table 9, p. 50, Table 12, p. 53, Table 15, p. 56, Table 18, p. 59, Table 21, p. 62, and Table 24, p. 65 of the study report.