PMRA Submission Number {.....}

EPA MRID Number 41479801

Data Requirement:

PMRA Data Code:

EPA DP Barcode: 378627

OECD Data Point:

EPA Guideline: 835.1240

Test material:

Common name:

Oryzalin.

Chemical name:

IUPAC name:

3,5-Dinitro-4-(dipropylamino)benzenesulfonamide.

3,5-Dinitro-N⁴,N⁴-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).

Primary Reviewer: Kindra Bozicevich

Cambridge Environmental

Signature:

Date: 10/25/10

Secondary Reviewer: Joan Harlin

Cambridge Environmental

Signature:

Date: 10/25/10

QC/QA Manager: Joan Gaidos

Cambridge Environmental

Signature:

Date: 10/25/10

Final Reviewer: Chuck Peck

EPA Reviewer

Signature: Cent

Date: 19 MAY 2011
Signature: Lenf Sutton
Date: _____

Final Reviewer: Cheryl Sutton, Ph.D.

EPA Reviewer

Company Code:

Active Code:

Use Site Category:

EPA PC Code: 104201

CITATION: Saunders, D.G. 1990. Oryzalin aged soil leaching study. Unpublished study performed, sponsored, and submitted by Plant Science Chemical Development, DowElanco (now Dow AgroChemicals), Greenfield, Indiana. Laboratory Project Number AAC8923. Experimental initiation November 14, 1989 and experimental completion March 6, 1990 (p. 3). Final report issued March 28, 1990.

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EXECUTIVE SUMMARY

The aged column leaching of [benzene-U-¹⁴C]-labelled 3,5-dinitro-N⁴,N⁴-dipropylsulfanilamide (oryzalin; radiochemical purity 99.5%) was investigated using three U.S. soils: a sandy loam soil [pH 7.7, organic carbon 0.9%] from Indiana was used for the aged treated soil, while a sand soil [pH 7.7, organic carbon 0.3%] from Texas and a loam soil [pH 6.5, organic carbon 1.0%] from Indiana were used in the leaching columns. The study was conducted according to USEPA Subdivision N Series 163-1 and in compliance with USEPA 40 CFR Part 160. Sandy loam soil was treated with [14C]oryzalin at an application rate equivalent to the soil concentration that would be obtained if 6.0 lb/A of oryzalin were applied and incorporated evenly to a depth of 3.0 cm. The soil was adjusted to a moisture content of 75% of 1/3 bar field capacity and the sample was connected to an air flow trapping system (ca. 2 mL/minute). A two-section charcoal trap was used for trapping volatiles and a gas dispersion tube was used to trap ¹⁴CO₂. The bottle and trap were wrapped in aluminium foil and aged in a temperature-controlled room at 25 ± 1 °C for 30 days. The charcoal and CO_2 traps were replaced after ca. 14, 18, and 25 days of incubation. Following aging, the soil was dried by drawing air through the soil at ca. 2 L/min. for ca. 4 days. The soil was then stored at -20°C for ca. 17 days, then air-dried, ground, and mixed. For the leaching phase, duplicate soil columns were constructed of pieces of Teflon tubing (3.6 cm i.d. x 30 cm long) that were pressed into polyvinylchloride pipe fittings packed with glass wool. The distribution of the soil in each column was as follows (from the bottom of the column to the top): untreated sandy loam soil (0 to 0.5 cm); aged, treated sandy loam soil (0.5 to 3.5 cm); and, untreated sand or loam soil (3.5 to 30.0 cm). The columns were kept inverted, with the leachate flowing up, to insure that the columns were kept in a saturate mode. The study did not indicate how it maintained leachate flow upwards (e.g., use of a vacuum). The columns were saturated with 0.01M CaCl₂ solution, then leached with 0.01M CaCl₂ solution in four portions (12.7 cm or 130 mL each; equivalent to 50.8 cm of rainfall) at 25 ± 1 °C. Leachate volumes were collected for each fraction and stored at 4°C. The soil columns were inverted, allowed to drain for ca. 5 days, and sectioned into five segments of approximate equal length (6 cm).

Leachate volumes were extracted either by partitioning with dichloromethane:ethyl acetate (50:50; v:v) or extracting with ethyl acetate. The extracts were diluted and in some cases, concentrated prior to analysis for total radioactivity using liquid scintillation counting (LSC). Additional extracts were purified prior to analysis using thin-layer chromatography (TLC) to confirm the identity of oryzalin and its transformation product 4-hydroxy-3,5-dinitrobenezesulfonamide (OR-20). Negative ion fast atom bombardment mass spectrometry was also used as a confirmatory method. Following aging, the charcoal traps were emptied, air-dried, and analyzed using LSC following combustion. Gas dispersion tubes to trap ¹⁴CO₂ were analyzed directly using LSC. Portions of the aged soils were combusted and analyzed using LSC. After drying, the column segments were ground and mixed, and a subsample was combusted and analyzed using LSC.

During aging, the temperature was maintained at 24.3-25.7°C, air-flow rates were maintained at 1.8-2.1 mL/minute, and the samples were wrapped in foil to protect from light. During the

PMRA Submission Number {.....}

EPA MRID Number 41479801

leaching phase, the temperature was maintained at 24.7-25.2°C, and the infiltration rate ranged from 1.30 to 3.45 cm/hour. Lighting conditions during the leaching phase were not reported.

Following the 30-day aging phase, the overall mass balance was 97.58% of the applied radioactivity. It was determined that 97.32% of the applied oryzalin was recovered in the aged soils, 0.22% was recovered as ¹⁴CO₂, and 0.05% was recovered from the charcoal trapping solutions. Aged soils that were extracted showed that *ca.* 89% of the radioactivity was extracted and partitioned into ethyl acetate. Little radioactivity remained in the extracted aqueous solution (<0.2%), and nonextractable radioactivity accounted for *ca.* 10%. TLC analysis of the aged soil extracts showed that the majority of extracted radioactivity was oryzalin (>80% of the applied). Transformation product OR-20 accounted for 1.5-1.7% of the applied. There was no evidence of degradation during storage.

Following the leaching phase, overall mass balances ranged from 91.9 to 97.0% of the applied radioactivity. Radioactivity recovered in the soil segments totalled 89.6% of the applied in column 1 (sand), 84.2% in column 2 (sand), 92.5% in column 3 (loam), and 93.1% in column 4 (loam). The majority of the radioactivity was observed in the upper 0-6 cm segment for all soil columns. For columns 1 and 2, which were packed with unaged sand, residues detected in the soil columns were 32.7-32.9% at 0-6 cm, 17.1-19.7% at 6-12 cm, 18.5-21.4% at 12-18 cm, 10.3-12.6% at 18-24 cm, and 3.2-5.4% at 24-30 cm. For columns 3 and 4, which were packed with unaged loam, residues detected in the soil columns were 58.2-78.9% at 0-6 cm, 8.5-22.4% at 6-12 cm, 2.9-7.2% at 12-18 cm, 1.4-3.5% at 18-24 cm, and 0.8-1.8% at 24-30 cm.

A total of 7.1%, 7.8%, 2.9%, and 3.9% of the applied radioactivity was found in the leachate fractions from columns 1, 2, 3, and 4, respectively. Leachates fractions A and D from each column were extracted, which removed 0.5-2.1% of the radioactivity leaving ≤0.5% in the aqueous fraction. TLC analysis of the leachate extracts showed that the majority of extracted radioactivity was the transformation product OR-20 (25.7-61.9%); OR-20 was identified as a minor degradate in the aerobic soil metabolism study. Only two fractions contained amounts of parent oryzalin greater than 5%. These fractions also contained an unidentified minor transformation product. Negative ion FAB mass spectrometry confirmed the identity of transformation product OR-20 in the leachate extract samples.

Study Acceptability: This study is classified as **not acceptable**. Pesticide residues were aged in a different type of soil (sandy loam) than was used in the leaching columns (sand and loam). OCSPP Guidelines (835.1240) require that the soil used for leaching studies with "aged residues" have a sand content > 70%; the sandy loam soil had a sand content of 66%. Guidelines also specify that the aging period of one half-life is recommended, but should not exceed 120 days. The half-life estimated in the aerobic soil metabolism study (MRID 41322801) was between 1.5 and 2.1 months, slightly longer than the aging period of 30 days used in the study. The lighting conditions used in the leaching phase of the study were not reported. The inner diameter and length of the soil columns used during the leaching phase were not in accordance with OCSPP guidelines.

PMRA Submission Number {.....}

EPA MRID Number 41479801

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: The study was submitted under USEPA Subdivision N

Series 163-1 (p. 1). Significant deviations from the

objectives of Subdivision N guidelines were:

More than one type of soil was packed into each

soil column for the leaching phase.

The lighting conditions used in the leaching phase

of the study were not reported.

The inner diameter and length of the soil columns

used during the leaching phase were not in

accordance with OCSPP guidelines.

COMPLIANCE: The study was conducted in compliance with USEPA 40 CFR Part 160 (p.

3). Signed and dated Data Confidentiality, GLP, and Quality Assurance

statements were provided (pp. 2-4). A Certificate of Authenticity

statement was not provided.

A. MATERIALS:

1. Test Material [Benzene- U-¹⁴C]oryzalin (p. 8).

Chemical Structure: See DER Attachment 1.

Description: Technical grade.

Purity: Radiochemical purity: 99.5% (p. 8).

Analytical purity: Not reported.

Lot No. 553-KBO-211.

Specific activity: 11.67 µCi/mg.

Location of the label: Uniformly labeled in the benzene ring.

Storage conditions of

test chemicals: Not reported.

PMRA Submission Number {.....} EPA MRID Number 41479801

Physico-chemical properties of oryzalin:

Parameter	Details	Comments
Molecular formula	Not reported.	
Molecular weight	Not reported.	
Water Solubility	Not reported.	
Melting point	Not reported.	
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.	

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description	Sand	Sandy loam ¹	Loam
Geographic location	Hidalgo County, Texas	Johnson County, Indiana	Hancock County, Indiana
8Pesticide use history at the collection site	Not reported.		
Collection procedures	Not reported.		
Sampling depth (cm)	Not reported.		
Storage conditions	Stored at 4°C.	Stored at 4°C for ca. 11 months. Afterwards, 800 g of soil were placed into a glass dish with 80 mL water, and the dish was covered with Saran wrap and stored at ambient temperature for ca. 2 weeks. The soils were then air-dried.	Stored at 4°C.
Storage length ²	ca. 4 years.	ca. 1 year.	ca. 2 years.
Soil preparation (eg: 2 mm sieved; air dried etc.)	Air-dried, gently crushed, and sieved (#20 mesh).	Air-dried, gently crushed, and sieved (#10 mesh).	

Data were obtained from pp. 3, 8-9 and Table I, p. 18 of the study report.

^{1.} Following arrival at the test facility, lime was added to the soil to raise the pH to 7.7.

^{2.} Storage length was determined by the reviewer as the interval between sampling (July 1985 for the sand, August 1987 for the loam, and November 1988 for the sandy loam) and experimental initiation (November 1989).

Table 2: Properties of the soil.

Property	Sand	Sandy loam	Loam
Soil Series	Neuces	Fox	Crosby
Soil texture ¹	Sand	Sandy loam	Loam
% Sand	89.2	66	28
% Silt	5.6	21	48
% Clay	5.2	13	24
рН	7.7	7.7	6.5
Organic carbon (%) ²	0.3	0.9	1.0
Organic matter (%)	0.5	1.5	1.8
CEC (meq/100g)	3.5	8.8	10.5
Moisture at field capacity (%)	4.87	12.90	20.36
Bulk density (g/cc)	1.48	1.28	1.11
Biomass (CFU/g)	Not reported.		
Soil taxonomic classification	Not reported.		
Soil mapping unit (for EPA)	Not reported.		

Data were obtained from Tables I-II, pp. 18-19 of the study report.

C. STUDY DESIGN:

1. Preliminary study: No preliminary studies were reported.

2. Definitive study experimental conditions: For aging, an aliquot (50 g) of sandy loam soil was added to a 500-mL glass bottle with a 24/40 ground glass joint and treated with an aliquot (10 mL) of [14 C]oryzalin, dissolved in acetonitrile (p. 10; Figure 1, p. 47). The solvent was allowed to evaporate, and an additional aliquot (350 mg) of untreated soil was added and mixed with the treated soil. The application rate was equivalent to the soil concentration that would be obtained if 6.0 lb/A of oryzalin were applied and incorporated evenly to a depth of 3.0 cm. Water (38.7 mL; equivalent to a moisture content of 75% of 1/3 bar field capacity) was added, and the bottle was connected to an air flow trapping system. Compressed air was passed through a needle valve for flow adjustment (ca. 2 mL/minute) and bubbled through water to saturate the air. A two-section charcoal trap (glass tubes 0.75 cm o.d. x 9 cm) at the exit of the soil bottle was used for trapping volatiles. The air was then passed through a gas dispersion tube to trap 14 CO₂. The bottle and trap were wrapped in aluminium foil to protect from light, and maintained in a temperature-controlled room at 25 ± 1°C for 30 days. Temperature and air-flow were periodically measured. The charcoal and CO₂ traps were replaced after ca. 14, 18, and 25 days.

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.

PMRA Submission Number {.....}

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Following aging, the bottle was disconnected from the flow system and a charcoal tube connected to a BDX-44 sampling pump was inserted (p. 11). Air was drawn through the tube at $ca.\ 2\ L/min.$ for $ca.\ 4$ days. The bottle was then stoppered and stored at -20°C for $ca.\ 17$ days. The soil was removed from the bottle, air-dried, ground, and mixed using a mortar and pestle, and aliquots were analyzed for total radioactivity using LSC following combustion.

The soil columns were constructed of pieces of Teflon tubing (3.6 cm i.d. x 30 cm long) that were pressed into polyvinylchloride pipe fittings packed with glass wool (p. 11; Figures 2-3, pp. 48-49). The 0.01M CaCl₂ solution for leaching was contained in 250-mL separatory funnels above the columns. The leaching study was conducted with the columns inverted so that the aged treated soil was at the bottom of the columns and the leachate passed up through the columns. This was done to ensure that the columns remained saturated. The study did not indicate how it maintained leachate flow upwards (*e.g.*, use of a vacuum). The distribution of the soil in each column was as follows (from the bottom of the column to the top): untreated sandy loam soil (0 to 0.5 cm); aged, treated sandy loam soil (0.5 to 3.5 cm); and untreated sand or loam soil (3.5 to 30.0 cm). The soils were packed into the columns with gentle tapping.

For column leaching, the columns were saturated with $0.01M \, \text{CaCl}_2$ solution (156-194 mL) prior to initiation on January 8^{th} (p. 12). The columns were then leached with $0.01M \, \text{CaCl}_2$ solution in four portions (12.7 cm or 130 mL each; equivalent to 50.8 cm of rainfall) at $25 \pm 1^{\circ}\text{C}$ between January 9^{th} and January 12th. Leachate volumes were collected for each fraction and stored at 4°C . The soil columns were inverted, allowed to drain for ca. 5 days, and sectioned into five segments of approximate equal length (6 cm). The soils were extruded from the columns using a stainless steel rod with a 3.6-cm diameter stainless steel disc attached.

3. Supplementary study: No supplementary experiments were described.

4. Description of analytical procedures:

Extraction/clean up/concentration methods: Aliquots of leachates (80 mL) from the first and last fractions from each column were transferred to 125 mL separatory funnels containing 2 g of NaCl and extracted by partitioning with 50:50 (v:v) dichloromethane:ethyl acetate (3 x 30 mL; p. 13). The extracts were combined in a volumetric flask, diluted to 100 mL, and an aliquot (4 mL) was analyzed for total radioactivity using LSC. The aqueous layer was transferred to a volumetric flask, diluted to 100 mL, and an aliquot (2 mL) was analyzed using LSC.

An additional extraction on leachate samples was conducted by transferring an aliquot (100 mL) of the diluted leachate to a separatory funnel and adding 12M HCl (1.0 mL) prior to extraction with ethyl acetate (2 x 40 mL; p. 13). The ethyl acetate was drained through a small bed of sodium sulfate, and collected in a volumetric flask. The samples were diluted to 100 mL and an aliquot (4 mL) was analyzed using LSC. The aqueous layer was drained into a volumetric flask and diluted to 100 mL, and an aliquot (2 mL) was analyzed using LSC.

PMRA Submission Number {.....}

EPA MRID Number 41479801

The dichloromethane:ethyl acetate (50:50; v:v) and ethyl acetate extracts were combined in a boiling flask and reduced to *ca.* 0.5 mL by rotary evaporation prior to analysis using TLC (p. 13). The residues remaining in the flask were dissolved in methanol (5 mL) prior to analysis using LSC.

Additional leachate volumes remaining from Column 1 (fractions A and D) plus 80 mL each of fractions B and C were combined, added to 2 g of NaCl + 2 mL of 1N HCl, and extracted twice with dichloromethane:ethyl acetate (50:50, v:v; 40 mL; p. 13). The extract was reduced to *ca*. 0.5 mL by vacuum rotary evaporation, and purified twice by TLC (reversed-phase plate developed with methanol:water:HOAC (60:40:1, v:v:v) and silica gel developed with toluene:acetone:HOAC (50:50:2, v:v:v)).

Volatile residue determination: Following aging, the charcoal traps were emptied into separate counting vials (front sections divided into three portions; back sections divided into two portions), the charcoal was air-dried and then analyzed using LSC following combustion (p. 12). Gas dispersion tubes to trap ¹⁴CO₂ were analyzed directly using LSC.

Total ¹⁴C measurement: Samples were analyzed for total radioactivity using LSC.

Non-extractable residues, if any: Portions $(4 \times 10 \text{ g})$ of the aged soils were transferred to counting vials, and aliquots were combusted $(2 \times 1 \text{ g}; p. 12)$. After drying, the column segments were ground and mixed using a mortar and pestle, and a subsample (ca. 10 g) was transferred to a counting vial prior to combustion $(4 \times 1 \text{ g})$.

Derivatization method, if used: No derivatization methods were employed.

Identification and quantification of parent compound: Concentrated leachate extracts were analyzed for oryzalin using silica gel TLC plates developed with toluene:acetone:HOAC (70:30:1, v:v:v; p. 13). Radioactive zones were visualized using autoradiography. Radioactive zones were scraped into methanol:AOAC (80:20, v:v; 5 mL) prior to analysis using LSC. An analytical standard of oryzalin was available for use (purity 98.3%; Lot L1252A; p. 8).

Identification and quantification of transformation products, if appropriate: Samples were analyzed for transformation products as described for the parent compound. The reference compound 4-hydroxy-3,5-dinitro-benezesulfonamide (OR-20; purity not reported) was available for use (p. 9).

The identity of the transformation product was confirmed using negative ion fast atom bombardment mass spectrometry (VG Model ZAB-ZSE; p. 13). The sample was ionized by dissolution in magic bullet (5:1 dithiothreitol:dithioerythritol) and bombardment with a 2 microamp beam of Cs ions of 28 keV energy.

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: Limits of Detection (LOD) and Limits of Quantification (LOO) were not reported.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: During aging, the temperature was maintained at 24.3-25.7°C, and air-flow rates were maintained at 1.8-2.1 mL/minute (p. 14; Table III, p. 20). The temperature was maintained at 24.7-25.2°C during the leaching phase; supporting data were not provided (p. 12). During leaching, the infiltration rate ranged from 1.30 to 3.45 cm/hour (Table XV, p. 34). During aging, the samples were wrapped in foil to protect from light. Lighting conditions during the leaching phase were not reported.

B. MASS BALANCE: Following the aging phase, the overall mass balance was 97.58% of the applied radioactivity (Table VII, p. 24).

Following the leaching phase, overall mass balances ranged from 91.9-97.0% of the applied radioactivity (Table XIX, p. 40).

C. LEACHING: Following the 30-day aging phase, it was determined that 97.32% of the applied oryzalin was recovered in the aged soils, 0.22% was recovered as ¹⁴CO₂, and 0.05% was recovered from the charcoal trapping solutions (Tables IV-VII, pp. 21-24). Aged soils that were extracted showed that ca. 89% of the radioactivity was extracted and partitioned into ethyl acetate (pp. 14-15; Table X, p. 27). Little radioactivity remained in the extracted aqueous solution (<0.2%), and nonextractable radioactivity accounted for ca. 10%. TLC analysis of the aged soil extracts showed that the majority of extracted radioactivity was oryzalin (>80% of the applied; Table XII, p. 31; Figure 4, p. 50). Transformation product OR-20 accounted for 1.5-1.7% of the applied. There was no evidence of degradation during storage (Table X, p. 27; Table XII, p. 30).

Following the leaching phase, radioactivity recovered in the soil segments totalled 89.6% of the applied in column 1 (sand), 84.2% in column 2 (sand), 92.5% in column 3 (loam), and 93.1% in column 4 (loam)(Table XVIII, p. 39). The majority of the radioactivity was observed in the upper 0-6 cm segment for all soil columns. For columns 1 and 2, which were packed with unaged sand, residues detected in the soil columns were 32.7-32.9% at 0-6 cm, 17.1-19.7% at 6-12 cm, 18.5-21.4% at 12-18 cm, 10.3-12.6% at 18-24 cm, and 3.2-5.4% at 24-30 cm. For columns 3 and 4, which were packed with unaged loam, residues detected in the soil columns were 58.2-78.9% at 0-6 cm, 8.5-22.4% at 6-12 cm, 2.9-7.2% at 12-18 cm, 1.4-3.5% at 18-24 cm, and 0.8-1.8% at 24-30 cm.

A total of 7.1%, 7.8%, 2.9%, and 3.9% of the applied radioactivity was found in the leachate fractions from columns 1, 2, 3, and 4, respectively (Table XVI, p. 35). Leachates fractions A and D from each column were extracted, which removed 0.5-2.1% of the radioactivity, leaving

PMRA Submission Number {.....} EPA MRID Number 41479801

≤0.5% in the aqueous fraction (Table XXI, p. 42). TLC analysis of the leachate extracts showed that the majority of extracted radioactivity was OR-20 (25.7-61.9% of the applied; Table XXII, pp. 43-45; Figure 5, p. 51). Only two fractions contained amounts of oryzalin greater than 5%. These fractions also contained an unidentified minor transformation product. Negative ion FAB mass spectrometry confirmed the identity of transformation product OR-20 in the leachate extract samples.

Supplementary Study: No supplementary studies were described.

III. STUDY DEFICIENCIES

- 1. Pesticide residues were aged in a different type of soil (sandy loam) than was used in the leaching columns (sand and loam). This confounds the
- 2. In this study, a sandy loam soil (66% sand and 0.9% organic carbon) was air-dried, treated and aged (moist conditions) for 30 days then packed into a total of four soil columns. OCSPP guidelines specify that for leaching studies with aged residue, soils should have a sand content >70% and an organic carbon content between 0.5-1.5%.
- 3. OCSPP guidelines specify that the soil to be aged should be fresh (not previously air-dried). For leaching, the columns should be packed with air-dried soil that is the same type as was used for aging.
- 4. OCSPP guidelines specify that the aging period of one half-life is recommended, but should not exceed 120 days. The half-life estimated in the aerobic soil metabolism study (MRID 41322801) was between 1.5 and 2.1 months, slightly longer than the aging period of 30 days used in the study.
- 5. The lighting conditions used in the leaching phase of the study were not reported. OCSPP guidelines specify that the soil columns should be kept in the dark during leaching.
- 6. The soil columns used during the leaching phase had an inner diameter of 3.6 cm and were 30 cm in length (p. 11). OCSPP guidelines specify that soil columns should have an inner diameter of at least 4 cm and a minimum height of 35 cm.

IV. REVIEWER'S COMMENTS

1. Soil collection procedures were not reported. OCSPP guidelines specify that the soils should be taken from the top layer (A horizon) to a maximum depth of 20 cm. Also, a detailed history of the field sites from where the test soils were collected was not available.

PMRA Submission Number {.....} EPA MRID Number 41479801

- 2. A reference substance with known leaching behavior was not used to evaluate the relative mobility of oryzalin.
- 3. The columns were packed with untreated soils via gentle tapping (p. 11). OCSPP guidelines specify that a spoon, plunger or vibration apparatus should be used to pack the soil columns in order to obtain uniform packing.
- 4. The method used to maintain a constant column head during leaching upwards through the soil columns was not reported.

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. 2008. Fate, Transport and Transformation Test Guidelines, OCSPP 835.1240, Leaching Studies. Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-08-019.

PMRA Submission Number {	{}	EPA MRID Number 41479801

Attachment 1: Structure of Test Material

Oryzalin [OR-1; EL-119]

IUPAC Name: 3,5-Dinitro-4-(dipropylamino)benzenesulfonamide.

3,5-Dinitro-N⁴,N⁴-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 [ring-UL-¹⁴C]Oryzalin [benzene-U-¹⁴C]Oryzalin [¹⁴C]Oryzalin

* = Location of the radiolabel.

PMRA Submission Number {	l	EPA MRID Number 41479801
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Identified Compounds

Oryzalin [OR-1; EL-119]

IUPAC Name: 3,5-Dinitro-4-(dipropylamino)benzenesulfonamide.

3,5-Dinitro-N⁴,N⁴-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:** $C_{12}H_{18}N_4O_6S$

* structure complexity/form was sacrificed to obtain SMILES string

OR-20

IUPAC Name: 4-Hydroxy-3,5-dinitro-benzenesulfonamide.

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

SMILES String: Oc1c(cc(cc1N(=O)=O)S(N)(=O)=O)N(=O)=O (EpiSuite version 4.0).

formula: