Data Evaluation Record on the anaerobic biotransformation of dimethyl disulfide in water-soil system

PMRA Submission Number {......} EPA MRID Number 47052820

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IUPAC name: Dimethyl disulfide.
CAS name: Dimethyl disulfide.
CAS No: 624-92-0.
Synonyms: DMDS; dimethyldisulfide; DMDS TC, dimethyl disulfide TC, ATOMAL, 2,3-dithiabutane; methyl disulfide; (methyldithio)methane; (methyldisulfanyl)methane; (methyldithio)methane.methyldithion ethane.
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EXECUTIVE SUMMARY

The biotransformation of *bis*-[methyl-^{14}C]-labeled dimethyl disulfide (radiochemical purity 96.6%) was studied in deoxygenated, deionized water-sandy loam soil (water not characterized prior to use; soil pH 7.4, organic carbon 0.5%) systems from California for 71 days under anaerobic (static, nitrogen atmosphere) conditions in darkness at 20°C. Based on the water volume, [^{14}C]dimethyl disulfide was applied at 280 mg a.i./L. The soil:water ratio was *ca.* 1:1.4 (*ca.* 25 g wet wt. soil:35 mL water). This study was conducted in accordance with OPPTS Guideline 835.3300, Soil Biodegradation, and in compliance with USEPA GLP Standards (40 CFR, Part 160). The test apparatus consisted of a sealed bottle (250-mL, 120 x 55 mm, neck diameter 17 mm) containing flooded soil that was kept under a static nitrogen atmosphere. Soil and nitrogen-sparged water were pre-incubated for several days (interval not specified), then following treatment, duplicate flasks were collected after 0 (5 min.), 3, 7, 14, 21 and 71 days of incubation. Upon collection, the incubation bottle was attached to a vacuum system and nitrogen was drawn (100-150 mL/minute, 4 hours) sequentially through the bottle headspace, 1N KOH solution, a solid-phase carbon trap and, finally, through a second 1N KOH solution. Volatiles collection was modified for one system at the final (71-day) interval, so that air was drawn through the bottle headspace, then sequentially through 1N KOH solution, a solid-phase carbon trap, a GC/RAM oxidative reactor tube and, finally, through a second 1N KOH solution. Selected KOH solutions were pH-neutralized and nitrogen-sparged through a solid-phase carbon trap. Water layers were decanted and analyzed directly. Soil was sequentially extracted once with deionized water, followed by twice with acetonitrile, and, finally, again with water. The contents of the solid-phase carbon traps were divided into equal portions and each extracted two or three times with hexane. Water layers, soil extracts, extracted soil, incubation bottle rinses (methanol), KOH trapping solutions, hexane extracts and extracted solid sorbent were analyzed for total radioactivity using LSC. Hexane extracts from the solid sorbent were analyzed by GC/MS and reverse-phase HPLC, with dimethyl disulfide the only compound detected. Water layers, soil extracts and KOH solution (prior to and after neutralization) were analyzed by reverse-phase HPLC. Two major transformation products,

- methane thiol (MT) and
- methanesulfonic acid (MSA),

were detected, but identifications were not confirmed. Methane thiol was detected through re-oxidation to dimethyl disulfide. No minor nonvolatile products were identified.

No determinations, such as redox potentials or dissolved oxygen concentrations, were made to verify that anaerobic conditions were achieved and maintained.

Overall recovery of radiolabeled material averaged 87.9 ± 6.8% (range 72.3-97.9%) of the applied, with no consistent pattern of decline in recoveries over the 71-day study. Following application of [^{14}C]dimethyl disulfide into the water layer *ca.* 68% of the applied volatilized during the 4-hour purge, while remaining [^{14}C]residues partitioned between the water layer and sandy loam soil with mean (n = 2) distribution ratios (water:soil) of 3:1 at day 0 (4+ hours) and 1:1 thereafter.

Dimethyl disulfide dissipated from the water-soil system via transformation and diffusion of parent. The 4-hour purge (100-150 mL/minute) interval to collect volatiles upon sampling probably removed most parent present from the test system. Significant levels of parent dimethyl disulfide were detected in the water layers, but quantitative results were not provided; consequently total levels of parent dimethyl disulfide in the systems and dissipation half-lives presented in this review are underestimated. Volatilized **dimethyl disulfide** was detected at a mean 67.5% of the applied at day 0 (4 hours) and was 42.5% (n = 1) at study termination. **Observed DT50** values for dissipation (volatilization/transformation) of dimethyl disulfide were *ca.* 10 days from the total system and <4 hours from the water layer; a DT50 from the soil could not be estimated. Calculated (all intervals) linear (Excel 2000) and nonlinear (Sigmaplot v 9) half-lives for dissipation of dimethyl sulfide from the total system were 79 and 20 days, respectively; low correlation coefficients ($r^2 < 0.40$) preclude any confidence in the results.

MT and **MSA** were both detected in 14- and 21-day KOH trapping solutions; only one replicate sample per interval was analyzed. At 14 and 21 days posttreatment, **MT** comprised 16.0% and 15.8% of the applied, respectively, and **MSA** comprised 5.4% and 16.2%, respectively. **MSA** was also detected in the water layers, but quantitative results were not provided. Unidentified [^{14}C]residues in the water layer decreased from 21.4% of applied (n = 2) at day 0 (4+ hours) to 11.0% at 21 days and were 11.9% (n = 1) at termination. No transformation products were identified in the soil extracts. Extractable soil [^{14}C]residues increased from 6.4% of the applied (n = 2) at day 0 (4 hours) to 8.5% at 7 days, then decreased to 3.1% (n = 1) at 71 days. Nonextractable [^{14}C]residues increased from 0.1% at day 0 (4 hours) to 5.1% at termination. A methanol rinse of the incubation bottles recovered ≤0.7% of the applied at any interval.

Total radioactivity detected in the KOH solutions increased from 0.7% of applied at day 0 (4 hours) to 7.3% at 7 days, 25.8% at 14 days, 35.8% at 21 days and was 18.0% at termination. Analysis of the KOH solutions determined that the trapping solution absorbed volatile [^{14}C]organics, including MT and MSA, as discussed above, and parent dimethyl disulfide ("early intervals", supporting results were not provided), in addition to $^{14}CO_2$. Barium chloride precipitation analysis of 14- and 21-day KOH solutions determined $^{14}CO_2$ comprised 1.1-2.6% of the applied; no other intervals were analyzed. For the 71-day system, which utilized the modified volatiles trapping system (GC/RAM oxidation reactor tube), [^{14}C]methane was detected, but only at 1% of applied.

Transformation pathways consistent with the products detected in this study were provided by the study authors. In addition to significant levels of diffusion of parent dimethyl disulfide from the water-soil system, the compound was found to degrade to methane thiol, methanesulfonic acid, methane and CO_2 with low levels of formation of bound soil residues.

Results Synopsis:

Test system used: Deionized water-sandy loam soil from California.
Linear half-life in water: ND (not determined).
Linear half-life in soil: ND.
Linear half-life in the total system: 78.9 days ($r^2 = 0.2062$) – not definitive.

Non-linear half-life in water: ND.
Non-linear half-life in soil: ND.
Non-linear half-life in total system: 19.6 days ($r^2 = 0.3926$) – not definitive.

Observed DT50 in water: <4 hours.
Observed DT50 in soil: ND.
Observed DT50 in total system: *ca.* 10 days.

Major transformation products:
Methane thiol (MT - 16.0 percent of applied detected at Day 14 sample – maximum over all samples could not be determined).
Methanesulfonic acid (MSA - 16.2 percent of applied detected at Day 21 sample- maximum over all samples could not be determined).

Minor transformation products:
CO_2 (maximum 2.6% of applied at two intervals analyzed, 14 and 21 days).
Methane (1% at sole interval analyzed, 71 days – maximum over all samples could not be determined).

Study Acceptability: This study is classified as Supplemental. The following significant deviations from good scientific practices or Subdivision N guidelines were noted:

- total levels of parent dimethyl disulfide in the system could not be determined because quantitative results for parent in the water layers were not provided,
- the pattern of formation and decline of transformation products was not adequately addressed,
- material balances were incomplete with up to *ca.* 28% of the applied unaccounted for, and
- it was not confirmed that the system was anaerobic at the time of treatment or during the study.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with OPPTS Guideline 835.3300, Soil Biodegradation (p. 13; Appendix 1, p. 48). The following significant deviations from good scientific practices or the objectives of Subdivision N guidelines were noted:

[^{14}C]Residues in the water layers comprised 10.8-21.6% of the applied. Parent dimethyl disulfide and MSA were detected at the 0- and 21-day intervals (only intervals analyzed), but quantitative results were not provided. Consequently, total levels of parent dimethyl disulfide in the systems could not be determined and dissipation half-lives presented in this review are underestimated.

In addition to MSA levels in the water layers not being reported and/or quantified at all intervals, only one KOH trapping solution sample at both the 14- and 21-day intervals was analyzed for transformation products and both methane thiol and methanesulfonic acid were found to be major (≥10% of applied) products. Therefore, the pattern of formation and decline of the degradates was not established.

Material balances were incomplete with up to 27.7% of the applied unaccounted for. The study author attributed low material balances to volatilization of parent dimethyl disulfide from the system and formation of methane, which the volatiles trapping system was not designed to collect; however, analysis for [^{14}C]methane in one system at the final sampling interval detected the compound at only 1% of applied.

The test soil was not flooded for 30 days prior to treatment, and no determinations, such as redox potentials or dissolved oxygen concentrations, were made to verify that anaerobic conditions were achieved and maintained.

COMPLIANCE: This study was conducted in compliance with USEPA GLP Standards 40 CFR, Part 160 (p. 3). Signed and dated Data Confidentiality, GLP, Quality Assurance and Study Authentication statements were provided (pp. 2-5).

A. MATERIALS:

1. Test Material	*bis*-[Methyl-^{14}C]dimethyl disulfide (p. 14).
Chemical Structure:	See DER Attachment 2.
Description:	Technical, in ethanol solution (p. 14).
Purity: Radiochemical purity:	96.6% (p. 14).

Lot/Batch No.	49520-1-4C (p. 14).
Analytical purity:	Not reported.
Initial specific activity:	12.79 mCi/mmol (2.667 mCi/mL; p. 14; Table 3, p. 30).
Final specific activity:	Reviewer-calculated 0.0205 mCi/mmol (0.0043 mCi/mL); 0.156 mg/mL [^{14}C]dimethyl disulfide + 97.4 mg/mL unlabeled dimethyl disulfide (purity 99.5%, Lot No.: 14514BA; p. 14, Table 3, p. 30).
Location of the radiolabel:	At each methyl C.
Storage conditions of test chemical:	<0°C in darkness (p. 14; Appendix 1, p. 49).

Physico-chemical properties of dimethyl disulfide:

Parameter	**Value**	**Comment**
Molecular weight	94.2 g/mole	
Molecular formula	$C_2H_6S_2$.	
Water solubility	*ca.* 3 g/L.	At 25°C.
Vapor pressure	28.7 mm Hg.	At 25°C.
UV Absorption	At 297.5 nm, molar absorptivity (ε_λ) = 37.32 (M^{-1}, cm^{-1}).	MRID 47052802.
pKa	Not reported.	
K_{ow}/log K_{ow}	Not reported.	
Stability of compound at room temperature	Not reported.	

Data obtained from p. 14 of the study report and Appendix 2, p. 29 in MRID 47052802.

2. Water-soil collection, storage and properties

Table 1: Description of water-soil collection and storage.

Description		**Details**
Geographic location	Water:	Not applicable; deionized (Milli-Q) water used as test water.
	Soil:	Rolinda, California.
Pesticide use history at the collection site		No pesticides or fertilizer for at least 4 years previous to collection.
Collection procedures for	Water:	Not applicable.
	Soil:	Not reported.
Sampling depth for	Water:	Not applicable.
	Soil:	Not reported.
Storage conditions	Water:	Not applicable.
	Soil:	Maintained at *ca.* 4°C in unsealed bags prior to use.
Storage length	Water:	Not applicable.
	Soil:	≤3 months.
Preparation	Water:	Not applicable.
	Soil:	2-mm sieved.

Data obtained from p. 15; Figure 1, p. 35; Appendix 1, p. 52 of the study report.

Table 2: Properties of the water.

Property	**Details**
Temperature (°C)	Not applicable as deionized (Milli-Q) water was used as the test water.
pH	Not determined.
Redox potential (mV)	Not determined.
Oxygen concentration (%)	Not determined.
Dissolved organic carbon (%)	Not determined.
Hardness (mg $CaCO_3$/L)	Not determined.
Electrical conductivity (mmhos/cm)	Not determined.
Microbial biomass/population (units)	Not determined.

Data obtained from p. 15; Figure 1, p. 35 of the study report.

Table 3: Properties of the soil.

Property	**Details**
Soil texture	Sandy loam.
% Sand (2000-50 μm):	Not reported.
% Silt (50-2 μm):	Not reported.
% Clay (<2 μm):	6
pH (soil:water, 1:1)	7.4
Organic carbon (%)[1]	0.5
Organic matter (%)	0.8
CEC (meq/100 g)	6.9
Redox potential (mV)	Not determined.
Moisture at 1/3 atm (%)	Not reported.
Bulk density (g/cm^3)	Not reported.
Microbial biomass/population (units)	Not reported.[2]

Data obtained from p. 15; Appendix 1, p. 52 of the study report.

[1] Percent organic carbon determined by primary reviewer using the following formula: organic carbon (%) = organic matter (%)/1.72.

[2] Although the study protocol specified that microbial biomass was to be determined in the test soil prior to treatment, no results were provided (Appendix 1, p. 52).

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: Preliminary experiments were conducted and determined that the standard "flow through" test system would not be suitable (p. 8). This resulted in development of a test system that would minimize diffusion of dimethyl disulfide.

In one of the experimental systems, a static KOH trapping solution was maintained inside the incubation bottle (p. 21). LSC analysis determined that 16% of the applied radioactivity was recovered in the KOH solution after 8 days of incubation, and 85-91% at 16-27 days. Since, dimethyl disulfide was not expected in the KOH solution, the study author proposed that [^{14}C]methane thiol was being formed; however, methane thiol was known to oxidize to dimethyl disulfide (p. 21). Consequently, an internal KOH trapping solution was not used.

In an additional preliminary experiment, that appeared to utilize the trapping system used for the definitive experiment, [^{14}C]residues recovered in the KOH trapping solution comprised 16.8% and 29.6% of the applied at 14 and 21 days posttreatment, respectively, with $^{14}CO_2$ only accounting for 3.0% and 4.6% of the applied, respectively (Table 5, p. 32).

2. Experimental conditions:

Table 4: Study design.

Parameter	**Details**
Duration of the test	71 days.
Water:	

Parameter		**Details**
Filtered/unfiltered water: Type and size of filter used, if any:		Deoxygenated (nitrogen-sparged), deionized (Milli-Q) water used as test water.
Amount of soil and water per treatment	Water:	35 mL (2- to 3-cm layer).
	Soil:	*ca.* 25 g wet wt.
Water/soil ratio		*ca.* 1.4:1 (35 mL:*ca.* 25 g wet wt.).
Application rates (mg a.i./L)	Nominal:	279 mg a.i./L (9.75 mg a.i./system).
	Actual:	280 mg a.i./L (9.81 mg a.i./35 mL water).
Control conditions, if used		No sterile controls were used.
No. of replications	Control, if used:	No sterile controls were used.
	Treated:	Duplicate treated water-soil systems at each collection interval.
Test apparatus (type/material/volume):		250-mL bottle (120 x 55 mm, neck diameter 17 mm, material composition not reported), sealed with a Teflon (PTFE)-lined septum cap
Details of traps for CO_2 and organic volatiles, if any:		<u>Two-stage SKC Anasorb CSC (coconut shell charcoal) tube</u> (100 mg front:50 mg back, 150 mg total sorbent). <u>1N KOH</u> (two traps) to trap CO_2; the first KOH trap (25 mL in septum-sealed, 60-mL borosilicate, glass vial) preceded the solid sorbent tube, with a second KOH trap (50 mL in glass, gas-washing bottle) placed after the solid sorbent tube (illustrated in Figure 1, p. 35).
If no traps were used, is the system closed?		Systems were incubated closed and attached to a volatiles trapping system upon collection.
Identity and concentration of co-solvent		Ethanol; final concentration 0.3% based on water volume (100 µL ethanol in 35 mL water).
Test material application method	Volume of the test solution used/treatment:	100 µL.
	Application method (*e.g.*: mixed/not mixed):	Test solution was applied, via glass syringe, "through" the water layer across the top of the soil layer.
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.
Microbial biomass/population (units) of controls	Water:	No sterile controls were used.
	Soil:	
Microbial biomass/population (units) of treated	Water:	Treated systems were not analyzed for biomass.[1]
	Soil:	
Experimental conditions	Temperature (°C):	20 ± 2°C.
	Continuous darkness (Yes/No):	Yes.
Other details, if any		At the time of preparation of the water-soil systems, soil moisture was *ca.* 3%.

Data were obtained from pp. 8-9, 14-16; Tables 1-4, pp. 28-31; Figure 1, p. 35; Appendix 1, pp. 52-53 of the study report.

[1] Although the study protocol specified that microbial biomass was to be determined in treated and untreated soil at study termination, no results were provided (Appendix 1, p. 52).

3. Anaerobic conditions: Soil was transferred to the incubation bottles and the headspace purged (flow rate not reported) with nitrogen for 30 seconds (p. 15). Deoxygenated (nitrogen-sparged), deionized (Milli-Q) water was then added over the soil and nitrogen was bubbled through the water layer for 30 seconds, with a final purge of the headspace for 10 seconds. Then the bottles were sealed and maintained at 20 ± 2EC in darkness for "several" days (interval not specified) prior to treatment (p. 15; Appendix 1, p. 53). No determinations, such as redox potentials or dissolved oxygen concentrations, were made to verify that anaerobic conditions were achieved and maintained.

4. Supplementary experiments: None reported.

5. Sampling:

Table 5: Sampling details.

Criteria	Details
Sampling intervals (days posttreatment)	0 (5 min.), 3, 7, 14, 21 and 71 days.
Sampling method	Duplicate treated water-soil systems at each interval.
Method of collection of CO_2 and organic volatile compounds	Upon sampling, the 1N KOH/solid-phase carbon tube/1N KOH volatiles traps were connected to the incubation bottle via an outlet needle. An inlet needle connected the incubation bottle to a nitrogen gas-filled Atmosbag. The nitrogen gas was then drawn (100-150 mL/minute, 4 hours) through the incubation bottle and traps via vacuum pump, with the Atmosbag re-filled with nitrogen gas as needed.
Sampling intervals/times for:	
Sterility check, if sterile controls are used:	No sterile controls were used.
Redox potential, dissolved oxygen, pH:	Not measured.
Sample storage before analysis	**Water layer** and **soil** were separated and soil extracted the day of collection. Any storage of water layer and/or soil extracts prior to analysis was not reported.
Other observations, if any	None.

Data were obtained from pp. 15-17; Table 4, p. 31; Figure 1, p. 35 of the study report.

C. ANALYTICAL METHODS:

Separation of the soil and water: Duplicate aliquots (volume not reported) of the water layer were taken and analyzed for total radioactivity by LSC prior to decanting from the soil (pp. 17-18). Duplicate aliquots (volume not reported) of the 0- and 21-day water layers were analyzed directly by HPLC as described below (pp. 17, 20).

Extraction/clean up/concentration methods: Soil was transferred to a 250-mL, wide-mouth Nalgene bottle and sequentially extracted once with deionized water (75 mL), followed by twice with acetonitrile (50 mL x 2) and a final extraction again with water (50 mL, p. 17). Each extraction was done via mechanical shaking (mechanism type not reported) for 15 minutes; after which, soil and extract were separated by centrifugation (3,500 rpm, 10 minutes). Duplicate aliquots (volume not reported) of each extract were analyzed for total radioactivity by LSC (pp. 17-18).

Incubation bottle rinse. After removal of the soil, the incubation bottles were rinsed with methanol (25 mL) to recover any residual [^{14}C]residues, with duplicate aliquots (volume not reported) analyzed for total radioactivity by LSC (p. 17).

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the water layers, soil extracts, extracted soil, bottle rinse and volatiles trapping materials (Table 4, p. 31).

Determination of non-extractable residues: Aliquots (weight, replicates not reported) of extracted, wet soil were analyzed for total radioactivity by LSC following combustion (pp. 17-18).

Determination of volatile residues: KOH solutions. Duplicate aliquots (volume not reported) the KOH trapping solutions were analyzed for total radioactivity by LSC (pp. 17-18). Aliquots of selected KOH solutions from the "first" trap that preceded the solid-phase carbon trap were also analyzed by HPLC and GC/MS as described below (pp. 18, 20; Figure 1, p. 35).

Neutralization of KOH solutions. The study author proposed that methane thiol was being formed and re-oxidized to dimethyl disulfide (p. 21). To recover [^{14}C]dimethyl disulfide formed from the re-oxidation of [^{14}C]methane thiol, aliquots of selected KOH solutions were adjusted to neutral pH with HCl, then purged with nitrogen and the released [^{14}C]residues drawn through a solid-phase (CSC) carbon trap. The nitrogen-sparged neutralized KOH solution was analyzed by HPLC and the solid sorbent extracted and analyzed as described below.

Solid-phase (CSC) carbon trap. The trap was opened and the sorbent divided into two, approximately equal, portions; "front" and "rear" of the trap (p. 16). Each portion was extracted two to three times with hexane; extraction solvent volumes were 5.0 mL (Table 7, p. 34). Extraction was done via mechanical shaking (mechanism not specified) for 15 minutes; after which, extract was drawn off via pipette. Duplicate aliquots (volume not reported) of each extract were analyzed for total radioactivity by LSC, and an aliquot (volume not reported of the initial hexane extract was analyzed by HPLC and GC/MS as described below (pp. 16-17). Aliquots (weight, replicates not reported) of the extracted sorbent were analyzed for total radioactivity by LSC following combustion (p. 17).

Derivatization method, if used: None was reported.

Identification and quantification of parent compound: Aliquots of the 0- and 21-day water layer samples, 7-day solid sorbent hexane extract, 21-day KOH trapping solution (trap that preceded solid-phase carbon trap), and 14- and 21-day KOH trapping solutions after pH neutralization were analyzed using reverse-phase HPLC under the following conditions: Betasil C-8 column (4.6 x 100 mm, 5 μm), column temperature ambient, either isocratic mobile phase combining 0.1% formic acid in methanol (A) and 0.1% aqueous formic acid (B) at A:B, 70:30 (v:v, run time 10 min.) or gradient mobile phase [percent A:B at 0-3 min. 0:100 (v:v), 5-8 min. 70:30, 10 min. 0:100], injection volume 50-100 μL, flow rate 1 mL/minute, and radioactivity detector (mechanism type not specified, p. 20). Parent [^{14}C]dimethyl disulfide was by comparison to the retention time of labeled reference standard (Figures 7-9, pp. 41-43).

Aliquots of the 14- and 21-day initial solid sorbent hexane extracts and KOH trapping solutions (same intervals) were analyzed using GC/MS under the following conditions: Varian 3800 GC/1200 MS system, Supelco SPB-1 Sulfur column (0.32 mm x 30 m, 4μ film thickness), flow rate 1.2 mL/minute, temperature gradient 40-200°C at 40°C/minute, electron ionization (EI), ion mode positive, electron energy -70 eV, detector and discharge voltage 1,500 V, manifold temperature 40°C, ion source temperature 150°C, transfer line temperature 200°C, scan mode centroid, scan time 0.25 second (pp. 18-19). Parent [^{14}C]dimethyl disulfide was identified by comparison to the retention time of reference standard (Figures 4-5, pp. 38-39).

Identification and quantification of transformation products: Methanesulfonic acid (MSA). MSA was detected and quantified using reverse-phase HPLC as described for the parent compound; however, a chromatogram of reference standard MSA was not provided (pp. 20, 22; Figures 8-9, pp. 42-43). Identification of MSA was confirmed via LC/MS-ESI (conditions not reported) in 21-day neutralized KOH solution (p. 22; Figure 10, p. 44). Although a LC/MS chromatogram of reference standard MSA was not provided, the chromatograms of the 21-day sample [^{14}C]MSA were comparable to chromatograms of reference standard MSA (LC/MS-ESI) provided in the dimethyl disulfide aerobic soil metabolism study (Appendix 2, pp. 78-79 in MRID 47052819) submitted concurrently with this study.

Methane thiol (as re-oxidized [^{14}C]dimethyl disulfide) was detected and quantified via GC/MS and HPLC as described for parent compound (pp. 21-22; Figure 4, p. 38; Figures 6-7, pp. 40-41; Figure 9, p. 43).

Identification of $^{14}CO_2$. Aliquots (1 mL) of the KOH solutions were combined with 1M barium chloride solution (KOH:$BaCl_2$, 1:1, v:v) and refrigerated overnight (p. 18). The samples were then vortexed for *ca.* 10 seconds, allowed to stand (interval not reported) and centrifuged (3,000 rpm, *ca.* 2 minutes). Total radioactivity in the KOH solutions was determined via LSC prior to and after barium chloride precipitation. The resulting precipitate was also re-suspended in 1N HCl solution and analyzed by LSC.

Methane. To determine if methane was present, the volatile trapping system was modified for one of the 71-day water-soil systems in the following manner:

- the Atmos bag (nitrogen gas) was removed from the incubation bottle inlet,
- the initial KOH trapping solution of 25 mL in a septum-sealed, 60-mL borosilicate, glass vial was changed to 50 mL in a glass, gas-washing bottle, and
- following the solid-phase (CSC) carbon trap, headspace gases were passed through a GC/RAM oxidation reactor tube (700°C) and a second KOH trapping solution (p. 23).

This system was designed to trap [^{14}C]methane thiol and $^{14}CO_2$ in the initial KOH trapping solution, parent [^{14}C]dimethyl disulfide on the solid-phase carbon sorbent, then oxidize any [^{14}C]methane to $^{14}CO_2$.

No reference compounds were reported for identifying transformation products of dimethyl disulfide.

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

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: After the initiation of anaerobic conditions (flooding with deoxygenated, deionized water; static nitrogen atmosphere), the water-soil systems were incubated for "several" days (interval not specified) prior to treatment. No determinations, such as redox potentials or dissolved oxygen concentrations, were made to verify that anaerobic conditions were achieved and maintained. Additionally, no records were provided to establish that the incubation temperature was maintained at 20 ± 2°C throughout the study (Appendix 1, p. 51).

B. MATERIAL BALANCE: Overall recovery of radiolabeled material averaged 87.9 ± 6.8% (range 72.3-97.9%, n = 11) of the applied, with no consistent pattern of decline in total applied radioactivity throughout the incubation (DER Attachment 2, Reviewer's Comment No. 1). Four hours following application of [^{14}C]dimethyl disulfide into the water layer *ca.* 67-69% of the applied had volatilized, while the remaining [^{14}C]residues partitioned between the water layer and sandy loam soil with mean (n = 2) distribution ratios (water:soil) of 3:1 at day 0 (4+ hours) and 1:1 at 3-71 days (DER Attachment 2).

Table 6. Biotransformation of *bis*-[methyl-^{14}C]dimethyl disulfide, expressed as percentage of applied radioactivity (n = 1 or mean ± s.d., n = 2[1]), in deionized water-California sandy loam soil under anaerobic conditions.

Compound		**Sampling times (days)**					
		0[2]	**3**	**7**	**14**	**21**	**71**
Dimethyl disulfide (all volatilized)	System[3]	67.5 ± 1.2	54.4 ± 5.2	56.3 ± 5.3	35.1 ± 2.4	31.6 ± 7.1	42.5
Methane thiol	System[4]	--[5]	--	--	16.0[9]	15.8[9]	--
MSA	System[6]	--	--	--	5.4[9]	16.2[9]	--
CO_2		--	--	--	1.9 ± 0.8	2.5 ± 0.0	--
Unidentified [^{14}C]residues in KOH solutions		0.7 ± 0.0	2.9 ± 0.1	7.3 ± 1.4	4.8, 21.7[7]	7.3, 27.5[7]	18.0
Total in KOH solutions		0.7 ± 0.0	2.9 ± 0.1	7.3 ± 1.4	25.8 ± 1.5	35.8 ± 5.8	18.0
Extractable soil residues[8]		6.4 ± 0.6	7.9 ± 0.9	8.5 ± 0.1	6.2 ± 0.3	5.5 ± 0.3	3.1
Nonextractable soil residues[10]		0.1 ± 0.0	1.6 ± 0.2	2.4 ± 0.8	4.4 ± 0.3	5.0 ± 0.9	5.1
Total recovery	Volatiles	68.2 ± 1.2	57.3 ± 5.2	63.6 ± 3.9	60.9 ± 0.9	67.4 ± 1.3	60.5
	Water	21.4 ± 0.2	13.6 ± 2.3	14.6 ± 2.0	14.3 ± 1.1	11.0 ± 0.2	11.9
	Soil	6.5 ± 0.6	9.4 ± 1.0	10.8 ± 0.7	10.6 ± 0.6	10.4 ± 1.1	8.2
	Flask rinse	0.4 ± 0.1	0.6 ± 0.0	0.7 ± 0.0	0.7 ± 0.0	0.7 ± 0.1	0.2
	System	96.4 ± 1.5	80.8 ± 8.5	89.7 ± 5.1	86.5 ± 0.8	89.5 ± 0.4	80.8

Data obtained from DER Attachment 2.

[1] Reviewer's Comment No. 1.

[2] The 0-day treated soil samples were taken for analysis "within 5 minutes of fortification"; however, incubation flask headspace gases were then evacuated via vacuum purge (100-150 mL/minute) for a 4-hour interval (pp. 15-16).

[3] Recovered in volatiles solid-phase carbon traps and pre-cartridge KOH traps via purging upon collection. Also recovered via combustion in sorbent traps. Recoveries in initial water layer (p.22) and KOH traps (p. 21) not quantified.

[4] Recovered from KOH trapping solution following re-oxidation to dimethyl disulfide (p. 23).

[5] Not reported/not determined.

[6] Recovered in KOH trapping solution (p. 22). Recoveries in initial water layer not quantified (p 22).

[7] [^{14}C]Residues identified in both replicates shown.

[8] None identified. Detected from ACN1, ACN2, water 1, and water 2 extracts.

[9] Detected in one replicate only.

[10] None identified. Detected from soil combustion.

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Dimethyl disulfide dissipated from the water-soil system via transformation and diffusion of parent. The 4-hour purge (100-150 mL/minute) interval to collect volatiles upon sampling probably removed most parent dimethyl disulfide present from the test system; however, the study author reported that "the majority of the radioactivity left in the water corresponded to unswept DMDS", but provided no quantitative results (p. 22; Figure 8, p. 42). Volatilized [^{14}C]dimethyl disulfide was detected at 66.3-68.6% of the applied at day 0 (4 hours) and was 42.5% (n = 1) at 71 days (final interval, DER Attachment 2).

HALF-LIFE/DT50/DT90: The observed DT50 value (based on mean detected at each interval) for dissipation of dimethyl disulfide via volatilization (combined diffusion/purging) from the total system was *ca.* 10 days. Calculated (all intervals) linear (Excel 2000) and nonlinear (Sigmaplot v 9) half-lives for dissipation of dimethyl sulfide from the total system were 79 and 20 days, respectively (DER Attachment 2).

The observed DT50 value for dissipation of dimethyl disulfide from the water layer was <4 hours, while a DT50 value could not be determined in the soil due to lack of data.

Half-lives/DT50/DT90

Phase	Half-life/DT50[1] (days)	First order linear regression equation	r^2	DT50[2] (days)	DT90[2] (days)
Deionized water					
Linear/natural log	ND[3]	--	--	--	--
Nonlinear/normal	ND	--	--	--	--
Observed DT50	<4 hours	--	--	--	--
California sandy loam soil					
Linear/natural log	ND	--	--	--	--
Nonlinear/normal	ND	--	--	--	--
Observed DT50	ND	--	--	--	--
Total system					
Linear/natural log	78.9	y = -0.0088x + 4.0161	0.2062	--	--
Nonlinear/normal	19.6	--	0.3926	14.3	47.4
Observed DT50	*ca.* 10	--	--	--	--

[1] Determined by the primary reviewer using Excel 2000 (linear) and Sigmaplot v 9.0 (nonlinear) and individual sample data obtained from Table 7, p. 34 of the study report (DER Attachment 2).

[2] Determined by the study author using kinetic modeling (KinGui software, Bayer CropScience) and assuming the [^{14}C]residues detected in the water layer at day 0 posttreatment (4 hours) were parent [^{14}C]dimethyl disulfide (Appendix 2, pp. 59-67).

[3] Could not determined due to lack of data.

TRANSFORMATION PRODUCTS: Two major nonvolatile transformation products,

- methane thiol (MT) and
- methanesulfonic acid (MSA),

were detected; no minor products were identified. MT and MSA were both detected in 14- and 21-day KOH trapping solutions; only one replicate sample per interval was analyzed. At 14 and 21 days posttreatment, MT comprised 16.0% and 15.8% of the applied, respectively, and MSA comprised 5.4% and 16.2%, respectively (DER Attachment 2).

The study author reported that MSA was detected in the 0- and 21-day water layers (only intervals analyzed), but no quantitative results were provided (p. 22; Figure 8, p. 42). Unidentified [^{14}C]residues in the water layer decreased from 21.2-21.6% of applied at day 0 (4+ hours) to 10.8-11.2% at 21 days and were 11.9% at 71 days (DER Attachment 2).

The study author reported that no transformation products were detected in the soil extracts (p. 23), but no supporting data were provided.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: Extractable soil [^{14}C]residues increased from 5.8-7.0% of the applied at day 0 (4 hours) posttreatment to 7.0-8.7% at 3-7 days, then decreased to 5.2-5.7% at 21 days and 3.1% at 71 days (DER Attachment 2). Nonextractable [^{14}C]residues increased from 0.1% at day 0 (4 hours) to 4.1-5.8% at 14-21 days and were 5.1% at 71 days. Flask rinses recovered only 0.2-0.7% of the applied at any interval (DER Attachment 2).

VOLATILIZATION: Parent dimethyl disulfide reportedly accounted for all volatilized [^{14}C]residues recovered by the solid-phase carbon traps (p. 22).

Total radioactivity detected in the KOH solutions increased from 0.7% of applied at day 0 (4 hours) to 5.9-8.7% at 7 days, 24.3-27.3% at 14 days, 30.0-41.6% at 21 days and was 18.0% at 71 days (DER Attachment 2). Analysis of the KOH solutions determined that the trapping solution absorbed volatile [^{14}C]organics, including MT and MSA discussed above, in addition to $^{14}CO_2$. The study author reported that at the "early time points" (<10% of applied), the majority of the [^{14}C]residues were comprised of parent dimethyl disulfide (p. 21), but no supporting data were provided. Barium chloride precipitation analysis of 14- and 21-day KOH solutions determined $^{14}CO_2$ comprised 1.1-2.6% of the applied; no other intervals were analyzed (Table 5, p. 32, DER Attachment 2).

The volatile trapping system for the one of the system replicates taken at the final sampling interval was modified to include an oxidation reactor tube and [^{14}C]methane was detected, but only at 1% of applied (p. 23).

TRANSFORMATION PATHWAY: The study author provided transformation pathways that were consistent with the transformation products detected in this study (Figure 12, p. 46). In addition to significant levels of diffusion of parent dimethyl disulfide from the water-soil system, the compound was found to degrade to methane thiol, methanesulfonic acid, methane and CO_2 with low levels of formation of bound soil residues.

Table 7: Chemical names and CAS numbers for the transformation products of dimethyl disulfide.

Applicants Code Name	CAS Number	Chemical Name[1]	Chemical Formula	MW (g/mol)	Smiles String
MT	--[2]	methane thiol	--	--	--
MSA	75-75-2[3]	methanesulfonic acid	CH_4O_3S	95.98	--[2]

Data obtained from p. 21 of the study report and Appendix 2, p. 76 in MRID 47052819.

1 Identifications based on comparison to retention times (GC/MS, HPLC) of reference standards.

2 Information not provided.

3 Information obtained from aerobic soil metabolism study (MRID 47052819) submitted concurrently with this study.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: No supplementary experiments were reported.

III. STUDY DEFICIENCIES

1. [^{14}C]Residues in the water layers comprised 10.8-21.6% of the applied, and while parent dimethyl disulfide and MSA were detected at the 0- and 21-day intervals (only intervals analyzed) quantitative results were not provided (p. 22; Figure 8, p. 42). Consequently, total levels of parent dimethyl disulfide in the systems and dissipation half-lives presented in this review are underestimated.

2. Only one KOH trapping solution sample at both the 14- and 21-day intervals was analyzed for transformation products methane thiol and methanesulfonic acid and both compounds were found to be major (≥10% of applied) products. Therefore, the pattern of formation and decline of the degradates was not established.

3. Material balances were incomplete with up to 27.7% of the applied unaccounted for. The study author attributed low material balances to volatilization of parent dimethyl disulfide from the system and formation of methane which the volatile trapping system was not designed to collect (p. 21). However, analysis for [^{14}C]methane in one system at the final sampling interval detected the compound at only 1% of applied (p. 23).

IV. REVIEWER'S COMMENTS

1. Mean results and standard deviations presented in this review were determined by the primary reviewer using Microsoft Excel 2000 (9.0.2720) software (DER Attachment 2). Standard deviations were determined using the "biased" or "n" method which determines the standard deviation of the entire sample population. Material balance summations and mean results reported by the study author (Table 7, p. 34) were verified by the primary reviewer and there was consistent agreement (within ± 0.1% of applied) between the study author's reported mean values and those determined by the primary reviewer (DER Attachment 2).

2. The test soil was inadequately characterized; the percent sand and silt were not reported so the textural classification could not be confirmed.

3. The test application rate of 390 mg a.i./kg soil selected for this study was reported as equivalent to a field rate of 800 lbs a.i./A (initial anticipated commercial application rate), assuming a soil incorporation depth of 6 inches and bulk density of 1.5 g/cm^3 (p. 8; Tables 1-2, pp. 28-29).

4. Figure 11 (p. 45) was not referenced by the study author and is a GC/MS analysis of headspace gases from a sampling interval (59 days) not referenced in this study.

V. REFERENCES

1. 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.

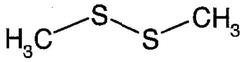
2. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Attachment 1: Structures of Parent Compound and Transformation Products

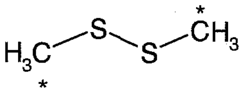
Dimethyl disulfide [DMDS; dimethyldisulfide; DMDS TC, dimethyl disulfide TC, ATOMAL, 2,3-dithiabutane; methyl disulfide; (methyldithio)methane; (methyldisulfanyl)methane; (methyldithio)methane.methyldithion ethane]

IUPAC Name: Dimethyl disulfide.
CAS Name: Dimethyl disulfide.
CAS Number: 624-92-0
SMILES String: S(SC)C (EPI Suite, v3.12 SMILES String).

Unlabeled



***bis*-[Methyl-^{14}C]dimethyl disulfide**

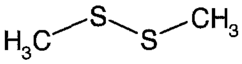


* = Location of the radiolabel.

Identified Compounds

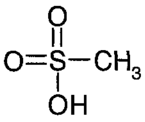
Dimethyl disulfide [DMDS; dimethyldisulfide; DMDS TC, dimethyl disulfide TC, ATOMAL, 2,3-dithiabutane; methyl disulfide; (methyldithio)methane; (methyldisulfanyl)methane; (methyldithio)methane.methyldithion ethane]

IUPAC Name: Dimethyl disulfide.
CAS Name: Dimethyl disulfide.
CAS Number: 624-92-0
SMILES String: S(SC)C (EPI Suite, v3.12 SMILES String).



Methanesulfonic acid [MSA]

IUPAC Name: Methanesulfonic acid.
CAS Name: Not reported.
CAS Number: 75-75-2.



Methane thiol [MT]

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

No structure provided.

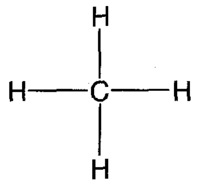
Carbon Dioxide

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

$O=C=O$

Methane

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



$$H-\overset{\displaystyle H}{\underset{\displaystyle H}{C}}-H$$

Attachment 2: Excel and SigmaPlot Spreadsheets

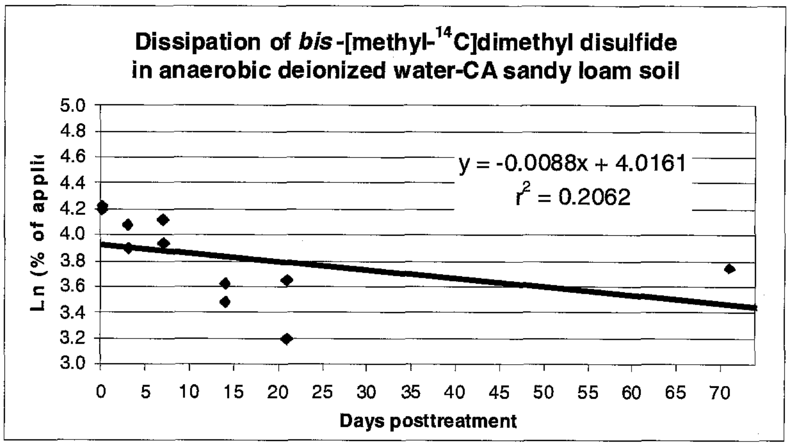
Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052820
Guideline: 162-3

Anaerobic aquatic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in deionized water-California sandy loam soil systems.
Half-life determination: total system.

Half-life (days)	**78.9**	**(0- to 71-day data)**

Days Posttreatment	Dimethyl disulfide (% of Applied)	Dimethyl disulfide Ln (% applied)
0	100.0	4.605170186
0.17	66.3	4.194189897
0.17	68.6	4.228292535
3	59.5	4.085976313
3	49.2	3.895893623
7	61.5	4.119037175
7	51.0	3.931825633
14	32.7	3.487375078
14	37.5	3.624340933
21	24.5	3.198673118
21	38.7	3.6558396
71	42.5	3.749504076

"Time 0" presumed to be 100%; first sampling interval after 4 hours of volatiles collection.
Study authors reported that radioactivity recovered in the solid sorbent (CT) traps was identified as dimethyl disulfide; data imported from **Volatiles** worksheet.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.454144844
R Square	0.206247539
Adjusted R Square	0.126872293
Standard Error	0.35587024
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Sig F*
Regression	1	0.329069047	0.3291	2.598386143	0.1380489
Residual	10	1.266436274	0.1266		
Total	11	1.59550532			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	4.016144881	0.126192781	31.825	2.20696E-11	3.7349698	4.29732	3.734969794	4.29731997
X Variable 1	-0.008786903	0.005451098	-1.612	0.138048902	-0.020933	0.0033589	-0.02093271	0.0033589

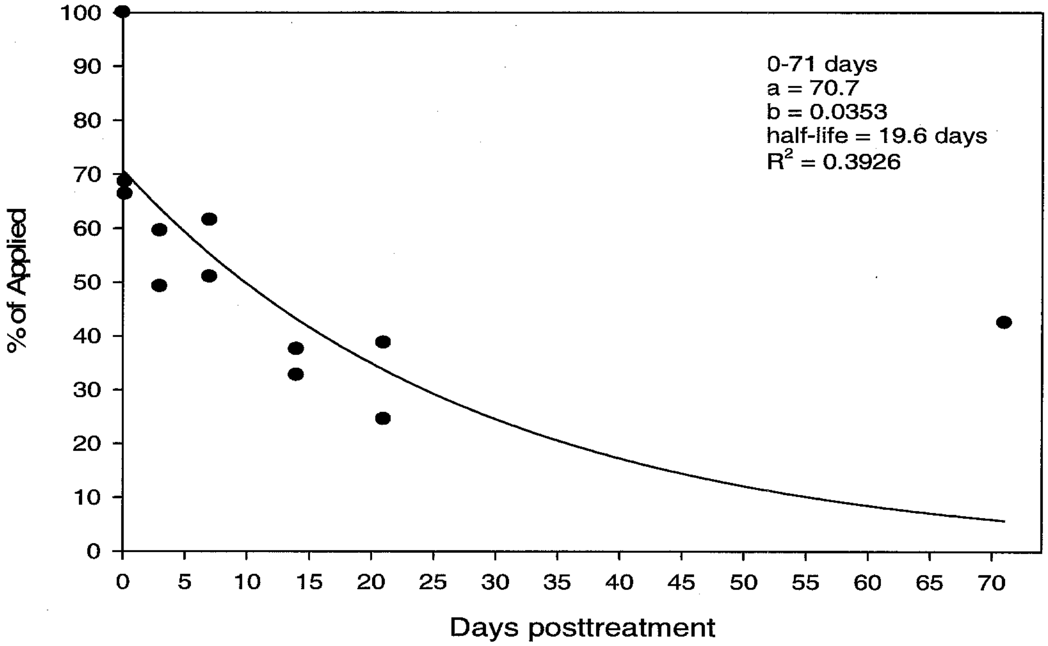
Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052820
Guideline: 162-3

Anaerobic aquatic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in deionized water-C
Nonlinear half-lives (exponential decay/single compartment, 2 parameter):

Deionized water-California loamy sand soil:

Phase	water	soil	system
Half-life (days)	ND[1]	ND	19.6
r squared			0.3926

[1] Not determined due to lack of data.



bis-[methyl-^{14}C]dimethyl disulfide in anaerobic deionized water-CA sandy loam soil (1/2 model, nonlinear)

"Time 0" presumed to be 100%; first sampling interval after 4 hours of volatiles collection.

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052820
Guideline: 162-2
Deionized water-California sandy loam soil
***bis*-[methyl-^{14}C]-label**

```
Nonlinear Regression

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
xnear0(q) = max(abs(q))-abs(q)
yatxnear0(q,r) = xatymax(q,xnear0(r))
[Parameters]
a = yatxnear0(y,x)  "Auto {{previous: 70.6633}}
b = if(x50(x,y)-min(x)=0, 1,  -ln(.5)/(x50(x,y)-min(x)))  "Auto {{previous: 0.0352581}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance=0.0001
stepsize=100
iterations=100

R = 0.62655013   Rsqr = 0.39256507          Adj Rsqr = 0.33182157

Standard Error of Estimate = 16.6068

             Coefficient  Std. Error        t              P
a           70.6633       7.8568          8.9939         <0.0001
b            0.0353       0.0138          2.5634           0.0282

Analysis of Variance:
             DF           SS                MS              F               P
Regression  1        1782.3187       1782.3187         6.4627          0.0293
Residual   10        2757.8680        275.7868
Total      11        4540.1867        412.7442

PRESS = 3898.5995

Durbin-Watson Statistic = 1.1040

Normality Test:   K-S Statistic = 0.2085      Significance Level = 0.6206

Constant Variance Test:    Passed    (P = 0.2734)

Power of performed test with alpha = 0.0500: 0.5976
```

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052820
Guideline: 162-2
Deionized water-California sandy loam soil
***bis*-[methyl-^{14}C]-label**
The power of the performed test (0.5976) is below the desired power of 0.8000.
You should interpret the negative findings cautiously.

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	70.6633	29.3367	1.7665	2.0051	2.4600
2	70.2493	-3.9493	-0.2378	-0.2685	-0.2557
3	70.2493	-1.6493	-0.0993	-0.1121	-0.1065
4	63.5706	-4.0706	-0.2451	-0.2621	-0.2495
5	63.5706	-14.3706	-0.8653	-0.9251	-0.9178
6	55.2086	6.2914	0.3788	0.3985	0.3811
7	55.2086	-4.2086	-0.2534	-0.2666	-0.2538
8	43.1341	-10.4341	-0.6283	-0.6855	-0.6661
9	43.1341	-5.6341	-0.3393	-0.3701	-0.3536
10	33.7003	-9.2003	-0.5540	-0.6344	-0.6144
11	33.7003	4.9997	0.3011	0.3448	0.3290
12	5.7811	36.7189	2.2111	2.3398	3.2998

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.5797	0.2238	1.3210
2	0.0099	0.2158	-0.1341
3	0.0017	0.2158	-0.0559
4	0.0049	0.1251	-0.0943
5	0.0612	0.1251	-0.3470
6	0.0085	0.0963	0.1244
7	0.0038	0.0963	-0.0828
8	0.0447	0.1599	-0.2906
9	0.0130	0.1599	-0.1543
10	0.0627	0.2375	-0.3429
11	0.0185	0.2375	0.1836
12	0.3281	0.1070	1.1424

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	70.6633	53.1573	88.1692	29.7288	111.5978
2	70.2493	53.0590	87.4395	29.4488	111.0497
3	70.2493	53.0590	87.4395	29.4488	111.0497
4	63.5706	50.4837	76.6576	24.3222	102.8191
5	63.5706	50.4837	76.6576	24.3222	102.8191
6	55.2086	43.7274	66.6899	16.4660	93.9513
7	55.2086	43.7274	66.6899	16.4660	93.9513
8	43.1341	28.3381	57.9301	3.2832	82.9850
9	43.1341	28.3381	57.9301	3.2832	82.9850
10	33.7003	15.6681	51.7325	-7.4620	74.8626
11	33.7003	15.6681	51.7325	-7.4620	74.8626
12	5.7811	-6.3241	17.8864	-33.1510	44.7133

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052820
Guideline: 162-3

Anaerobic aquatic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in deionized water-California sandy loam soil systems. Determination of unidentified residues in KOH solutions.

Day	KOH trap solutions								
	Initial	$^{14}CO_2$			MT	MSA	Unidentified		
	% AR	% AR	Mean	s.d.	% AR	% AR	% AR	Mean	s.d.
0	0.7						0.7		
	0.7						0.7	0.7	0.0
3	3.0						3.0		
	2.8						2.8	2.9	0.1
7	5.9						5.9		
	8.7						8.7	7.3	1.4
14	27.3	1.1			16.0	5.4	4.8		
	24.3	2.6	1.9	0.8			21.7	13.3	8.5
21	41.6	2.4			15.8	16.2	7.3		
	30.0	2.5	2.5	0.0			27.5	17.4	10.1
71	18.0						18.0		

Results from Tables 5-6, pp. 32-33 of the study report.
In Table 6 (p. 33), study author reported that "% Volatiles in Dose" = MT, and
"% of Dose Unidentified in Water" was = MSA (pp. 22-23).
Results for "Day 21 Rep. 1" and "Day 21 Repeat" were averaged.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052820
Guideline: 162-3

Anaerobic aquatic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in deionized water-California sandy loam soil systems.
[14C]Residue water phase:soil ratios.
Total [^{14}C]residues in soil.

	Soil				
	Ext.	**Nonext.**	**Total in Soil**		
Day	% AR	% AR	% AR	Mean	s.d.
0	5.8	0.1	5.9		
	7.0	0.1	7.1	6.5	0.6
3	8.7	1.7	10.4		
	7.0	1.4	8.4	9.4	1.0
7	8.5	1.6	10.1		
	8.4	3.1	11.5	10.8	0.7
14	6.5	4.7	11.2		
	5.9	4.1	10.0	10.6	0.6
21	5.7	5.8	11.5		
	5.2	4.1	9.3	10.4	1.1
71	3.1	5.1	8.2		

[14C]Residue water phase:soil ratios.

	Water	**Soil**	**Ratio**	**Ratio**	**W:S ratio**		**S:W ratio**	
Day	% AR	% AR	**W:S**	**S:W**	**Mean**	**s.d.**	**Mean**	**s.d.**
0	21.6	5.9	4	0				
	21.2	7.1	3	0	3	0	0	0
3	15.9	10.4	2	1				
	11.3	8.4	1	1	1	0	1	0
7	16.6	10.1	2	1				
	12.6	11.5	1	1	1	0	1	0
14	15.4	11.2	1	1				
	13.2	10.0	1	1	1	0	1	0
21	10.8	11.5	1	1				
	11.2	9.3	1	1	1	0	1	0
71	11.9	8.2	1	1				

Results imported from **Mat bal** worksheet.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052820
Guideline: 162-3

Anaerobic aquatic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in deionized water-California sandy loam soil systems.
Summations and determination of means/standard deviations for volatilized radioactivity.

	KOH trap solutions					Solid-phase (CSC) carbon trap														Total Volatiles		
						Extractable								Nonextractable			Total Volatile organics					
	KOH#1	KOH#2	Total			F#1	F#2	F#3	B#1	B#2	Total											
Day	% AR	% AR	% AR	Mean	s.d.	% AR	% AR	% AR	% AR	% AR	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	0.6	0.1	0.7			60.0	4.4	0.4	0.3	0.0	65.1			1.2			66.3			67.0		
	0.5	0.2	0.7	0.7	0.0	59.7	5.5	0.7	1.6	0.1	67.6	66.4	1.3	1.0	1.1	0.1	68.6	67.5	1.2	69.3	68.2	1.2
3	2.9	0.1	3.0			54.3	3.6	0.4	0.3	0.0	58.6			0.9			59.5			62.5		
	2.7	0.1	2.8	2.9	0.1	43.5	2.7	0.3	1.9	0.1	48.5	53.6	5.1	0.7	0.8	0.1	49.2	54.4	5.2	52.0	57.3	5.2
7	5.8	0.1	5.9			55.1	4.5	0.5	0.3	0.0	60.4			1.1			61.5			67.4		
	8.5	0.2	8.7	7.3	1.4	46.3	3.3	0.3	0.3	0.0	50.2	55.3	5.1	0.8	1.0	0.2	51.0	56.3	5.3	59.7	63.6	3.9
14	27.2	0.1	27.3			29.3	2.3	0.3	0.2	0.0	32.1			0.6			32.7			60.0		
	24.1	0.2	24.3	25.8	1.5	32.9	3.2	0.4	0.2	0.0	36.7	34.4	2.3	0.8	0.7	0.1	37.5	35.1	2.4	61.8	60.9	0.9
21	41.5	0.1	41.6			21.8	1.8	0.2	0.2	0.0	24.0			0.5			24.5			66.1		
	29.8	0.2	30.0	35.8	5.8	34.2	3.0	0.5	0.2	0.0	37.9	31.0	7.0	0.8	0.7	0.2	38.7	31.6	7.1	68.7	67.4	1.3
71	17.0	1.0	18.0			38.7	3.0	0.3	0.1	0.0	42.1			0.4			42.5			60.5		

KOH#1 and **KOH#2** refer to "Pre-cartridge KOH" and "KOH Trap", respectively.
F#1, **F#2**, **F#3**, **B#1** and **B#2** refer to "front sorbent #1, #2 and #3" and "back sorbent #1 and #2", respectively.
Nonextractable refers to "cartridge combustion".
Results from Table 7, p. 34 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052820
Guideline: 162-3

Anaerobic aquatic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in deionized water-California sandy loam soil systems.
Confirmation of summations (material balances) and determination of means/standard deviations for applied radioactivity.

				Soil																								
				Extractable													Volatiles									Study Reported		
	Water			H2O 1	ACN 1	ACN 2	H2O 2	Total			Nonextractable			Flask rinse			KOH			CT			Material Balance			Material Balance		
Day	% AR	Mean	s.d.	%AR	%AR	%AR	%AR	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.	% AR	Mean	s.d.
0	21.6			4.9	0.8	0.1	0.0	5.8			0.1			0.4			0.7			66.3			94.9			94.9		
	21.2	21.4	0.2	6.0	0.9	0.1	0.0	7.0	6.4	0.6	0.1	0.1	0.0	0.3	0.4	0.1	0.7	0.7	0.0	68.6	67.5	1.2	97.9	96.4	1.5	97.9	96.4	1.5
3	15.9			7.0	1.3	0.3	0.1	8.7			1.7			0.5			3.0			59.5			89.3			89.3		
	11.3	13.6	2.3	5.5	1.1	0.3	0.1	7.0	7.9	0.9	1.4	1.6	0.2	0.6	0.6	0.0	2.8	2.9	0.1	49.2	54.4	5.2	72.3	80.8	8.5	72.3	80.8	8.5
7	16.6			6.9	1.3	0.2	0.1	8.5			1.6			0.7			5.9			61.5			94.8			94.8		
	12.6	14.6	2.0	6.7	1.4	0.2	0.1	8.4	8.5	0.1	3.1	2.4	0.8	0.7	0.7	0.0	8.7	7.3	1.4	51.0	56.3	5.3	84.5	89.7	5.1	84.5	89.7	5.1
14	15.4			5.0	1.1	0.3	0.1	6.5			4.7			0.7			27.3			32.7			87.3			87.3		
	13.2	14.3	1.1	4.5	1.1	0.2	0.1	5.9	6.2	0.3	4.1	4.4	0.3	0.7	0.7	0.0	24.3	25.8	1.5	37.5	35.1	2.4	85.7	86.5	0.8	85.7	86.5	0.8
21	10.8			4.4	0.9	0.2	0.2	5.7			5.8			0.7			41.6			24.5			89.1			89.1		
	11.2	11.0	0.2	4.2	0.8	0.1	0.1	5.2	5.5	0.3	4.1	5.0	0.9	0.6	0.7	0.1	30.0	35.8	5.8	38.7	31.6	7.1	89.8	89.5	0.3	89.8	89.5	0.4
71	11.9			2.1	0.4	0.2	0.4	3.1			5.1			0.2			18.0			42.5			80.8			80.8		

Overall	87.9	6.8		87.9	6.8
maximum	97.9			97.9	
minimum	72.3			72.3	
n =	11			11	

CT = solid sorbent trap, residues of which were identified as parent DMDS.
Results from Table 7, p. 34 of the study report; **Volatiles** results imported from **Volatiles** worksheet.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and stdevp(A1:A2).

Attachment 3: Transformation Pathway Presented by Registrant and Illustration of Test System

Figure 12 Dimethyl Disulfide Anaerobic Soil Metabolism

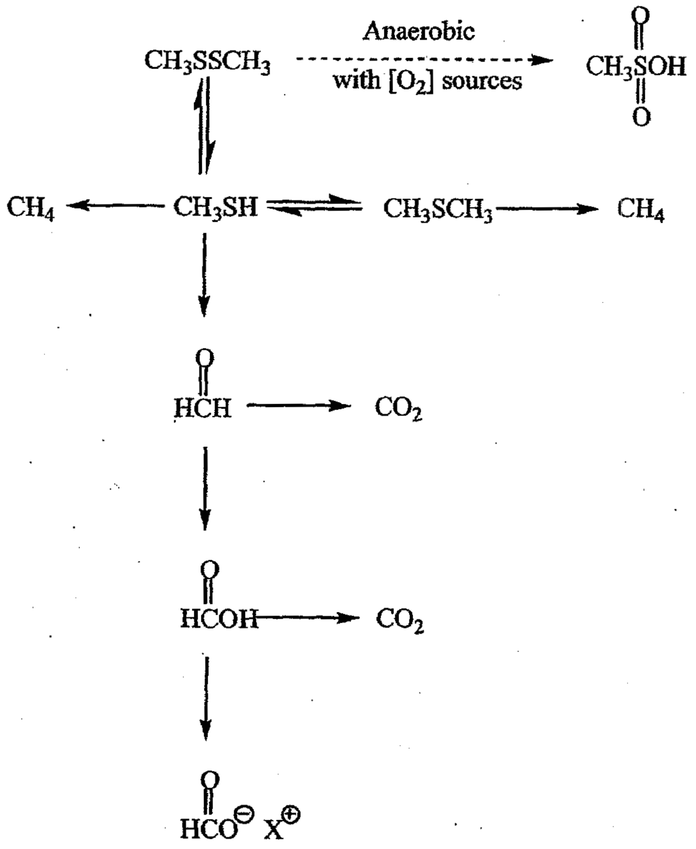
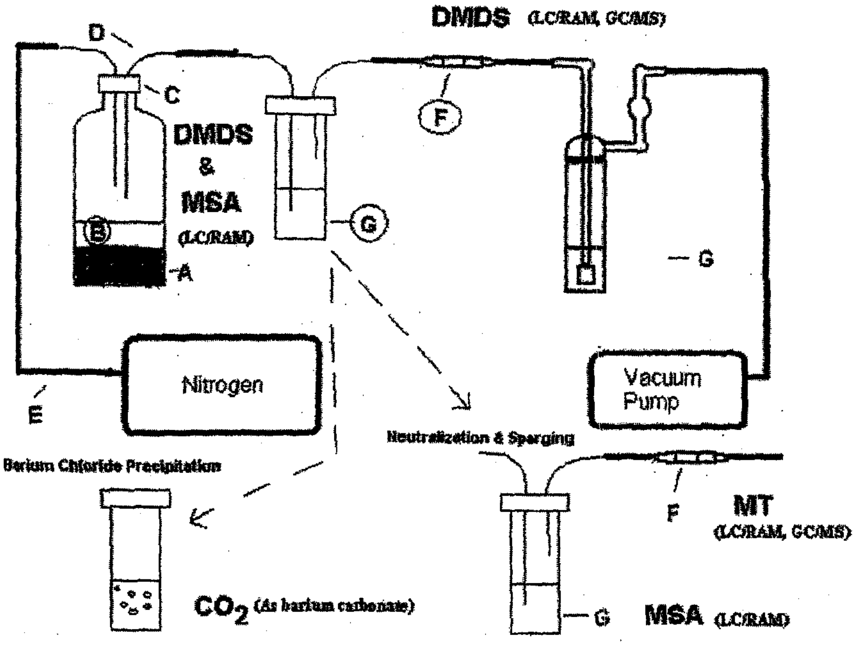


Figure 3 **Identification of Major Radioactive Components in the Test System**



A: Soil
B: Nitrogen Sparged Milli-Q Water
C: PTFE-lined septum cap
D: Stainless Steel Needles (joined to tubing with trimmed plastic syringe barrel sections)
E: Tygon™ connecting tube
F: Anasorb CSC Cocunut Shell Carbon cartridge
G. 1N KOH traps (pre-cartridge & post-cartridge)