Data Evaluation Record on the adsorption-desorption of oryzalin in soil

PMRA Submission Number {.....} EPA MRID Number 41479802

Data Requirement: PMRA Data Code:
EPA DP Barcode: 378627
OECD Data Point:
EPA Guideline: 835.1230

Test material:

Common name: Oryzalin.

Chemical name:

IUPAC name: 3,5-Dinitro-4-(dipropylamino)benzenesulfonamide.
3,5-Dinitro-N^4,N^4-dipropylsulfanilamide.

CAS name: 4-(Dipropylamino)-3,5-dinitrobenzenesulfonamide.

CAS No.: 19044-88-3.

Synonyms OR-1; EL-119.

SMILES String: C1C(S(=O)(=O)N)=CC(N(O)O)=C(N(CCC)CCC)C=1N(O)O (EpiSuite version 4.0).

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Cambridge Environmental

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Company Code:
Active Code:
Use Site Category:
EPA PC Code: 104201

CITATION: Saunders, D.G. and F.L. Powers. 1987. Adsorption and desorption of oryzalin on soil. Unpublished study performed by Lilly Research Laboratories, Greenfield, Indiana; sponsor unidentified; submitted by DowElanco (now Dow AgroChemicals), Greenfield, Indiana. Laboratory Project ID EWD8726. Experimental initiation date August 31, 1987 and completion date October 1, 1987 (p. 8). Final report issued October 29, 1987.

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EXECUTIVE SUMMARY

The adsorption/desorption characteristics of [ring-UL-^{4}C]-labeled 3,5-dinitro-N^4,N^4-dipropylsulfanilamide (oryzalin; radiochemical purity >99%) were studied in four U.S. soils, a sand [pH 7.7, organic carbon 0.3%] from Texas; and a sandy loam [pH 5.7, organic carbon 0.8%], a loam [pH 6.5; organic carbon 1.0%], and a clay loam [pH 6.9; organic carbon 1.2%], each from Indiana, in a batch equilibrium experiment. The studies were conducted according to USEPA Subdivision N Series 163-1. GLP compliance documents were not provided. The adsorption phase of the study was carried out by equilibrating air-dried, sieved soil with oryzalin at nominal concentrations of 0.016, 0.08, 0.4, and 2.0 mg a.i./kg soil for the sand soil and 0.064, 0.32, 1.6, and 8.0 mg a.i./kg soil for the sandy loam, loam, and clay loam soils. The test soils were equilibrated in the dark at 25 ± 1°C for 22 hours. The equilibrating solution used was 0.01M $CaCl_2$ solution with soil solution ratios of 1:2 (w:v) for the sand soil and 1:8 (w:v) for the sandy loam, loam, and clay loam soils. The desorption phase of the study was carried out by replacing 22 mL of the adsorption solution with an equivalent volume of 0.01M $CaCl_2$ solution and equilibrating for 22 hours. Two desorption steps were conducted for all soils.

Following the adsorption and desorption phases, the supernatant solutions were separated by centrifugation and analyzed for total radioactivity using liquid scintillation counting (LSC). Following the second desorption step, the soils were extracted twice with methanol and the extracts were combined, diluted and analyzed using LSC. Subsamples of the "A" replicate extract samples were transferred to separatory funnels containing 5% aqueous NaCl and extracted twice with dichloromethane. The extracts were collected and the solvent was evaporated by rotary vacuum. The identity of oryzalin was confirmed using thin layer chromatography (TLC) analysis. The samples were not analyzed for transformation products.

The experimental temperature employed during the study was reported to be maintained at 25 ± 1°C; supporting details were not provided. The pHs of the test solutions during the definitive study were not reported. TLC analysis of the soil extracts showed oryzalin was stable in the test samples; supporting data were not provided.

Mass balances at the end of the adsorption phase were not determined. Mass balances at the end of the adsorption and desorption phases were 100.0 ± 2.1% (range 96.8-102.7%) for the sand soil, 99.8 ± 2.7% (range 96.5-105.5%) for the sandy loam soil, 95.6 ± 3.0% (range 89.2-98.4%) for the loam soil, and 96.7 ± 3.2% (range 92.7-103.1%) for the clay loam soil.

The percent of the applied oryzalin residues that were adsorbed to the test soils was estimated by the reviewer using radioactivity estimates calculated by the study authors. Average percent adsorptions were 52-60%, 39-55%, 51-63%, and 62-74% for the sand, sandy loam, loam, and clay loam soils, respectively. Average reviewer-calculated adsorption K_d values were 2.68, 7.35, 11.31, and 18.4 for the sand, sandy loam, loam, and clay loam soils, respectively; corresponding adsorption K_{oc} values were 893, 919, 1131, and 1533. Based on linear regression analysis, reviewer-calculated adsorption K_d values were 2.2, 5.0, 8.4, and 12.9 for the sand, sandy loam, loam, and clay loam soils, respectively. Reviewer-calculated adsorption K_F values were 2.11,

4.77, 7.98, and 12.0 for the sand, sandy loam, loam, and clay loam soils, respectively; corresponding adsorption K_{Foc} values were 703, 596, 798, and 1000.

The percent of oryzalin desorbed from the test soils, as percent of the radioactivity adsorbed, was estimated by the reviewer using radioactivity estimates calculated by the study authors. Average percent desorptions ranged from 36-41%, 36-48%, 27-38%, and 20-31% for the sand, sandy loam, loam, and clay loam soils, respectively, following the second desorption. Registrant-calculated desorption K_d values (based on the two desorptions) were 3.2, 10.3, 15.7, and 25.6 for the sand, sandy loam, loam, and clay loam soils, respectively; corresponding desorption K_{oc} values were not reported. Registrant-calculated Freundlich desorption K and K_{oc} values were not reported.

Using the Standardized Soil Mobility Classification Guidance according to the Food and Agriculture Organization (FAO) of the United Nations adopted by USEPA and using reviewer calculated adsorption K_{oc} values, oryzalin is characterized as being moderately mobile in the sandy and sandy loam soils, and slightly mobile in the loam and clay loam soils. There were strong correlations (r^2 > 90%) between the average K_d values and the organic matter, CEC, and clay content.

Results Synopsis:

Soil type:		**Sand**	**Sandy loam**	**Loam**	**Clay loam**
Adsorption					
Average K_d		2.68 ± 0.4	7.35 ± 1.9	11.31 ± 2.2	18.4 ± 4.0
Average K_{oc}		893	919	1,131	1,533
Regression	K_d	2.2	5.0	8.4	12.9
	r^2	0.9984	0.9953	0.9976	0.9953
	p-value	8.93E-17	3.81E-14	1.02E-15	3.73E-14
Freundlich Regression	Freundlich K_F	2.11	4.77	7.98	12.0
	p-value	3.34E-09	2.51E-14	5.26E-15	1.60E-14
	r^2	0.9988	0.9994	0.9993	0.9989
	1/n	0.93	0.87	0.90	0.89
	p-value	7.42E-16	2.37E-17	3.62E-17	3.65E-16
Freundlich K_{Foc}		703	596	798	1000
Desorption					
Average K_d		3.2	10.3	15.7	25.6
Average K_{oc}		Not reported.			
Freundlich K_F		Not reported.			
Freundlich K_{Foc}		Not reported.			

Study Acceptability: This study is classified as **acceptable**. No significant deviations from good scientific practices were noted. Limits of Detection (LOD) and Limits of Quantification (LOQ) were not reported.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: The study was conducted according to USEPA Subdivision N Series 163-1 (p. 1). The following significant deviation was noted:

> Limits of Detection (LOD) and Limits of Quantification (LOQ) were not reported.

COMPLIANCE: GLP compliance documents were not provided. A signed and dated No Data Confidentiality statement was provided (p. 2). GLP, Quality Assurance, and Certificate of Authenticity statements were not provided.

A. MATERIALS:

1. Test Material	[Ring-UL-^{14}C]Oryzalin (p. 5).
Chemical Structure:	See DER Attachment 1.
Description:	Technical grade.
Purity:	
Radiolabeled	Radiochemical purity: >99% (p. 5). Lot Number: 553-KBO-211. Analytical purity: Not reported. Specific radioactivity: 11.6 µCi/mg. Location of the label: Uniformly ring labeled.
Storage conditions of test chemicals:	Not reported.

Physico-chemical properties of oryzalin:

Parameter	Value	Comment
Molecular weight	Not reported.	
Molecular formula	Not reported.	
Water Solubility	2.6 µg/mL	
Vapor Pressure/Volatility	Not reported.	
UV Absorption	Not reported.	
pKa	Not reported.	
K_{ow}/log K_{ow}	Not reported.	
Stability of compound at room temperature, if provided	Not reported.	

Data were obtained from p. 6 of the study report.

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description	Sand	Sandy loam	Loam	Clay loam
Geographic location	Hidalgo County, Texas	Johnson County, Indiana	Hancock County, Indiana	Hancock County, Indiana
Pesticide use history at the collection site	Not reported.			
Collection procedures	Not reported.			
Sampling depth (cm)	Unspecified (“A” horizon).			
Storage conditions	Stored at 4°C.			
Storage length[1]	Not reported.			
Soil preparation	Air-dried, gently crushed, and sieved (#20 mesh).	Air-dried, gently crushed, and sieved (#10 mesh).		

Data were obtained from p. 5 and Table I, p. 12 of the study report.

Table 2: Properties of the soils.

Property	Sand	Sandy loam	Loam	Clay loam
Soil series	Nueces	Fox	Crosby	Brookston
Soil texture (USDA)[1]	Sand	Sandy loam	Loam	Clay loam
% Sand	89.2	66	28	24
% Silt	5.6	22	48	44
% Clay	5.2	12	24	32
pH	7.7	5.7	6.5	6.9
Organic carbon (%)[2]	0.3	0.8	1.0	1.2
Organic matter (%)	0.5	1.4	1.8	2.0
CEC (meq/100 g)	3.5	4.9	10.5	21.2
Moisture at field capacity (%)	4.87	11.86	20.36	25.96
Bulk density (g/cc)	1.48	1.28	1.11	1.15
Biomass (mg microbial C/100 g or CFU or other)	Not reported.			
Soil taxonomic classification	Not reported.			
Soil mapping unit (for EPA)	Not reported.			

Data were obtained from Tables I-II, pp. 12-13 of the study report.
1 Textural classifications were confirmed by the reviewer using the NRCS soil texture calculator http://soils.usda.gov/technical/aids/investigations/texture/ which calculates texture based on the percent sand and clay.
2 Organic carbon was determined by the reviewer as % organic matter ÷ 1.72.

1. Preliminary study: To determine the equilibration time to be used in the definitive study, aliquots (2 x 5 g) of sandy loam and aliquots (2 x 5 g) of clay loam soil were fortified with oryzalin at a concentration of 0.04 µg/mL and placed on a mixing wheel in the dark at 25 ± 1°C (pp. 6-7). Following 4, 8, 16, 22, 48, and 72 hours of mixing, the samples were centrifuged, and aliquots (2 mL) of the supernatants were analyzed for total radioactivity using LSC. It was determined that oryzalin adsorbed quickly to the test soils, with the majority of the adsorption occurring within 4 hours (p. 8; Table III, p. 14). Additional adsorption was observed through the remaining 72 hours.

Based on the results of the preliminary studies, an equilibration time of 22 hours was selected for use in the definitive study (p. 8).

2. Definitive study experimental conditions:

Table 3: Study design for the adsorption phase.

Parameters		**Sand**	**Sandy loam**	**Loam**	**Clay loam**
Condition of soil (air dried/fresh)		Air-dried.			
Have these soils been used for other laboratory studies? (specify which)		No.			
Soil (g/replicate)		20	5	5	5
Equilibrium solution used (eg: 0.01N $CaCl_2$)		Sterile 0.01M $CaCl_2$.solution.			
Control used (with salt solution only) (Yes/No)		No.			
Test material concentrations [1]	Nominal application rates (mg a.i./kg soil)	0.016, 0.08, 0.4, 2.0	0.064, 0.32, 1.6, 8.0	0.064, 0.32, 1.6, 8.0	0.064, 0.32, 1.6, 8.0
	Analytically measured concentrations (mg a.i./kg soil)	Not reported.			
Identity and concentration of co-solvent, if any		Acetone; concentration not reported.			
Soil:solution ratio (w:v)		1:2	1:8	1:8	1:8
Initial pH of the equilibration solution, if provided		Not reported.			
No. of replications	Controls	Single replicate.			
	Treatments	Triplicate replicates at all test concentrations.			
Equilibration	Time (hours)	22			
	Temperature (°C)	25 ± 1			
	Darkness (Yes/No)	Yes.			
	Shaking method	Ferris wheel mixer that rotated at 16 rpm and inverted the tubes every 2 seconds.			
	Shaking time (hours)	22			
Method of separation of supernatant (eg., centrifugation)		Centrifugation.			
Centrifugation	Speed (rpm)	3000			
	Duration (min)	30			
	Method of separation of soil and solution	Aliquots of the supernatants were removed via pipette.			

Data were obtained from pp. 5-7 and Appendix E, pp. 44, 50, 56, and 62 of the study report.
1 Test material concentrations were calculated by the reviewer by converting µg/mL to mg a.i./kg using the following equations: [(test concentration (µg/mL) × total volume of test material (mL)] ÷ amount of soil (g); eg. lowest test concentration for the sand soil [0.008 µg/mL × 40 mL] ÷ 20 g = 0.016 mg a.i./kg soil.

Table 4: Study design for the desorption phase.

Parameters		**Sand**	**Sandy loam**	**Loam**	**Clay loam**
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption		Yes.			
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.016/0.064	0.00968	0.03583	0.04262	0.05051
	0.08/0.32	0.04789	0.16745	0.20723	0.24813
	0.4/1.6	0.22580	0.72749	0.95778	1.16054
	2.0/8.0	1.04174	3.15332	4.29724	5.26675
No. of desorption steps		2			
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M $CaCl_2$)		0.01M $CaCl_2$; 22 mL.			
Soil:solution ratio (w:v)		1:2	1:8	1:8	1:8
Replications	Controls	Single replicate.			
	Treatments	Triplicate replicates at all test concentrations.			
Desorption equilibration	Time (hours)	22			
	Temperature (°C)	25 ± 1			
	Darkness	Yes.			
	Shaking method	Ferris wheel mixer that rotated at 16 rpm and inverted the tubes every 2 seconds.			
	Shaking time (hours)	22			
Centrifugation	Speed (rpm)	3000			
	Duration (min)	30			
	Method of separation of soil and solution	Aliquots of the supernatants were removed via pipette.			
Second desorption step		Followed same procedure as described for the first desorption step.			

Data were obtained from pp. 6-7 and Appendix E, pp. 44, 50, 56, and 62 of the study report.

Supplementary study: Adsorption of oryzalin to the glass test vessels was determined by preparing thirteen centrifuge tubes without soil as described in the definitive study (p. 8). The tubes were placed on a mixing wheel for 22 hours in the dark at 25 ± 1°C. Aliquots (2 mL) of the supernatants were analyzed for total radioactivity using LSC following centrifugation. No adsorption of oryzalin to the glass test vessels was observed (p. 9; Table IV, p. 15).

3. Description of analytical procedures:

Extraction/clean up/concentration methods: Following the second desorption step, the soils were extracted by mixing for *ca*. 16 hours with methanol (2 x 40 mL; pp. 7-8). Following each extraction, the samples were centrifuged, and the extracts were combined and diluted to 100 mL prior to analysis. A subsample (50 mL) of the extract for the "A" replicate samples was transferred to 250 mL separatory funnels containing 5% aqueous NaCl (100 mL), and were

extracted with dichloromethane (2 x 30 mL). The extracts were collected in 125-mL boiling flasks, and the solvent was evaporated by rotary vacuum to *ca*. 0.5 mL prior to analysis using TLC.

Total ^{14}C measurement: Following the adsorption, each desorption step, and extraction, aliquots were analyzed for total radioactivity using LSC (pp. 7-8).

Non-extractable residues, if any: Non-extractable residues were not analyzed.

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

Identification and quantification of parent compound: Soil extracts were analyzed by TLC using silica gel plates (LK6F, Whatman) developed with toluene (p. 8). Radioactive zones were detected by autoradiography using Kodak XAR-5 film.

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

Detection limits (LOD, LOQ) for the parent compound: Limits of Detection (LOD) and Limits of Quantification (LOQ) were not reported.

Detection limits (LOD, LOQ) for the transformation products, if appropriate: Samples were not analyzed for transformation products of oryzalin. Oryzalin was stable (TLC analysis) in the test samples.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The experimental temperature employed during the study was reported to be maintained at 25 ± 1°C; supporting details were not provided (p. 6). The pHs of the test solutions during the definitive study were not reported. TLC analysis of the soil extracts showed oryzalin was stable in the test samples; supporting data were not provided (p. 10).

B. MASS BALANCE: Mass balances at the end of the adsorption phase were not determined. Mass balances at the end of the adsorption and desorption phases were 100.0 ± 2.1% (range 96.8-102.7%) for the sand soil, 99.8 ± 2.7% (range 96.5-105.5%) for the sandy loam soil, 95.6 ± 3.0% (range 89.2-98.6%) for the loam soil, and 96.7 ± 3.2% (range 92.7-103.1%) for the clay loam soil (Table VII, pp. 18-19, DER Attachment 2; see Study Deficiencies).

Table 5: Recovery of oryzalin residues, expressed as percentage of applied radioactivity, in soil after adsorption/desorption (n = 3).

Matrices	**Sand**	**Sandy loam**	**Loam**	**Clay loam**
At the end of the adsorption phase				
Supernatant solution	Not determined.			
Solid phase (extracted)	Not applicable.			
Non-extractable residues in soil, if measured	Not applicable.			
Total recovery	Not applicable.			
At the end of the desorption phase				
Supernatant solution	Not determined.			
Solid phase	Not determined.			
Non-extractable residues in soil, if measured	Not applicable.			
Total recovery	100.0 ± 2.1	99.8 ± 2.7	95.6 ± 3.0	96.7 ± 3.2

Data were obtained from Table VII, pp. 18-19 of the study report and DER Attachment 2. Means and standard deviations were calculated by the reviewer using Excel.

Table 6: Concentration of oryzalin residues in the solid and liquid phases at the end of adsorption (mean ± s.d.; n = 3).

Concentration (mg a.i./kg soil)	Sand			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]
0.016/0.064	0.00968 ± 0.0	0.00318 ± 0.0	60.2 ± 2.4	0.03583 ± 0.0	0.00363 ± 0.0	54.6 ± 0.2
0.08/0.32	0.04789 ± 0.0	0.01615 ± 0.0	59.6 ± 0.6	0.16745 ± 0.0	0.01957 ± 0.0	51.1 ± 0.4
0.4/1.6	0.22580 ± 0.0	0.08755 ± 0.0	56.2 ± 0.8	0.72749 ± 0.0	0.11123 ± 0.0	44.4 ± 1.3
2.0/8.0	1.04174 ± 0.0	0.48126 ± 0.0	51.9 ± 0.5	3.15332 ± 0.1	0.61534 ± 0.0	38.5 ± 1.3
Concentration (mg a.i./kg soil)	Loam			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]
0.064	0.04262 ± 0.0	0.00295 ± 0.0	63.1 ± 1.2	0.05051 ± 0.0	0.00209 ± 0.0	73.9 ± 0.7
0.32	0.20723 ± 0.0	0.01544 ± 0.0	61.4 ± 0.7	0.24813 ± 0.0	0.01097 ± 0.0	72.6 ± 0.4
1.6	0.95778 ± 0.0	0.08650 ± 0.0	56.8 ± 0.7	1.16054 ± 0.0	0.06421 ± 0.0	67.9 ± 0.7
8.0	4.29724 ± 0.0	0.49083 ± 0.0	50.9 ± 0.4	5.26675 ± 0.1	0.38384 ± 0.0	61.6 ± 1.2

Data were obtained from Appendix E, pp. 44, 50, 56, and 62 of the study report and DER Attachment 2. Means and standard deviations were calculated by the reviewer using Excel.

1. Estimated using Total DPM Soil / Total DPM Added from Appendix E, pp. 44, 50, 56, and 62 of the study report.

Table 7: Concentration of oryzalin residues in the solid and liquid phases at the end of the second desorption step (mean ± s.d., n = 3).

Concentration (mg a.i./kg soil)	Sand			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]
0.016/0.064	0.00623 ± 0.0	0.00186 ± 0.0	35.6 ± 1.2	0.02305 ± 0.0	0.00179 ± 0.0	35.7 ± 1.3
0.08/0.32	0.03153 ± 0.0	0.00878 ± 0.0	34.2 ± 0.4	0.10855 ± 0.0	0.00883 ± 0.0	35.2 ± 0.8
0.4/1.6	0.14129 ± 0.0	0.04601 ± 0.0	37.4 ± 0.9	0.43445 ± 0.0	0.04687 ± 0.0	40.3 ± 0.9
2.0/8.0	0.61507 ± 0.0	0.24155 ± 0.0	41.0 ± 0.8	1.64979 ± 0.1	0.24851 ± 0.0	47.7 ± 1.1
Concentration (mg a.i./kg soil)	Loam			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]
0.064	0.03115 ± 0.0	0.00160 ± 0.0	26.9 ± 1.9	0.04065 ± 0.0	0.00120 ± 0.0	19.5 ± 1.0
0.32	0.14473 ± 0.0	0.00824 ± 0.0	30.2 ± 1.1	0.19346 ± 0.0	0.00668 ± 0.0	22.0 ± 1.3
1.6	0.62653 ± 0.0	0.04433 ± 0.0	34.6 ± 0.6	0.84760 ± 0.0	0.03858 ± 0.0	27.0 ± 0.8
8.0	2.67820 ± 0.0	0.23106 ± 0.0	37.7 ± 0.4	3.65823 ± 0.1	0.20970 ± 0.0	30.6 ± 1.3

Data were obtained from Appendix E, pp. 45-48, 51-54, 57-60, and 63-66 of the study report and DER Attachment 2. Means and standard deviations were calculated by the reviewer using Excel.

1. Estimated using Total DPM Soil reported in Appendix E, pp. 45-48, 51-54, 57-60, and 63-66 of the study report.

Table 8: Reviewer-calculated adsorption constants of oryzalin in the soils.

Soil	Adsorption											
	K_d (average and SD)	Regression Analysis			%OC	K_{oc}	Regression Analysis					K_{Foc}
		K_d	r^2	p-value			K_F	r^2	p-value	1/n	p-value	
Sand	2.68 ± 0.4	2.2	0.9984	8.93E-17	0.3	893	2.11	0.9988	3.34E-09	0.93	7.42E-16	703
Sandy loam	7.35 ± 1.9	5.0	0.9953	3.81E-14	0.8	919	4.77	0.9994	2.51E-14	0.87	2.37E-17	596
Loam	11.31 ± 2.2	8.4	0.9976	1.02E-15	1.0	1131	7.98	0.9993	5.26E-15	0.90	3.62E-17	798
Clay loam	18.4 ± 4.0	12.9	0.9953	3.73E-14	1.2	1533	12.0	0.9989	1.60E-14	0.89	3.65E-16	1000

Data were obtained from DER Attachment 2.

K_d values were reviewer-calculated using following equation: $K_d = [(C_0V_0-C_{aq}V_0)/m]/C_{aq}$, where

K_d = adsorption coefficient (mL/g);
C_0= Initial mass concentration of the test solution in contact with the soil (µg/mL);
V_0 = Initial volume of the aqueous phase in contact with the soil during the adsorption test (40 mL);
C_{aq} = mass concentration of the test substance in the aqueous phase at adsorption equilibrium (µg/mL); and
m = quantity of the soil phase, expressed in dry mass of soil (20 g).

K_{oc} values were reviewer-calculated using following equation: $K_{oc} = (K_d/\%OC) \times 100$, where

K_{oc} = organic carbon normalized adsorption coefficient (mL/g_{oc});
K_d = average adsorption coefficient (mL/g); and
%OC = percent organic carbon in the soil.

K_F values were reviewer-calculated using following equation: $(C_0V_0-C_{aq}V_0)/m = K_F \times (C_{aq})^{1/n}$; where

C_0= Initial mass concentration of the test solution in contact with the soil (µg/mL);
V_0 = Initial volume of the aqueous phase in contact with the soil during the adsorption test (40 mL);
C_{aq} = mass concentration of the test substance in the aqueous phase at adsorption equilibrium (µg/mL);
m = quantity of the soil phase, expressed in dry mass of soil (20 g);
K_F = Freundlich adsorption coefficient (µg/g)/(µg/mL)$^{1/n}$; and
1/n = Freundlich exponent.

K_{Foc} values were reviewer-calculated using following equation: $K_{Foc} = (K_F/\%OC) \times 100$, where

K_{Foc} = organic carbon normalized Freundlich adsorption coefficient (µg/g organic carbon)(µg/mL)$^{1/n}$;
K_F = Freundlich adsorption coefficient (µg/g)(µg/mL)$^{1/n}$; and
%OC = percent organic carbon in the soil.

Table 9: Study author-calculated desorption constants of oryzalin in the soils following the second desorption step.

Soil	Second Desorption					
	K_d	K_F	1/n	r^2	K_{oc}	K_{Foc}
Sand	3.2	NR	0.735	0.9786	NR	NR
Sandy loam	10.3	NR	0.617	0.9890	NR	NR
Loam	15.7	NR	0.575	0.9806	NR	NR
Clay loam	25.6	NR	0.515	0.9773	NR	NR

Data were obtained from Table VI, p. 17 of the study report and DER Attachment 2. Kd values estimated as average of values obtained from Appendix E, pp. 45-48, 51-54, 57-60, and 63-66 of the study report.
K_d - Desorption coefficients; K_F - Freundlich desorption coefficients; 1/n - Slope of Freundlich desorption isotherms; K_{oc} - Coefficient desorption per organic carbon (K_d or K x 100/% organic carbon); r^2 - Regression coefficient of Freundlich equation.
NR = Not reported.

C. ADSORPTION: The percent of the applied oryzalin residues that were adsorbed to the test soils was estimated by the reviewer using radioactivity estimates calculated by the study authors. Average percent adsorptions ranged from 52-60%, 39-55%, 51-63%, and 62-74% for the sand, sandy loam, loam, and clay loam soils, respectively. Average reviewer-calculated adsorption K_d values were 2.7, 7.4, 11.3, and 18.4 for the sand, sandy loam, loam, and clay loam soils, respectively; corresponding adsorption K_{oc} values were 893, 919, 1131, and 1533 (DER Attachment 2). Based on linear regression analysis, reviewer-calculated adsorption K_d values were 2.2, 5.0, 8.4, and 12.9 for the sand, sandy loam, loam, and clay loam soils, respectively. Reviewer-calculated adsorption K_F values were 2.1, 4.8, 8.0, and 12.0 for the sand, sandy loam, loam, and clay loam soils, respectively; corresponding adsorption K_{Foc} values were 703, 596, 798, and 1000.

D. DESORPTION: The percent of oryzalin desorbed from the test soils, as percent of the radioactivity adsorbed, was estimated by the reviewer using radioactivity estimates calculated by the study authors. Average percent desorptions were 36-41%, 36-48%, 27-38%, and 20-31% for the sand, sandy loam, loam, and clay loam soils, respectively. Registrant-calculated desorption K_d values, based on the two desorptions, were 3.2, 10.3, 15.7, and 25.6 for the sand, sandy loam, loam, and clay loam soils, respectively. Registrant-calculated Freundlich desorption coefficients and K_{oc} values were not reported.

Using the Standardized Soil Mobility Classification Guidance according to the Food and Agriculture Organization (FAO) of the United Nations adopted by USEPA and using reviewer calculated adsorption K_{oc} values presented in Table 8 of this DER, oryzalin is characterized as being moderately mobile in the sandy and sandy loam soils, and slightly mobile in the loam and clay loam soils.

III. STUDY DEFICIENCIES

1. Limits of Detection (LOD) and Limits of Quantification (LOQ) were not reported.

IV. REVIEWER'S COMMENTS

1. The following K_F values were calculated by the study author following the adsorption phase:

Table 10: Study author-calculated constants of oryzalin in the soils.

Soil	Adsorption					
	K_d	K_F[1]	1/n	r^2	K_{oc}	K_{Foc}
Sand	2.7	2.1	0.930	0.9995	NR	NR
Sandy loam	7.5	4.9	0.869	0.9997	NR	NR
Loam	11.9	8.4	0.900	0.9996	NR	NR
Clay loam	19.7	12.9	0.889	0.9995	NR	NR
	First Desorption					
Sand	2.9	NR	NR	NR	NR	NR
Sandy loam	8.8	NR	NR	NR	NR	NR
Loam	14.2	NR	NR	NR	NR	NR
Clay loam	22.3	NR	NR	NR	NR	NR

Data were obtained from Table V, p. 16 of the study report and DER Attachment 2.
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 of Freundlich equation. NR = Not reported.
1 The study author calculated Freundlich adsorption K_F values using the following equation (pp. 9, 25 of the study report):

$\log C_{ad} = \log K_F + 1/n \log C_{aq}$, where
C_{ad} = soil concentration after adsorption (µg/g);
C_{aq} = concentration of supernatant after adsorption (µg/mL);
1/n = exponential constant or slope; and
K_F = Freundlich adsorption constant.

2. The following values for adsorption K_d vs. % organic carbon, pH, % clay, and CEC were calculated by the reviewer:

Table 11: Reviewer-calculated adsorption regression.

Parameter	Adsorption- Regression Analysis				
	Slope	p-value	Intercept	p-value	r^2
Kd vs. % organic carbon	0.055	0.055	0.280	0.210	0.893
Kd vs. pH	-0.024	0.804	6.943	0.020	0.038
Kd vs. % clay	1.770	0.018	0.718	0.819	0.964
Kd vs. CEC	1.173	0.029	-1.628	0.561	0.942

Data were obtained from DER Attachment 2.

3. It was not stated whether the samples were stored prior to analysis. Storage stability was not addressed.

V. REFERENCES

1. 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.

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

3. U.S. Environmental Protection Agency. 2006. Standardized Soil Mobility Classification Guidance.

4. U.S. Environmental Protection Agency. 2008. Fate, Transport and Transformation Test Guidelines, OPPTS 835.1230, adsorption/desorption (batch equilibrium). Office of Prevention, Pesticides and Toxic Substances, Washington, DC. EPA 712-C-08-019.

5. U.S. Environmental Protection Agency. 2009. Technical Advisory: Calculation and reporting of Partition Coefficient Data from Batch Equilibrium Experiments.

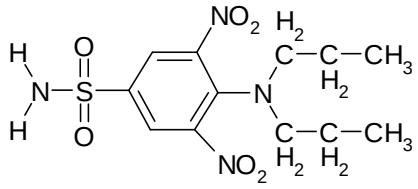
6. U.S. Environmental Protection Agency. 2009. Technical Direction on the Preparation of Data Evaluation Records (DER).

Attachment 1: Structure of Test Material

Oryzalin [OR-1; EL-119]

IUPAC Name: 3,5-Dinitro-4-(dipropylamino)benzenesulfonamide.
3,5-Dinitro-N^4,N^4-dipropylsulfanilamide.
CAS Name: 4-(Dipropylamino)-3,5-dinitrobenzenesulfonamide.
CAS Number: 19044-88-3.
SMILES String: C1C(S(=O)(=O)N)=CC(N(O)O)=C(N(CCC)CCC)C=1N(O)O (EpiSuite version 4.0).
Empirical formula: $C_{12}H_{18}N_4O_6S$ **Molecular formula:** $C_{12}H_{18}N_4O_6S$

Unlabeled



*** structure complexity/form was sacrificed to obtain SMILES string**
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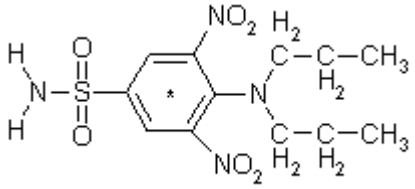
[benzene-U-^{14}C]Oryzalin
[^{14}C]Oryzalin



* = Location of the radiolabel.

Compound Identified

Oryzalin [OR-1; EL-119]

IUPAC Name: 3,5-Dinitro-4-(dipropylamino)benzenesulfonamide.
3,5-Dinitro-N^4,N^4-dipropylsulfanilamide.
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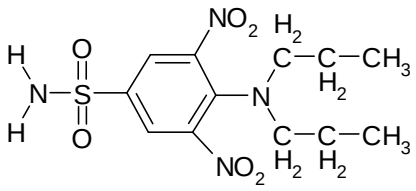
Empirical formula: $C_{12}H_{18}N_4O_6S$ **Molecular formula:** $C_{12}H_{18}N_4O_6S$



*** structure complexity/form was sacrificed to obtain SMILES string**