Data Evaluation Record on the aerobic biotransformation of dimethyl disulfide in soil

PMRA Submission Number {......}   EPA MRID Number 47052819

Data Requirement: PMRA Data Code:
         EPA DP Barcode: D339684
         OECD Data Point:
         EPA Guideline: 162-1

Test material:

Common name: Dimethyl disulfide.
Chemical name:
  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.
SMILES string: S(SC)C (EPI Suite, v3.12 SMILES String).

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EXECUTIVE SUMMARY

The biotransformation of *bis*-[methyl-^{14}C]-labeled dimethyl disulfide (radiochemical purity 98.7%) was studied in a loamy sand soil (pH, organic carbon not reported) from California and a sand soil (pH, organic carbon not reported) from Florida for 120 days under static aerobic conditions in darkness at 20°C and a soil moisture of 40% of maximum water holding capacity. Biotransformation of [^{14}C]dimethyl disulfide was also investigated in a clay loam soil (pH, organic carbon not reported) from France for 59 days and a clay soil (pH, organic carbon not reported) from Switzerland for 120 days under the same conditions. [^{14}C]Dimethyl disulfide was applied at 390 mg a.i./kg (equivalent to *ca.* 440 kg a.i./ha). This study was conducted in accordance with OPPTS Guideline 835.3300, Soil Biodegradation; European Union Commission Directive 95/36/EC (1995); OECD Guideline 307 (2000); and SETAC-Europe Procedures for Assessing the Environmental Fate and Ecotoxicology of Pesticides, Part 1 (1995); and in compliance with USEPA GLP Standards (40 CFR, Part 160). The test apparatus consisted of a sealed bottle (250-mL volume, 120 x 55 mm, neck i.d. 17 mm, 1-mm side-arm) connected via the side-arm to a 1-L Teflon bag holding oxygen gas. A culture tube containing 1N KOH was maintained inside the incubation bottle for the static absorption of CO_2, and a solid-phase carbon trap was positioned between the side-arm and the Teflon bag for the collection of volatile organics. Following treatment of the USA soils, duplicate treated samples of each soil type were taken for analysis after 0 (5 minutes), 1, 4 (Florida sand only), 7, 14, 21, 60/62 and 120 days, while the European soils were taken for analysis after 0 (5 minutes), 1, 4, 7, 11, 14, 21, 59 and 120 (Swiss clay only) days. Upon collection, the incubation bottle was attached to a vacuum system and air was drawn (100-150 mL/minute) sequentially through the bottle headspace, the side-arm and solid-phase carbon trap and finally through 0.5N KOH solution for 2 hours. For the European soils, the solid-phase carbon trap was replaced with a fresh trap prior to purging. Following the 2-hour purge, the inner, static 1N KOH trapping solution was removed. Soil was then sequentially extracted twice with acetonitrile, followed by twice with water, once with 0.5% aqueous sodium hypochlorite and, finally, again with water. The contents of the solid-phase carbon traps were divided into equal portions and each extracted three times with hexane. Soil extracts, extracted soil, KOH trapping solutions, hexane extracts and extracted solid sorbent were analyzed for total radioactivity using LSC (liquid scintillation counting). Hexane extracts from the solid sorbent were analyzed by normal-phase HPLC, with parent dimethyl disulfide the only compound detected. The two acetonitrile and initial two water extracts from the soil samples were respectively combined and analyzed by anion-exchange HPLC (High Performance Liquid Chromatography using Ultraviolet Spectrophotometric Detection, with one nonvolatile transformation product,

- **methanesulfonic acid (MSA),**

detected in all four soils. MSA was isolated from a clay (Switzerland) soil water extract and its identification confirmed via LC/MS and LC/MS/MS against reference standard.

Individual replicate results were not provided, and, while duplicate treated soil samples were collected at each interval, the study authors did not specify that the reported results were means of the replicates. Additionally, quantitative results for MSA were not reported, but approximated

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by the primary reviewer based on the percentages the study authors estimated the compound comprised in the extracts.

For all soil experiments, quantitative results for MSA were not directly reported. In the California Loamy Sand experiment, the study authors estimated that *ca.* 70% of residues recovered in the ACN extract, plus all radioactivity in the first water extract was MSA (p. 22; Figure 7, p. 39; DER Attachment 2). For the Florida sand experiment, the study authors estimated that *ca.* 50% of residues recovered in the ACN extract, plus all radioactivity in the first water extract was MSA (pp. 22-23; Figure 7, p. 39; DER Attachment 2). In both European soil experiment (France clay loam and Switzerland loam), the study authors estimated that residues recovered in the ACN extract and first water extract was MSA (p. 21; Figure 6, p. 38; Figures 8-9, pp. 40-41, DER Attachment 2).

Volatile CO_2 and other volatile organic compounds were also extracted and quantified in all of the experiments.via purging through a trap containing dilute aqueous KOH. The radioactive content of the dilute 1N and 0.5N KOH solutions in the inner vial and outer traps respectively will be determined through liquid scintillation counting (LSC) of the extracts in the solution. Furthermore, the radioactivity related to CO2 was quantified applying the LSC analysis to the barium chloride salt precipitate in the KOH solution. Volatile organic compounds were minor transformation products in the USA soils (California loamy sand soil and Florida sand soil) and major transformation products in the European soils (France clay loam and Switzerland clay soil). From the selected intervals analyzed, CO_2 was a minor transformation product in all soil experiments. However, in the European soils, it is unknown whether CO_2 was a major constituent of the volatile organic compounds transformation products.

Dimethyl disulfide dissipated from the soils via transformation and diffusion of parent. Upon sampling, the 2-hour purge to collect volatiles effectively removed any parent dimethyl disulfide present from the test system, with the exception of very minor amounts (<1.1% of applied) detected in the USA soils' acetonitrile extracts. **MSA** was a minor product in the USA soils, but a major product in the Euro soils.

No supporting records were provided to establish that aerobicity, soil moisture or temperature were maintained throughout the 59- and 120-day incubations.

<u>USA soils.</u> Overall recovery of radiolabeled material averaged 94.76 ± 3.83% (range 87.99-100.90%) and 92.22 ± 2.59% (range 88.70-97.27%) of the applied for the California loamy sand and Florida sand soils, respectively, with no consistent patterns of decline in recoveries for either soil over the 120-day incubations. **Dimethyl disulfide** was detected (combined diffusion/purging) at 79.15% and 73.24% of the applied for the California loamy sand and Florida sand soils, respectively, at study termination. The **observed DT50** via volatilization (combined diffusion/purging) occurred in <2 hours. However, observed DT50 values for total detected parent were >120 days (final interval). In a <u>supplemental experiment</u>, dimethyl disulfide diffused (passive) from the California loamy sand soil with an observed DT50 value of *ca.* 3 days, and calculated (0-14 days) linear and nonlinear half-lives of 3.4-3.5 days (r^2 = 0.9902-0.9942); diffusion from the sand soil was not investigated. **MSA** was detected at

approximate maximums of 3.26% and 4.95% of applied in the loamy sand and sand soils, respectively, at termination. Unidentified extractable [^{14}C]residues were <2% of applied for both soils. Extractable [^{14}C]residues were maximums of 3.86% and 6.61% of applied for the loamy sand and sand soils, respectively, at termination, while nonextractable [^{14}C]residues were <1.1% for both soils at all intervals. [^{14}C]Residues of volatile organic compounds in the KOH solutions were total maximums of 8.30-8.35% for the two soils, with $^{14}CO_2$ accounting for ≤20% of the recovered radioactivity (≤1.24% of applied) at the selected intervals analyzed.

European soils. Overall recoveries averaged 90.19 ± 5.04% (range 77.20-93.47%) and 93.17 ± 5.10% (range 81.52-100.92%) for the clay loam and clay soils, respectively, with the lowest recovery for each soil detected at the final sampling interval. **Dimethyl disulfide** was detected (combined diffusion/purging) at 90.47% of applied at day 0, 55.46% at 4 days, 45.67% at 7 days and 35.30% at 59 days (termination) for the clay loam soil, and at 89.16% at day 0, 54.65% at 7 days, 46.75% at 11 days and 38.82% at 120 days (termination) for the clay soil. For both soils, diffusion (passive) of parent increased to *ca.* 35% of applied at 7 days and was relatively steady state at *ca.* 35-44% thereafter. The **observed DT50** via volatilization (purging only) occurred in <2 hours. However, observed DT50 values for total detected parent were were *ca.* 6 and 10 days for the France clay loam and Switzerland clay soils, respectively. Calculated half-lives were determined; however, low correlation coefficients (r^2 <0.63) preclude any confidence in the results (see below). **MSA** was detected at an approximate maximum of 33.17% at 14 days in the clay loam soil decreasing to 32.97% at 21 days and was 2.02% at 59 days, and an approximate maximum 32.86% at 21 days in the clay soil decreasing to 26.80% at 59 days and 5.76% at 120 days. Unidentified extractable [^{14}C]residues were maximums of 6.00% and 3.46% for the France clay loam and Switzerland clay soils, respectively. Extractable soil [^{14}C]residues increased to maximums of 36.32-39.06% at 14-21 days for the two soils and were 6.83% at 59 days (termination) for the clay loam soil and 8.21% for the clay soil at 120 days (termination). Nonextractable [^{14}C]residues were maximums of 4.26% and 7.25% for the France clay loam and Switzerland clay soils, respectively, at termination. [^{14}C]Residues of volatile organic compounds in the KOH solutions were total maximums of 30.81% and 27.24% of applied for the France clay loam and Switzerland clay soils, respectively, at termination, with $^{14}CO_2$ accounting for up to 52.7% and 61.9% (5.82% and 6.72 % of applied) of the recovered radioactivity, respectively, at the selected intervals analyzed (final intervals were not analyzed).

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 soil, the compound was found to degrade to methanesulfonic acid and CO_2/ volatile organic compounds with low levels of formation of bound soil residues.

In a supplemental experiment, diffusion of [^{14}C]dimethyl disulfide from incubation bottles containing no soil was similar to the rate of diffusion seen with the loamy sand soil.

Results Synopsis:

Test system used: Loamy sand soil from California.
Linear half-life: ND (insufficient transformation).

Non-linear half-life: ND (insufficient transformation)
    Observed DT50:   >120 days.
Major transformation products:
    No major transformation products were isolated.
Minor transformation products:
    Methanesulfonic acid (MSA, maximum *ca.* 3.26% of applied).
    CO_2 + volatile organics other than parent (maximum 8.35% of applied).

Test system used: Sand soil from Florida.
Linear half-life: ND (insufficient transformation).
Non-linear half-life: ND. (insufficient transformation).
Observed DT50:   >120 days.
Major transformation products:
    No major transformation products were isolated.
Minor transformation products:
    Methanesulfonic acid (MSA, maximum *ca.* 4.95% of applied).
    CO_2 + volatile organics other than parent (maximum 8.30% of applied).

Test system used: Clay loam soil from France.
Linear half-life: 48.4 days ($r^2 = 0.4550$).
Non-linear half-life: 13.8 days ($r^2 = 0.6267$).
Observed DT50:   *ca.* 6 days.
Major transformation products:
    Methanesulfonic acid (MSA, maximum *ca.* 33.17% of applied).
    CO_2 + volatile organics not identified as parent (maximum 30.81% of applied).
Minor transformation products:
    No minor transformation products were identified.

Test system used: Clay soil from Switzerland.
Linear half-life: 122 days ($r^2 = 0.4145$).
Non-linear half-life: 68.6 days ($r^2 = 0.4227$).
Observed DT50:   *ca.* 10 days.
Major transformation products:
    Methanesulfonic acid (MSA, maximum *ca.* 32.86% of applied).
    CO_2 + volatile organics not identified as parent (maximum 27.24% of applied).
Minor transformation products:
    No minor transformation products were identified.

Study Acceptability: This study is classified as Supplemental. The following significant deficiencies were noted:

For the portion of this study conducted with USA soils:
- the experimental design did not allow for the distinction between diffusion of parent dimethyl disulfide and that induced during the post-sampling purge,

- while a supplemental experiment investigating diffusion of parent from the loamy sand (CA) soil was conducted, details regarding experimental procedures were not reported and no results other than analysis of the solid-phase traps were provided. Therefore, adequate comparisons between the experiments could not be made.
- Since DMDS residues were detected in the headspace immediately upon the beginning of the study, the route of degradation, as observed with the accumulation of degradate products in the soil over time, is unclear.
- the study may have been terminated before the pattern of decline of the test substance was established, and
- the test soils were inadequately characterized (only soil type, maximum water holding capacity and biomass were reported).

For the portion of this study conducted with Euro soils:
- the experimental design did not allow for the distinction between diffusion of parent dimethyl disulfide and that induced during the post-sampling purge,
- Since DMDS residues were detected in the headspace immediately upon the beginning of the study, the route of degradation, as observed with the accumulation of degradate products in the soil over time, is unclear.
- material balances were incomplete with up to 18-23% of the applied unaccounted for at study termination,
- the test soils were inadequately characterized (only soil type, maximum water holding capacity and biomass were reported), and

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with OPPTS Guideline 835.3300, Soil Biodegradation; European Union Commission Directive 95/36/EC (1995, amending Council Directive 91/414/EEC, Annex I, 7.1.1.1.1, 7.1.1.2.1); OECD Guideline 307 (2000); and SETAC-Europe Procedures for Assessing the Environmental Fate and Ecotoxicology of Pesticides, Part 1 (1995; Appendix 3, pp. 88-89, 93, 98). The following significant deviations from good scientific practices or the objectives of Subdivision N guidelines were noted:

The following applies to the portion of this study conducted with USA soils:

Dissipation of parent dimethyl disulfide via diffusion and volatilization effected by the post-sampling 2-hour purge interval were not distinguished. Although a supplemental experiment investigating diffusion of parent from the loamy sand soil was conducted, sufficient information regarding experimental procedures and results were not

provided to allow for adequate comparison of the experiments.

At 120 days (termination), parent [^{14}C]dimethyl disulfide was detected at 73.24-79.15% of the applied, and the experimental design did not allow for dissipation via diffusion to be assessed. Consequently, it could not be determined whether the study was terminated before the pattern of decline of the test substance in soil was established.

The test soils were inadequately characterized; only soil type, maximum water holding capacity and biomass were reported.

The following applies to the portion of this study conducted with Euro soils:

For the France clay loam and Switzerland clay soils, 22.8% and 18.5% of the applied, respectively, was unaccounted for at study termination. Mass balances reported by the study authors were not in agreement with those determined by the primary reviewer and the study authors provided no data to support their calculations.

At study termination, radioactivity recovered in the KOH trapping solution totaled 30.81% of applied at 59 days for the clay loam soil and 27.24% at 120 days for the clay soil, and, at the intervals analyzed, barium chloride precipitation indicated that $^{14}CO_2$ only accounted for, at most, *ca.* 53-62% of the sample radioactivity. Consequently, volatile organics, other than CO_2, may have been present at ≥10% of the applied and were not identified.

The test soils were inadequately characterized; only soil type, maximum water holding capacity and biomass were reported.

The France and Switzerland soils were classified as a clay loam and clay, respectively (USDA textural classifications, unconfirmed). FAO soil classifications were also provided allowing for adequate comparison to establish that the foreign test soils were comparable to soils that would be found at intended use sites for dimethyl disulfide in the United States.

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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 1.

Description: Technical, in ethanol solution (p. 14).

Purity: Radiochemical purity: 98.7% (p. 14; Figure 2, p. 34; Figure 5, p. 37).

Lot/Batch No.:   49520-1-4C (p. 14).

Analytical purity: Not reported.

Initial specific activity: 12.79 mCi/mmol (2.667 mCi/mL; Table 3, p. 31). The information provided on p. 14 appears to be incorrect, as the [^{14}C]dimethyl disulfide used in this study has the same ABC lot number and Cerexagri log number as that used in MRID 47052820 (p. 14; Table 3, p. 30) submitted concurrently with this study. The registrant should clarify if otherwise.

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. 31).

Location of the radiolabel: At each methyl C.

Storage conditions of test chemical: <0°C in darkness (p. 14; Appendix 3, p. 90).

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 $(\varepsilon_\lambda) = 37.32$ (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.

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2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description		Details
Geographic location	Loamy sand:	San Luis Obispo, California.
	Sand:	Quincy, Florida.
	Clay:	Intingen-AT, Switzerland.
	Clay loam:	Ruelisheim, France.
Pesticide use history at the collection site		No pesticides or fertilizer for at least 5 years previous to collection.
Collection procedures		Not reported.
Sampling depth (units)		Not reported.
Storage conditions		Maintained at *ca.* 4°C in unsealed bags prior to use.
Storage length		≤3 months.
Soil preparation		Soil moisture adjusted to *ca.* 40% of maximum water holding capacity, 2-mm sieved, and maintained at 20°C in darkness with access to air.

Data obtained from p. 15 and Appendix 3, p. 92 of the study report.

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Table 2: Properties of the soils.

Property	California	Florida	Switzerland	France
Soil texture	Loamy sand.	Sand.	Clay.	Clay loam.
% Sand (2000-50 µm):	Not reported.			
% Silt (50-2 µm):	Not reported.			
% Clay (<2 µm):	Not reported.			
pH	Not reported.			
Organic carbon (%)	Not reported.			
Organic matter (%)	Not reported.			
CEC (meq/100 g)	Not reported.			
Maximum holding capacity (%)	19.1	23.5	73.8	66.02
Moisture at 75% of 1/3 bar (%)	Not reported.			
Bulk density, disturbed (g/cm^3)	Not reported	Not reported	Not reported	1.0
Microbial biomass (mg OC/kg dry wt. soil)[1]	86	99	474	352
Soil taxonomic classification	Not reported	Not reported	Calcaric Cambisol	Dystric Cambisol
Sol mapping unit	Not reported.			

Data obtained from p. 15 of the study report.
1 OC = organic carbon (p. 15).
Soil bulk density and taxonomic classifications were obtained from registrant through clarification e-mail.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: Preliminary experiments were conducted and determined that the standard "flow through" test system would not be suitable (p. 9). This resulted in development of a test system that would minimize diffusion of dimethyl disulfide. No additional details regarding the preliminary experiments were provided.

2. Experimental conditions:

Table 3: Experimental design.

Parameter		All four soils
Duration of the test		59 days for the clay loam (French), and 120 days for the loamy sand (CA), sand (FL) and clay (Swiss) soils.
Soil condition: (Air dried/fresh)		Fresh.
Soil (g/replicate)		*ca.* 25 g dry wt.
Application rate (mg a.i./kg & equiv. kg a.i./ha)	Nominal:	392 mg a.i./kg (443 kg a.i./ha[1]).
	Actual:	390 mg a.i./kg (9.75 mg a.i./25 g dry wt. soil).
Control conditions, if used		No sterile controls were used.

Parameter		All four soils
No. of Replications	Controls, if used	No sterile controls were used.
	Treatment	Duplicate treated samples per soil type at each collection interval.
Test apparatus	Type/material/volume	250-mL bottle (120 x 55 mm, neck i.d. 17 mm, 1-mm side-arm, material composition not reported), sealed with a Teflon (PTFE)-lined septum cap and connected via the side-arm to a 1-L Teflon bag filled with oxygen gas (illustrated in Figure 1, p. 33).
	Details of traps for CO_2 and organic volatiles, if any	Two-stage SKC Anasorb CSC (coconut shell charcoal) tube (100 mg front:50 mg back, 150 mg total sorbent) connecting the incubation bottle side-arm and the Teflon bag to trap volatile organics. 1N KOH (10 mL) in borosilicate, glass culture tube (160 x 100 mm) placed inside the sealed incubation bottle to trap CO_2.
If no traps were used, is the system closed/open?		Systems incubated sealed under static oxygen conditions.
Identity and concentration of co-solvent		Ethanol; final concentration 0.4% based on soil dry wt.
Test material	Volume of the test solution used/treatment:	0.10 mL/*ca.* 25 g soil.
	Application method (*e.g.*: mixed/not mixed):	Test solution was applied to the soil surface via glass syringe, then the incubation bottle was immediately sealed and manually shaken, vigorously, for several seconds.
	Is the co-solvent evaporated?	No.
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.
Microbial biomass/population of the control (units)		Initial	Final
		No sterile controls were used.	
Microbial biomass/population of the treated soil (units)		Initial	Final
		Treated soil samples were not analyzed for biomass.[2]	
Experimental conditions	Temperature (°C):	20 ± 2°C, maintained via controlled-temperature chamber.
	Continuous darkness (Yes/No):	Yes.
	Moisture content:	40% of maximum water holding capacity.
	Moisture maintenance method:	Not reported.
Other details, if any		None

Data obtained from pp. 9, 15-17; Tables 1-3, pp. 29-31; Figure 1, p. 33; Appendix 1, pp. 46-47, 49-50; Appendix 3, pp. 89, 92 of the study report.
1 Primary reviewer used conversion factor of 1 ppm = 1.13 kg/ha.
2 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 3, p. 92).

3. Aerobic conditions: Treated soil samples were incubated sealed under a static oxygen atmosphere (pp. 15-16). The study authors proposed that oxygen consumption within the incubation bottle would result in a slight negative pressure that would cause the oxygen gas

within the attached Teflon bag to diffuse into the incubation bottle and maintain aerobic conditions (p. 16). No determinations, such as redox potentials, were made to verify that aerobic conditions were maintained.

4. Supplementary experiments: Diffusion from loamy sand (CA) soil. To estimate the rate of dimethyl disulfide diffusion [passive] from the USA soils, loamy sand (CA) soil was apparently treated with [^{14}C]dimethyl disulfide and incubated as previously described; however, no additional details were provided (p. 23). The solid-phase carbon traps were collected, without purging, at 0, 1, 2, 3, 4, 8 and 14 days posttreatment and analyzed (Appendix 1, pp. 43, 48).

Diffusion in absence of soil. To determine the rate of dimethyl disulfide diffusion in the absence of soil, [^{14}C]dimethyl disulfide was applied to incubation bottles containing no soil (pp. 17-18); no additional details were provided. The solid-phase carbon traps were collected, without purging, at various (unspecified) intervals and analyzed as described below.

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5. Sampling:

Table 4: Sampling details.

Criteria		Details
Sampling intervals (days posttreatment)	Loamy sand (CA):	0 (5 min.), 1, 7, 14, 21, 62 and 120.
	Sand (FL):	0 (5 min.), 1, 4, 7, 14, 21, 60 and 120.
	Clay loam (French):	0 (5 min.), 1, 4, 7, 11, 14, 21 and 59.
	Clay (Swiss):	0 (5 min.), 1, 4, 7, 11, 14, 21, 59 and 120.
Sampling method		Duplicate treated samples per soil type at each interval.
Method of collection of CO_2 and organic volatile compounds		Upon sampling, volatiles were collected as follows: 1) A needle, connected to a vacuum and gas-washing bottle containing 0.5N KOH (50 mL), was inserted into plastic tubing that connected the solid-phase carbon trap and the Teflon bag, then the oxygen in the bag was drawn out. 2) A stainless-steel needle was then inserted into the septum cap of the incubation flask and positioned a few millimeters above the soil surface. Air was then drawn (100-150 mL/minute) via vacuum for 2 hours through the bottle headspace, solid-phase carbon trap and trapping solution (0.5N KOH). 3) After collection of headspace volatiles, extraction solvent was added via the stainless-steel needle, the incubation bottle was opened and the culture tube containing the 1N KOH trapping solution inside was removed.
Sampling intervals/times for: Sterility check, if sterile controls are used: Moisture content: Redox potential, other:		 No sterile controls were used. Not reported. Not determined.
Sample storage before analysis		**Soil** was extracted upon sampling after the 2-hour volatiles collection period. Any storage of extracts prior to analysis was not reported.
Other observation, if any		At the 1- to 59-day intervals for the clay loam (French) and the 4- to 120-day intervals for the clay (Swiss) soils, the solid-phase carbon trap was replaced with a fresh carbon trap prior to volatiles collection via vacuum.

Data obtained from pp. 16-17 and 20-21; Appendix 1, pp. 46-47, 49-50 of the study report.

C. ANALYTICAL METHODS:

Extraction/clean up/concentration methods: Soils were sequentially extracted twice with acetonitrile, followed by twice with water, once with 0.5% aqueous sodium hypochlorite and a

final extraction again with water; all extraction solvent volumes were 50 mL (p. 18). Each extraction was done via manual shaking for 10 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 (p. 18). The two acetonitrile and initial two water extracts were respectively combined and analyzed by HPLC as described below.

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the soil extracts, extracted soil and volatiles trapping materials (Appendix 3, p. 95).

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

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. 17). Each portion was extracted three times with hexane; extraction solvent volumes were 5.0 mL. Extraction was done via mechanical shaking (mechanism not specified) for 15 minutes; after which the 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 as described below (pp. 17-18). 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 acetonitrile ("organic") and water ("aqueous") soil extracts were analyzed using anion-exchange (carbonate selective) HPLC under the following conditions: Dionex IonPac AS4A-SC column (4.0 x 250 mm, particle size not reported), column temperature 25°C, isocratic mobile phase of aqueous 1.8mM disodium carbonate/1.7mM sodium carbonate, run time 7.0 minutes, injection volume 25 μL, flow rate 1.0 mL/minute, UV detector (wavelength not specified), radioactivity detector (type not specified) fraction collection at 1-minute intervals (p. 19). Parent[^{14}C]dimethyl disulfide was identified by comparison to the retention time of unlabeled reference standard (Figures 5-9, pp. 37-41).

Aliquots of the initial solid sorbent hexane extract were analyzed using normal-phase HPLC under the following conditions: Supelco Spherisorb Silica column (4.6 x 150 mm, 5 μm), column temperature 25°C, isocratic mobile phase of hexane, run time 7.0 minutes, injection volume varied (not specified), flow rate 1.0 mL/minute, radioactivity detector (type not specified, p. 19). Parent[^{14}C]dimethyl disulfide was identified by comparison to the retention time of unlabeled reference standard (p. 24; Figure 2, p. 34; Figure 4, p. 36).

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Identification and quantification of transformation products: Transformation products were separated, quantified and identified using HPLC as described for the parent compound (p. 19; Figure 3, p. 35; Figures 6-9, pp. 38-41). The sole identified product, methanesulfonic acid (MSA), was isolated from 21-day clay (Swiss) soil water extract via fraction collection and analyzed via reverse-phase LC/MS and LC/MS/MS under the following conditions: ThermoHypersil-Keystone Betasil C8 column (4.6 x 100 mm, 5 μm), isocratic mobile phase of 0.1% aqueous formic acid, run time 10 minutes, column temperature 28°C, injection volume 25-1,000 μL, flow rate 0.5 mL/minute, MS:LC post-column split not reported, Packard Radiomatic C525TR Flo-One beta radioactivity detector, Micromass Ultima MS, electrospray ionization (ESI), ion mode negative, source temperature 130°C, desolvation temperature 350°C, mass range 50-125 amu (p. 24; Appendix 2, pp. 76-77; Figure 1, p. 78). Isolated [^{14}C]MSA was identified against reference standard (Appendix 2, p. 77; Figures 1-9, pp. 78-86).

Attempts to analyze 21-day clay (Switzerland) soil acetonitrile and water extracts using NMR were inconclusive (Appendix 4, p. 100).

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), vortexed for *ca.* 10 seconds, allowed to stand (interval not reported), then centrifuged (3,000 rpm, *ca.* 2 minutes; p. 19). Total radioactivity in the KOH solutions was determined via LSC prior to and after barium chloride precipitation.

Table 5: Reference compounds available for identifying transformation products of dimethyl disulfide.

Applicant code	Chemical Name	Purity[1]	Lot/Batch No.
MSA	Methanesulfonic acid	99.5%	13517AE

Data obtained from Figure 3, p. 35; Appendix 2, p. 76 of the study report.
1 Purity w/w unless otherwise designated.

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: No supporting records were provided to establish that aerobicity, soil moisture and temperature were maintained throughout the experiments.

B. MATERIAL BALANCE: Individual replicate results were not provided, and, while duplicate treated soil samples were collected at each interval, the study authors did not specify that the reported results were means of the replicates (Reviewer's Comment No. 1).

USA soils. Overall recovery of radiolabeled material averaged 94.76 ± 3.83% (range 87.99-100.90%, n = 7) of the applied for the loamy sand (CA) soil and 92.22 ± 2.59% (range 88.70-

97.27%, n = 8) for the sand (FL) soil, with no consistent patterns of decline in recoveries for either soil (DER Attachment 2).

Euro soils. Overall recoveries averaged 90.19 ± 5.04% (range 77.20-93.47%, n = 8) for the clay loam (France) soil and 93.17 ± 5.10% (range 81.52-100.92%, n = 9) for the clay (Switzerland) soil, with the lowest recovery for each soil detected at the final sampling interval (DER Attachment 2).

Table 6: Biotransformation of *bis*-[methyl-^{14}C]dimethyl disulfide, expressed as percentage of applied radioactivity (n =2[1]), in California loamy sand soil under aerobic conditions.

Compound	Sampling times (days)						
	0[2]	1	7	14	21	62	120
Dimethyl disulfide (all volatilized)[3]	94.34	82.80	86.76	87.19	90.96	82.03	79.15
Methanesulfonic acid (approximate)[4]	0.49	1.06	1.53	1.72	1.93	3.00	3.26
Unidentified extractable [^{14}C]residues[5]	0.14	0.31	0.50	0.56	0.50	0.61	0.60
Total extractable residues	0.63	1.37	2.03	2.28	2.43	3.61	3.86
Nonextractable residues [6]	0.02	0.05	0.12	0.10	0.09	0.15	0.13
1N KOH solution (CO_2 / other volatiles)[7]	0.58	3.78	0.49 / 7.46	0.32 / 6.51	0.63 / 6.79	8.35	8.31
Total recovery [8]	95.57	88.00	96.86	96.40	100.90	94.14	91.45

Data obtained from Table 5, p. 49 and DER Attachment 2.

1 Reviewer's Comment No. 1. Additionally, while duplicate treated soil samples were collected at each interval, the study authors did not specify that the reported results were means of the replicates.

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 2-hour interval (pp. 16-17).

3 Recovered in volatiles solid-phase carbon trap after purging.

4 Quantitative results for MSA were not reported. The study authors estimated that *ca.* 70% of residues recovered in the acetonitrile extract, plus all radioactivity in the first water extract from soil was MSA (p. 22; Figure 7, p. 39; Table 5 p. 49; DER Attachment 2).

5 Unidentified [^{14}C] residues account for 30 percent of the acetonitrile soil extraction, the second water extract from soil, and extracts from the sodium hypochlorite solution. Includes minor amounts (≤0.25% of applied) of parent [^{14}C]dimethyl disulfide detected in acetonitrile extracts (p. 22; Figure 7, p. 39).

6. Nonextractable residues measured include those in the Soil PES sample only.

7 KOH solution maintained inside incubation bottle (p. 24). At some, but not all, intervals, $^{14}CO_2$ was distinguished from other volatile [^{14}C]organics via barium chloride precipitation (Table 4, p. 32).

8. Total recovery = Dimethyl disulfide residues (all volatilized) + Total extractable residues + Nonextractable residues + CO_2/other volatile residues

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Table 7: Biotransformation of *bis*-[methyl-^{14}C]dimethyl disulfide, expressed as percentage of applied radioactivity (n =2[1]), in Florida sand soil under aerobic conditions.

Compound	Sampling times (days)							
	0[2]	1	4	7	14	21	60	120
Dimethyl disulfide (all volatilized)[3]	90.77	87.07	80.13	84.35	79.08	79.74	76.40	73.24
Methanesulfonic acid (approximate)[4]	0.85	1.63	2.28	2.74	2.57	3.32	3.95	4.95
Unidentified extractable [^{14}C]residues[5]	0.66	1.29	1.65	1.66	1.32	1.45	1.38	1.66
Total extractable residues	1.51	2.92	3.93	4.40	3.89	4.77	5.32	6.61
Nonextractable residues [6]	0.09	0.31	0.79	1.06	0.68	0.71	0.68	0.55
1N KOH solution (CO_2 / other volatiles)[7]	0.72	3.80	0.19 / 6.10	0.26 / 7.20	1.24 / 4.92	8.08	7.94	8.30
Total recovery [8]	93.09	94.10	91.14	97.27	89.81	93.30	90.34	88.70

Data obtained from Table 6, p. 50 and DER Attachment 2.

1 Reviewer's Comment No. 1. Additionally, while duplicate treated soil samples were collected at each interval, the study authors did not specify that the reported results were means of the replicates.

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 2-hour interval (pp. 16-17).

3 Recovered in volatiles solid-phase carbon trap after purging.

4 Quantitative results for MSA were not reported. The study authors estimated that *ca.* 50% of residues recovered in the ACN extract, plus all radioactivity in the first water extract was MSA (pp. 22-23; Figure 7, p. 39; Table 6, p. 50; DER Attachment 2).

5 Unidentified [^{14}C] residues account for 50 percent of the acetonitrile soil extraction, the entire second water extract from soil, and the entire extract from the sodium hypochlorite solution. Includes minor amounts ($\leq$1.08% of applied) of parent [^{14}C]dimethyl disulfide detected in acetonitrile extracts (pp. 22-23; Figure 7, p. 39).

6. Nonextractable residues measured include those in the Soil PES sample only.

7 KOH solution maintained inside incubation bottle (p. 24). At some, but not all, intervals, $^{14}CO_2$ was distinguished from other volatile [^{14}C]organics via barium chloride precipitation (Table 4, p. 32). The 21-day barium chloride analysis was not included in this table because the CO_2 / volatiles of 0.58 / 4.83 did not account for the initial 8.08% of applied in the KOH solution.

8. Total recovery = Dimethyl disulfide residues (all volatilized) + Total extractable residues + Nonextractable residues + CO_2/other volatile residues

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Table 8: Biotransformation of *bis*-[methyl-^{14}C]dimethyl disulfide, expressed as percentage of applied radioactivity (n =2[1]), in France clay loam soil under aerobic conditions.

Compound		Sampling times (days)							
		0[2]	1	4	7	11	14	21	59
Dimethyl disulfide (all volatilized)[4]	Passive diffusion	--[3]	10.01	28.61	35.12	37.60	37.29	38.60	35.27
	Purged	90.47	64.90	26.85	10.55	3.66	1.51	0.22	0.03
	Total	90.47	74.91	55.46	45.67	41.26	38.80	38.82	35.30
Methanesulfonic acid (approximate)[5]		1.45	6.17	21.68	29.10	32.50	33.17	32.97	2.02
Unidentified extractable [^{14}C]residues [6]		0.10	0.86	3.09	6.00	5.83	5.89	5.49	4.81
Total extractable residues		1.55	7.03	24.77	35.10	38.33	39.06	38.46	6.83
Nonextractable residues[7]		0.06	0.54	1.59	2.78	1.70	2.39	3.40	4.26
1N KOH solution (CO$_2$ / other volatiles)[8]		0.57	1.29 / 870	11.47	9.92	9.67	9.52	5.82 / 5.22	30.81
Total recovery[9]		92.65	92.47	93.29	93.47	90.96	89.77	91.72	77.20

Data obtained from Table 3, p. 47 and DER Attachment 2.

1 Reviewer's Comment No. 1. Additionally, while duplicate treated soil samples were collected at each interval, the study authors did not specify that the reported results were means of the replicates.

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 2-hour interval (pp. 16-17).

3 Solid-phase carbon trap not collected prior to purging.

4 Recovered in volatiles solid-phase carbon traps via passive diffusion prior to purging and after purging upon collection.

5 Quantitative results for MSA were not reported. The study authors estimated that residues recovered in the ACN extract and first water extract was MSA (p. 21; Figure 6, p. 38; Figures 8-9, pp. 40-41; Table 3, p. 47; DER Attachment 2).

6. Unidentified [^{14}C] residues account for the entire second water extract from soil, and the entire extract from sodium hypochlorite solution.

7. Nonextractable residues measured include those in the Soil PES sample only.

8 KOH solution maintained inside incubation bottle (p. 24). At some, but not all, intervals, ^{14}CO$_2$ was distinguished from other volatile [^{14}C]organics via barium chloride precipitation (Table 4, p. 32).

9. Total recovery = Dimethyl disulfide residues (all volatilized) + Total extractable residues + Nonextractable residues + CO$_2$/other volatile residues

Table 9: Biotransformation of *bis*-[methyl-^{14}C]dimethyl disulfide, expressed as percentage of applied radioactivity (n =2[1]), in Switzerland clay soil under aerobic conditions.

Compound		Sampling times (days)								
		0[2]	1	4	7	11	14	21	59	120
Dimethyl disulfide (all volatilized)[4]	Passive diffusion	--[3]	--	27.25	35.73	40.30	43.66	43.69	42.04	38.60
	Purged	89.16	79.13	34.43	18.92	6.45	2.43	0.05	0.06	0.22
	Total	89.16	79.13	61.68	54.65	46.75	46.09	43.74	42.10	38.82
Methanesulfonic acid (approximate)[5]		1.42	8.09	17.47	25.67	30.34	32.16	32.86	26.80	5.76
Unidentified extractable [14C]residues[6]		0.18	0.80	1.84	2.80	3.27	3.44	3.46	2.88	2.45
Total extractable residues		1.60	8.89	19.31	28.47	33.61	35.60	36.32	29.68	8.21
Nonextractable residues[7]		0.25	0.88	2.02	2.76	3.75	4.17	4.10	3.62	7.25
1N KOH solution (CO₂ / other volatiles)[8]		0.61	12.02	1.84 / 8.67	3.42 / 6.72	3.89 / 6.14	4.87 / 5.59	6.72 / 4.13	14.05	27.24
Total recovery[9]		91.62	100.92	93.54	96.02	94.14	96.32	95.01	89.45	81.52

Data obtained from Table 2, p. 46 and DER Attachment 2.
1 Reviewer's Comment No. 1. Additionally, while duplicate treated soil samples were collected at each interval, the study authors did not specify that the reported results were means of the replicates.
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 2-hour interval (pp. 16-17).
3 Solid-phase carbon trap not collected prior to purging.
4 Recovered in volatiles solid-phase carbon traps via passive diffusion prior to purging and after purging upon collection.
5 Quantitative results for MSA were not reported. The study authors estimated that residues recovered in the ACN extract and first water extract was MSA (p. 20; Figure 6, p. 38; Figures 8-9, pp. 40-41; Table 2, p. 46; DER Attachment 2).
6. Unidentified [14C] residues account for the entire second water extract from soil, and the entire extract from the sodium hypochlorite solution.
7. Nonextractable residues measured include those in the Soil PES sample only.
8 KOH solution maintained inside incubation bottle (p. 24). At some, but not all, intervals, [14]CO₂ was distinguished from other volatile [14C]organics via barium chloride precipitation (Table 4, p. 32).
9. Total recovery = Dimethyl disulfide residues (all volatilized) + Total extractable residues + Nonextractable residues + CO₂/other volatile residues

C. TRANSFORMATION OF PARENT COMPOUND: [14C]Dimethyl disulfide dissipated
from the soils via transformation and diffusion of parent. The 2-hour purge (100-150 mL/minute) interval to collect volatiles upon sampling effectively removed any parent dimethyl disulfide present from the test system, with the exception of very minor amounts (<1.1% of applied) detected in the USA soils' acetonitrile extracts (Figure 7, p. 39).

USA soils. At study termination (120 days), parent [14C]dimethyl disulfide was detected at 79.15% and 73.24% of the applied for the loamy sand (CA) and sand (FL) soils, respectively (Table 5, p. 49; Table 6, p. 50; DER Attachment 2).

In a supplemental diffusion (no purge) experiment with the loamy sand (CA) soil, [^{14}C]dimethyl disulfide was detected in volatiles traps at a mean 0.48% of applied at day 0, 17.91% at 1 day, 33.47% at 2 days, 49.35% at 3 days, 56.20% at 4 days, 75.40% at 8 days and was 94.53% at 14 days (final interval)(Table 4, p. 48 and DER Attachment 2). Diffusion from the sand (FL) soil was not investigated.

Euro soils. For the clay loam (France) soil, [^{14}C]dimethyl disulfide was detected at 90.47% of applied at day 0, 55.46% at 4 days, 45.67% at 7 days and was 35.30% at 59 days (final interval) (Table 3; p. 47; DER Attachment 2). Passive diffusion (no purge) of parent increased from 10.01% at 1 day to 35.12% at 7 days and was 35.27-38.60% thereafter.

For the clay (Switzerland) soil, [^{14}C]dimethyl disulfide was detected at 89.16% of applied at day 0, 54.65% at 7 days, 46.75% at 11 days and was 38.82% at 120 days (final interval) (Table 2, p. 46; DER Attachment 2). Passive diffusion (no purge) of parent increased from 27.25% at 4 days (first interval analyzed) to 40.30% at 11 days and was 38.60-43.69% thereafter.

HALF-LIFE/DT50/DT90: USA soils. Dissipation of parent dimethyl disulfide from the loamy sand (CA) and sand (FL) soils via volatilization (combined diffusion/purging) occurred in <2 hours. However, observed DT50 (50% decline time) values for total detected parent were >120 days (final interval).

In a supplemental experiment with the loamy sand (CA) soil, parent dimethyl disulfide diffused (passive) from the soil with an observed DT50 value of *ca.* 3 days and calculated (all intervals) linear (Excel 2000) and nonlinear (Sigmaplot v 9) half-lives of 3.4-3.5 days (Table 4, p. 48; DER Attachment 2).

In another supplemental experiment, the first-order kinetics algorithm, the KinGui model indicated the observed DT50 values due to combined diffusion and dissipation of dimethyl disulfide from the soils were *ca.* 2.8 days for both USA soils (California loamy sand and Florida sand soils) (Table 1, p. 45).

Euro soils. Dissipation of parent dimethyl disulfide from the clay loam (France) and clay (Switzerland) soils via volatilization (purging only) occurred in <2 hours. However, for the clay loam (France) soil, the observed DT50 (50% decline time) values for the total detected parent diffusion/purging) of *ca.* 6 days and calculated (all intervals) linear with the KinGui model. For the clay (Switzerland) soil, the observed DT50 (50% decline time) values for total detected parent was calculated using the KinGui model at *ca.* 10 days and calculated (all intervals) (Table 2, p. 46; Table 3; p. 47; DER Attachment 2). Half-lives of the DMDS total system are shown in the table below, and supporting plots and statistics are shown in Attachment 2.

In a supplemental experiment, the first-order kinetics algorithm, the KinGui model indicated the observed DT50 values due to combined diffusion and dissipation of dimethyl disulfide from the soils were *ca.* 3 days for the clay loam (France) soil and 2.5 days for the clay (Switzerland) soil (Table 1, p. 45).

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Half-lives/DT50/DT90

Compound	Half-life/DT50 [1] (days)	First order linear regression equation	r^2	DT50[2] (days)	DT90[2] (days)
California loamy sand soil					
Linear/natural log	ND[3]	--	--	--	--
Nonlinear/normal	ND	--	--	2.79	9.29
Observed DT50	>120	--	--	--	--
Florida sand soil					
Linear/natural log	ND	--	--	--	--
Nonlinear/normal	ND	--	--	2.77	9.19
Observed DT50	>120	--	--	--	--
France clay loam soil					
Linear/natural log (Total System DMDS Decline)	48.4	y = -0.0143x + 4.1712	0.4550	--	--
Nonlinear/normal (Total System DMDS Decline)	13.8	--	0.6267	2.69	8.93
Observed DT50 (Total System DMDS Decline)	ca. 6	--	--	--	--
Switzerland clay soil					
Linear/natural log (Total System DMDS Decline)	122	y = -0.0057x + 4.1794	0.4145	--	--
Nonlinear/normal (Total System DMDS Decline)	68.6	--	0.4227	3.04	10.09
Observed DT50 (Total System DMDS Decline)	ca. 10	--	--	--	--
California loamy sand/supplemental diffusion experiment					
Linear/natural log	3.4	y = -0.2010x + 4.6066	0.9902	--	--
Nonlinear/normal	3.5	--	0.9942	--	--
Observed DT50	ca. 3	--	--	--	--

1 Determined by the primary reviewer using Excel 2000 (linear) and Sigmaplot v 8.0 (nonlinear) and individual sample data obtained from Appendix 1, pp. 46-50 of the study report (DER Attachment 2).
2 Determined by the study authors using kinetic modeling (KinGui software, Bayer CropScience) and correcting for diffusion (Appendix 1, pp. 43-74).
3 ND = Not determined due to insufficient transformation of parent.

The aerobic soil metabolism half-life of DMDS can be estimated from soil degradates (methanesulfonic acid, unidentified extractable residue, non-extractable residue, and CO_2) formation rates in soil because of the high volatility of DMDS; DMDS was only detected in the head space of the biometer flask. Additionally, the aerobic soil metabolism studies for DMDS were designed as closed-head space test systems. The combination of the high volatility of

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DMDS and the closed-head space of the test systems led to no detection of DMDS in the soil as well as possible sterilization of the soil in the test system from a fumigation effect.

The DMDS concentration in soil was approximated in aerobic soil metabolism data (MRID 47052819) using the following equation:

$$DMDS_{estimate} = 1.00 - \sum(\text{soil degradation products})_{time}$$

where soil degradation products = methanesulfonic acid + unidentified extractable residue + unextractable residue + CO_2 (% of applied radioactivity) at each time interval.

The table below shows the estimated concentration of DMDS from the aerobic soil metabolism studies.

DMDS concentration estimate in soil in the aerobic soil metabolism study (MRID 47052819) using a total system mass balance

Time (Days)	Switzerland clay		France clay loam	
	Soil Degradation Products	Estimate DMDS	Soil Degradation Products	Estimate DMDS
0	2.46	97.54	2.18	97.82
1	21.79	78.21	8.86	91.14
4	23.17	76.83	37.83	62.17
7	34.65	65.35	47.8	52.2
11	41.25	58.75	49.7	50.3
14	44.64	55.36	50.97	49.03
21	47.14	52.86	47.68	52.32
59	47.35	52.65	75.18	24.82
120	42.7	57.3		

The DMDS degradation rate was estimated using non-linear regression with the 3 parameter exponential decay ($y = y_0 + ae^{-bx}$) models (SigmaPlot, Version 10). Plots contained in Attachment 3 illustrates the model fit for a 3-parameter exponential decay model fit to DMDS degradation in a France clay loam soil and Switzerland clay soil, respectively. The table below shows the computation of half-lives for DMDS in soil from the 3 parameter exponential decay model for both soils.

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Fitted parameters for exponential decay model for DMDS in aerobic soil metabolism Study (MRID 47052819) using a total system mass balance.

Soil	Model	Y_0 (% applied)	a (% applied)	b (days^{-1})	Estimated Half-life (days)	Adjusted R2
France Clay Loam	3-parameter exponential decay	48.0940	47.6464	0.2006	3.45	0.8022
Switzerland Clay		53.9264	38.9367	0.1844	3.75	0.9325

Another approach can be to assume the degradation of DMDS can be indirectly modeled from the formation of methanesulfonic acid. Methanesulfonic acid forms through the breaking of the disulfide bond in DMDS. The DMDS concentration in soil was approximated in aerobic soil metabolism data (MRID 47052819) using the following equation:

$$[DMDS]_{estimate} = 1.00 - [methanesulfonic\ acid]_{time}$$

The table below shows the estimated concentration of DMDS from the aerobic soil metabolism studies using this approach. Figures 4-2a and 4-2b illustrates the model fit for a 3-parameter exponential decay model fit to DMDS degradation France clay loam soil and Switzerland clay soil, respectively, using this approach. The table below shows the computation of half-lives for DMDS in soil from the 3 parameter exponential decay model for both soils.

DMDS concentration estimate in soil in the aerobic soil metabolism study (MRID 47052819) using methanesulfonic acid formation.

Time (Days)	Switzerland clay		France clay loam	
	Methanesulfonic acid	Estimate DMDS	Methanesulfonic acid	Estimate DMDS
0	1.42	98.58	1.45	98.55
1	8.09	91.91	6.17	93.83
4	17.47	82.53	21.68	78.32
7	25.67	74.33	29.1	70.9
11	30.34	69.66	32.5	67.5
14	32.16	67.84	33.17	66.83
21	32.86	67.14	32.97	67.03
59	26.8	**73.2**	35.3	64.7
120	5.76	**94.24**		

Bolded values were not included in the degradation kinetic analysis because they indicate DMDS formation. This situation is likely an artifact of from the degradation of methanesulfonic acid in soil.

Plots contained in Attachment 3 illustrates the model fit for a 3-parameter exponential decay model fit to DMDS degradation in a France clay loam soil and Switzerland clay soil, respectively, assuming that all DMDS degradation was due to the observed methanesulfonic acid

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formation in the soil. The table below shows the computation of half-lives for DMDS in soil from the 3 parameter exponential decay model for both soils.

Fitted parameters for exponential decay model for DMDS in aerobic soil metabolism study using methanesulfonic acid formation (MRID 47052819).

Soil	Model	Y_0 (% applied)	a (% applied)	b (days^{-1})	Estimated Half-life (days)	Adjusted R^2
France Clay Loam	3-parameter exponential decay	65.4818	34.1053	0.2422	2.86	0.80
Switzerland Clay		65.8673	32.38	0.1851	3.74	0.9948

TRANSFORMATION PRODUCTS: One nonvolatile transformation product,

- methanesulfonic acid (MSA),

was detected in all four soils. MSA was a minor product in the USA soils, but a major product in the Euro soils. MSA was isolated from clay (Switzerland) soil extract and identified via LC/MS and LC/MS/MS against reference standard (Appendix 2, pp. 76-86). Quantitative results for MSA were not reported, but approximated by the primary reviewer based on the percentages the study authors estimated that MSA comprised in the various extracts (DER Attachment 2).

USA soils. MSA was detected at approximate maximums of 3.26% and 4.95% of applied in the loamy sand (CA) and sand (FL) soils, respectively, at 120 days (DER Attachment 2). Unidentified extractable [^{14}C]residues were <2% of applied at any interval for both soils.

Euro soils. In the clay loam (France) soil, MSA was detected at an approximate maximum of 33.17% at 14 days decreasing to 32.97% at 21 days and was 2.02% at 59 days, while at a maximum 32.86% at 21 days in the clay (Switzerland) soil decreasing to 26.80% at 59 days and was 5.76% at 120 days. Unidentified extractable [^{14}C]residues were maximums of 6.00% and 3.46% for the clay loam and clay soils, respectively.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: USA soils. Extractable [^{14}C]residues were maximums of 3.86% and 6.61% of applied for the loamy sand (CA) and sand (FL) soils, respectively, at 120 days, while nonextractable [^{14}C]residues were <1.1% for either soil at all intervals (DER Attachment 2).

Euro soils. Extractable clay loam (France) soil [^{14}C]residues increased to 39.06% at 14 days and were 6.83% at 59 days, while nonextractable [^{14}C]residues were a maximum 4.26% at study termination (DER Attachment 2). Extractable clay (Switzerland) soil [^{14}C]residues increased to 36.32% at 21 days and were 8.21% at 120 days, while nonextractable [^{14}C]residues were a maximum 7.25% at termination.

VOLATILIZATION: Parent dimethyl disulfide reportedly accounted for all volatilized [^{14}C]residues recovered by the solid-phase carbon traps (p. 24). Analysis of the KOH solutions

Data Evaluation Record on the aerobic biotransformation of dimethyl disulfide in soil

via barium chloride precipitation at selected intervals showed that the trapping solution absorbed volatile [^{14}C]organics in addition to $^{14}CO_2$ (Table 4, p. 32).

USA soils. Maximum levels of [^{14}C]residues in the KOH solutions were 8.30-8.35% for the loamy sand (CA) and sand (FL) soils; barium chloride precipitation indicated that $^{14}CO_2$ accounted for ≤20% of the sample radioactivity at the intervals analyzed.

Euro soils. At study termination, [^{14}C]residues in the KOH solutions were maximums of 30.81% and 27.24% of applied for the clay loam (France) and clay (Switzerland) soils, respectively, with barium chloride precipitation indicating that $^{14}CO_2$ accounted for up to 52.7% and 61.9% of the sample radioactivity, respectively, at the intervals analyzed.

TRANSFORMATION PATHWAY: The study authors provided transformation pathways that were consistent with the transformation products detected in this study (Figure 10, p. 42). In addition to significant levels of diffusion of parent dimethyl disulfide from the soil, the compound was found to degrade to methanesulfonic acid and CO_2 with low levels of formation of bound soil residues.

Table 10: Chemical names and CAS numbers for the transformation products of dimethyl disulfide.[1]

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
MSA	75-75-2	Methanesulfonic acid	CH_4O_3S	95.98	--[2]

Data obtained from Appendix 2, p. 76 of the study report.
1 Identification via LC/MS and LC/MS/MS against reference standard.
2 Information not provided.

D. SUPPLEMENTARY EXPERIMENT-RESULTS: Diffusion from loamy sand (CA) soil. Results discussed above.

Diffusion in absence of soil. The study authors only reported that the results were similar to diffusion from the loamy sand (CA) soil with *ca.* 50% of parent diffused by 4 days posttreatment and >90% at 14 days (pp. 23-24).

III. STUDY DEFICIENCIES: The following significant deviations from good scientific practices or the objectives of Subdivision N guidelines were noted:

For the portion of this study conducted with USA soils:

- Dissipation of parent dimethyl disulfide via diffusion and volatilization effected by the post-sampling 2-hour purge interval were not distinguished.

- While a supplemental experiment investigating diffusion of parent from the loamy sand (CA) soil was conducted, details regarding experimental procedures were not reported

and no results other than analysis of the solid-phase traps were provided. Therefore, adequate comparisons between the experiments could not be made.

- At study termination (120 days), parent [^{14}C]dimethyl disulfide was detected at 73.24-79.15% of the applied, and the experimental design did not allow for dissipation via diffusion to be assessed. Consequently, it could not be determined that the study was not terminated before the pattern of decline of the test substance was established.

- The test soils were inadequately characterized; only soil type, maximum water holding capacity and biomass were reported.

For the portion of this study conducted with Euro soils:

- Dissipation of parent dimethyl disulfide via diffusion and volatilization effected by the post-sampling 2-hour purge interval were not distinguished.

- Since DMDS residues were detected in the headspace immediately upon the beginning of the study, the route of degradation, as observed with the accumulation of degradate products in the soil over time, is unclear.

- For the France clay loam and Switzerland clay soils, 22.8% and 18.5% of the applied, respectively, was unaccounted for at study termination. The study authors reported mass balances of 93.2-112.5% and 97.2-106.8% for the clay loam (French) and clay (Swiss) soils, respectively (pp. 20-21); however, supporting quantitative data were not provided.

- At study termination, radioactivity recovered in the KOH trapping solution totaled 30.81% of applied at 59 days for the clay loam (France) soil and 27.24% at 120 days for the clay (Switzerland) soil, and, at the intervals analyzed, barium chloride precipitation indicated that $^{14}CO_2$ only accounted for, at most, *ca.* 53-62% of the sample radioactivity. Therefore, volatile organics, other than CO_2, may have been present at ≥10% of the applied and were not identified.

- The test soils were inadequately characterized; only soil type, maximum water holding capacity and biomass were reported.

IV. REVIEWER'S COMMENTS

1. Individual replicate results were not provided, and, while duplicate treated soil samples were collected at each interval, the study authors did not specify that the reported results were means of the replicates. Overall mean results and standard deviations presented in this review were determined by the primary reviewer using Microsoft Excel 2000 (9.0.2720) software (DER Attachment 2). Standard deviations were determined using the "biased" or "n" method which determines the standard deviation of the entire sample population. Mean material balance summations were not reported for all sampling intervals by the study

authors and the ranges reported in the study text (pp. 20-22) were not in agreement with the ranges determined by the primary reviewer.

2. The test application rate of 392 mg a.i./kg 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 (pp. 9, 15; Tables 1-2, pp. 29-30).

3. The France and Switzerland soils were classified as a clay loam and clay, respectively (USDA textural classifications, unconfirmed). FAO soil classifications were also provided; the France and Switzerland soils were classified as Dystric Cambisol and Calcaric Cambisol, respectively. Cambisols fall under the category of the Inceptisol U.S. Taxonomic Classification, which are found domestically in the Southwest. Therefore, the mineral and chemical properties of these soils can be considered representative of that which is found domestically.

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-1, Aerobic Soil Metabolism Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

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

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).

$$H_3C-S-S-CH_3$$

Methanesulfonic acid [MSA]

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

$$O=S(=O)(OH)-CH_3$$

Carbon Dioxide

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

$$O=C=O$$
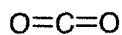
Attachment 2

Excel and Sigmaplot Spreadsheets – DMDS Total System Degradation/Dissipation Plots and Statistics

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052819
Guideline: 162-1

Aerobic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in four soils.
Half-life determination
France clay loam soil.
Half-life (days)   48.4   (0- to 59-day data)

Days Posttreatment	Dimethyl disulfide	
	(% of Applied)	Ln (% applied)
0	100.00	4.605170186
0.08	90.47	4.505018304
1	74.91	4.316287393
4	55.46	4.01566204
7	45.67	3.821441627
11	41.26	3.719893508
14	38.80	3.658420247
21	38.82	3.658935578
59	35.30	3.563882964

"Time 0" presumed to be 100%; first sampling interval after 2 hours of volatiles collection.
Study authors reported that radioactivity recovered in the solid sorbent (CT) traps was
identified as dimethyl disulfide; data imported from **Clay loam** worksheet.

Dissipation of *bis*-[methyl-^{14}C]dimethyl disulfide
in aerobic France clay loam soil

$y = -0.0143x + 4.1712$
$r^2 = 0.4550$

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.674539641
R Square	0.455003727
Adjusted R Square	0.377147116
Standard Error	0.312345151
Observations	9

ANOVA

	df	SS	MS	F	Sig F
Regression	1	0.570149827	0.5701	5.844124523	0.0462642
Residual	7	0.682916452	0.0976		
Total	8	1.253066279			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.171211443	0.129519275	32.205	7.19767E-09	3.8649472	4.4774756	3.864947243	4.47747564
X Variable 1	-0.014316223	0.005922004	-2.417	0.04626422	-0.02832	-0.0003129	-0.02831953	-0.0003129

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052819
Guideline: 162-1

Aerobic metabolism of bis-[methyl-^{14}C]dimethyl disulfide in four soils.
Half-life determination
Switzerland clay soil.
Half-life (days)   122   (0- to 120-day data)

Days Posttreatment	Dimethyl disulfide	
	(% of Applied)	Ln (% applied)
0	100.00	4.605170186
0.08	89.16	4.490432509
1	79.13	4.37109207
4	61.68	4.121959729
7	54.65	4.000949215
11	46.75	3.844814256
14	46.09	3.830596007
21	43.74	3.778263015
59	42.10	3.740047741
120	38.82	3.658935578

"Time 0" presumed to be 100%; first sampling interval after 2 hours of volatiles collection.
Study authors reported that radioactivity recovered in the solid sorbent (CT) traps was
identified as dimethyl disulfide; data imported from **Clay** worksheet.

Dissipation of bis-[methyl-^{14}C]dimethyl disulfide
in aerobic Switzerland clay soil

$y = -0.0057x + 4.1794$
$r^2 = 0.4145$

Ln (% of applied)

Days posttreatment
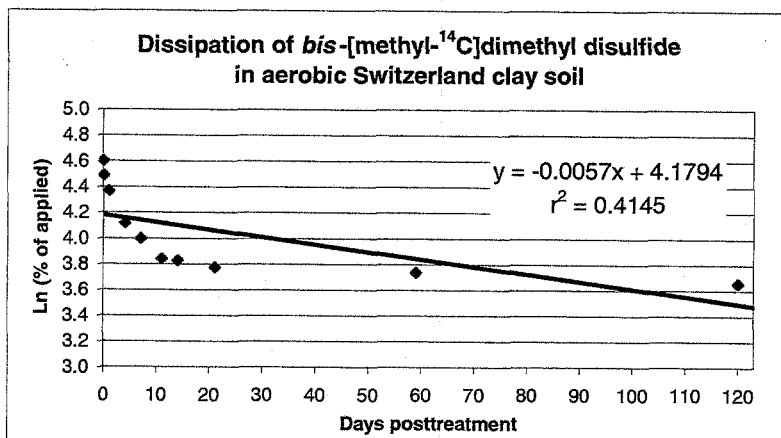
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.643795943
R Square	0.414473216
Adjusted R Square	0.341282368
Standard Error	0.273982778
Observations	10

ANOVA

	df	SS	MS	F	Sig F
Regression	1	0.425095219	0.4251	5.662910423	0.0445674
Residual	8	0.600532499	0.0751		
Total	9	1.025627718			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.179362097	0.103592745	40.344	1.56786E-10	3.9404766	4.4182475	3.940476645	4.41824755
X Variable 1	-0.00569994	0.002395248	-2.38	0.044567441	-0.011223	-0.0001765	-0.01122339	-0.0001765

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052819
Guideline: 162-1
Aerobic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in four soils.
Half-life determination
California loamy sand soil: supplemental diffusion experiment.
Half-life (days)   3.4   (0- to 14-day data)

Days Posttreatment	Dimethyl disulfide	
	(% of Applied)	Ln (% applied)
0	99.52	4.600358629
1	82.09	4.407816206
2	66.54	4.197803271
3	50.65	3.924939231
4	43.81	3.779862102
8	24.61	3.203152864
14	5.47	1.699278616

Results from Appendix 1, p. 48 of the study report.

Diffusion of *bis*-[methyl-^{14}C]dimethyl disulfide
in aerobic California loamy sand soil

$y = -0.2010x + 4.6066$
$r^2 = 0.9902$
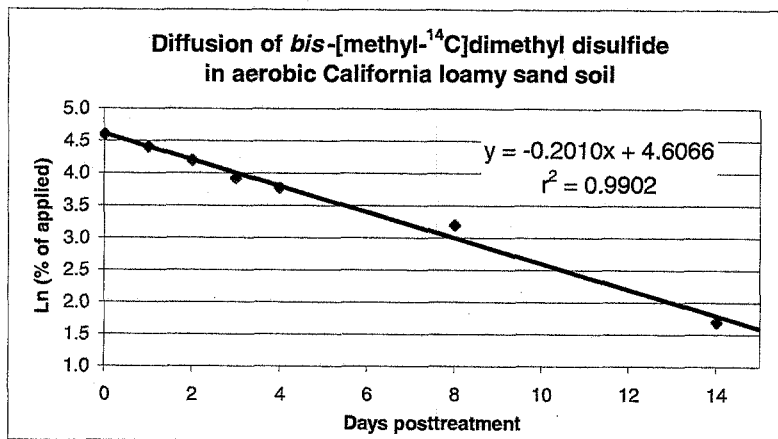
SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.99509932
R Square	0.990222656
Adjusted R Square	0.988267187
Standard Error	0.107093512
Observations	7

ANOVA

	df	SS	MS	F	Sig F
Regression	1	5.807755132	5.8078	506.3863315	3.221E-06
Residual	5	0.057345102	0.0115		
Total	6	5.865100233			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.60658168	0.057499381	80.115	5.74118E-09	4.4587751	4.7543883	4.458775057	4.7543883
X Variable 1	-0.201026901	0.008933326	-22.5	3.22072E-06	-0.223991	-0.1780631	-0.22399071	-0.1780631

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052819
Guideline: 162-1

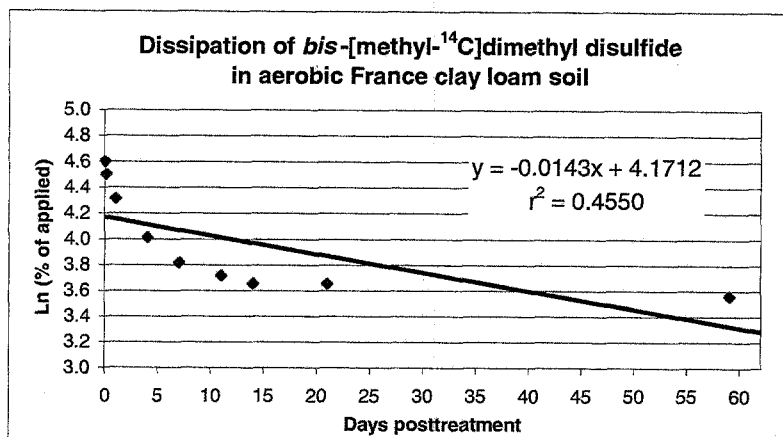**Aerobic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in four soils.**
Nonlinear half-lives (exponential decay/single compartment, 2 parameter):

California loamy sand soil:
Half-life (days)   ND[1]
r squared

California loamy sand soil diffusion experiment:
Half-life (days)   3.4
r squared   0.9902

Florida sand soil:
Half-life (days)   ND[1]
r squared

France clay loam soil:
Half-life (days)   13.8
r squared   0.6267

Switzerland clay soil:
Half-life (days)   68.6
r squared   0.4227

1 Not determined due to insufficient transformation.

bis-[methyl-^{14}C]dimethyl disulfide in aerobic France clay loam soil (1/2 model, nonlinear)
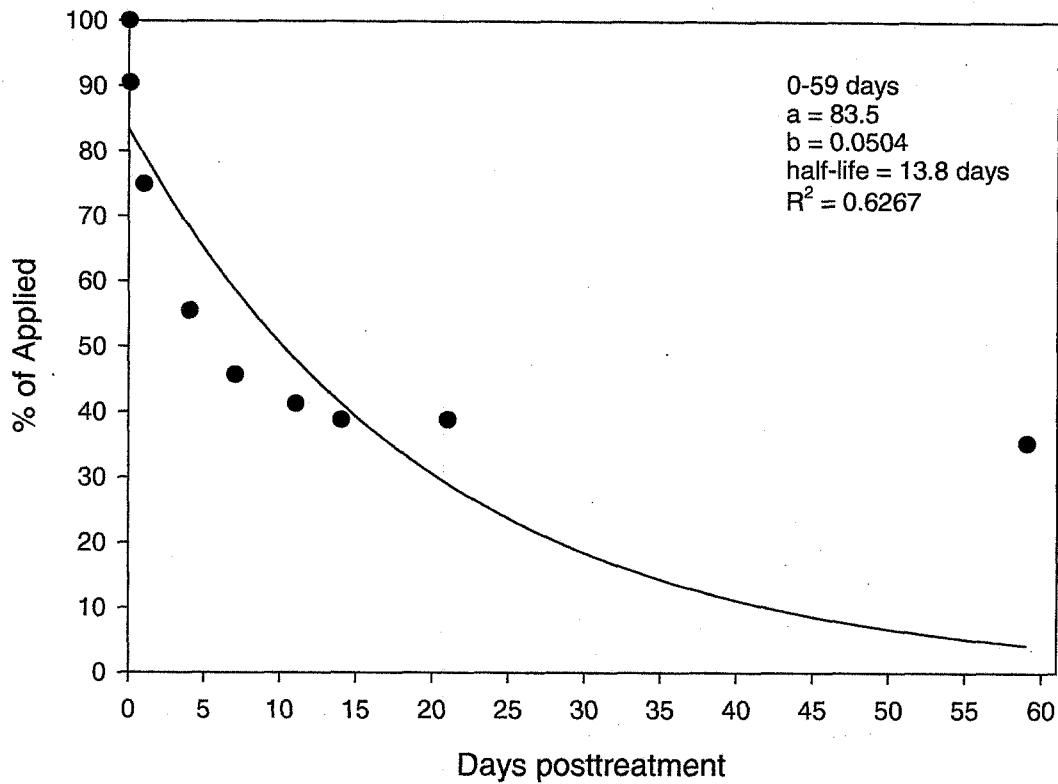
0-59 days
a = 83.5
b = 0.0504
half-life = 13.8 days
R^2 = 0.6267

Days posttreatment

"Time 0" presumed to be 100%; first sampling interval after 2 hours of volatiles collection.

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052819
Guideline: 162-1
France clay 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: 83.4698}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.0503869}}
[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 = 0.79167449   Rsqr = 0.62674849   Adj Rsqr = 0.57342685

Standard Error of Estimate = 15.9892

	Coefficient	Std. Error	t	P
a	83.4698	8.8896	9.3896	<0.0001
b	0.0504	0.0170	2.9707	0.0208

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	3004.9888	3004.9888	11.7541	0.0110
Residual	7	1789.5800	255.6543		
Total	8	4794.5688	599.3211		

PRESS = 2570.7553

Durbin-Watson Statistic = 0.5309

Normality Test: K-S Statistic = 0.1877   Significance Level = 0.8742

Constant Variance Test: Passed   (P = 0.9129)

Power of performed test with alpha = 0.0500: 0.7503

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052819
Guideline: 162-1
France clay loam soil
bis-[methyl-^{14}C]-label
The power of the performed test (0.7503) 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	83.4698	16.5302	1.0338	1.2438	1.3047
2	83.1201	7.3499	0.4597	0.5502	0.5208
3	79.3682	-4.4582	-0.2788	-0.3191	-0.2976
4	68.2336	-12.7736	-0.7989	-0.8623	-0.8444
5	58.6611	-12.9911	-0.8125	-0.8812	-0.8653
6	47.9534	-6.6934	-0.4186	-0.4721	-0.4442
7	41.2260	-2.4260	-0.1517	-0.1766	-0.1639
8	28.9729	9.8471	0.6159	0.7457	0.7195
9	4.2702	31.0298	1.9407	2.0094	2.8598

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.3461	0.3091	0.8727
2	0.0655	0.3020	0.3425
3	0.0158	0.2363	-0.1655
4	0.0613	0.1416	-0.3429
5	0.0685	0.1499	-0.3634
6	0.0303	0.2139	-0.2317
7	0.0055	0.2621	-0.0977
8	0.1295	0.3178	0.4911
9	0.1456	0.0672	0.7679

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	83.4698	62.4493	104.4904	40.2108	126.7288
2	83.1201	62.3429	103.8973	39.9788	126.2614
3	79.3682	60.9874	97.7491	37.3286	121.4079
4	68.2336	54.0080	82.4592	27.8375	108.6297
5	58.6611	44.0207	73.3016	18.1171	99.2052
6	47.9534	30.4691	65.4377	6.2979	89.6089
7	41.2260	21.8700	60.5820	-1.2491	83.7011
8	28.9729	7.6575	50.2883	-14.4301	72.3759
9	4.2702	-5.5345	14.0748	-34.7888	43.3292

bis-[methyl-^{14}C]dimethyl disulfide in aerobic Switzerland clay soil (1/2 model, nonlinear)
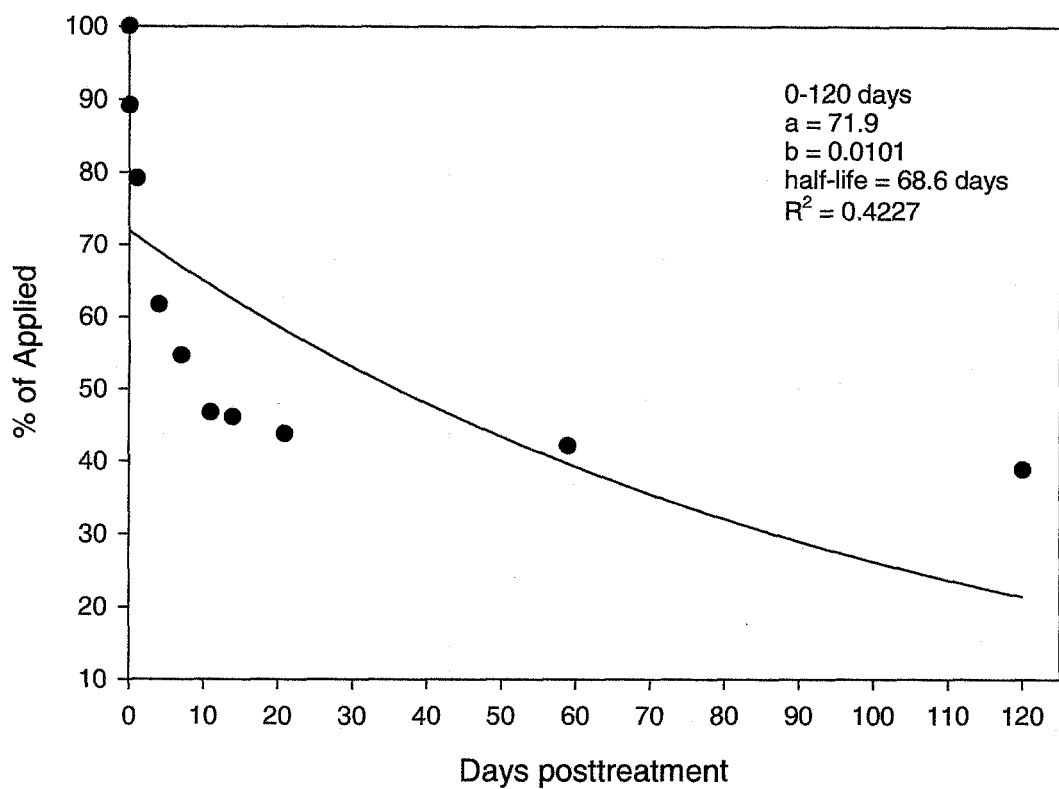
0-120 days
a = 71.9
b = 0.0101
half-life = 68.6 days
R^2 = 0.4227

"Time 0" presumed to be 100%; first sampling interval after 2 hours of volatiles collection.

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052819
Guideline: 162-1
Switzerland clay 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: 71.8519}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.0100955}}
[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 = 0.65018712   Rsqr = 0.42274329   Adj Rsqr = 0.35058620

Standard Error of Estimate = 17.5113

	Coefficient	Std. Error	t	P
a	71.8519	7.4042	9.7042	<0.0001
b	0.0101	0.0051	1.9685	0.0845

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	1796.5315	1796.5315	5.8587	0.0418
Residual	8	2453.1670	306.6459		
Total	9	4249.6986	472.1887		

PRESS = 4222.2212

Durbin-Watson Statistic = 0.4094

Normality Test: K-S Statistic = 0.1720   Significance Level = 0.9007

Constant Variance Test: Passed   (P = 0.5588)

Power of performed test with alpha = 0.0500: 0.5367

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052819
Guideline: 162-1
Switzerland clay soil
bis-[methyl-^{14}C]-label
The power of the performed test (0.5367) 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	71.8519	28.1481	1.6074	1.7738	2.1302
2	71.7915	17.3685	0.9918	1.0938	1.1095
3	71.1302	7.9998	0.4568	0.5006	0.4757
4	69.0082	-7.3282	-0.4185	-0.4511	-0.4274
5	66.9495	-12.2995	-0.7024	-0.7492	-0.7267
6	64.2998	-17.5498	-1.0022	-1.0618	-1.0716
7	62.3816	-16.2916	-0.9303	-0.9850	-0.9829
8	58.1253	-14.3853	-0.8215	-0.8781	-0.8641
9	39.6057	2.4943	0.1424	0.1795	0.1683
10	21.3947	17.4253	0.9951	1.4126	1.5253

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.3425	0.1788	0.9939
2	0.1293	0.1778	0.5159
3	0.0251	0.1671	0.2131
4	0.0165	0.1393	-0.1719
5	0.0386	0.1210	-0.2696
6	0.0690	0.1091	-0.3750
7	0.0587	0.1079	-0.3419
8	0.0549	0.1247	-0.3262
9	0.0095	0.3705	0.1291
10	1.0131	0.5038	1.5369

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	71.8519	54.7777	88.9262	28.0094	115.6945
2	71.7915	54.7662	88.8169	27.9680	115.6150
3	71.1302	54.6232	87.6372	27.5055	114.7550
4	69.0082	53.9394	84.0770	25.9071	112.1093
5	66.9495	52.9039	80.9951	24.1954	109.7037
6	64.2998	50.9618	77.6378	21.7729	106.8267
7	62.3816	49.1148	75.6484	19.8769	104.8863
8	58.1253	43.8638	72.3869	15.2998	100.9509
9	39.6057	15.0246	64.1867	-7.6687	86.8800
10	21.3947	-7.2675	50.0569	-28.1245	70.9140

Diffusion of *bis*-[methyl-^{14}C]dimethyl disulfide in aerobic California loamy sand soil (1/2 model, nonlinear)
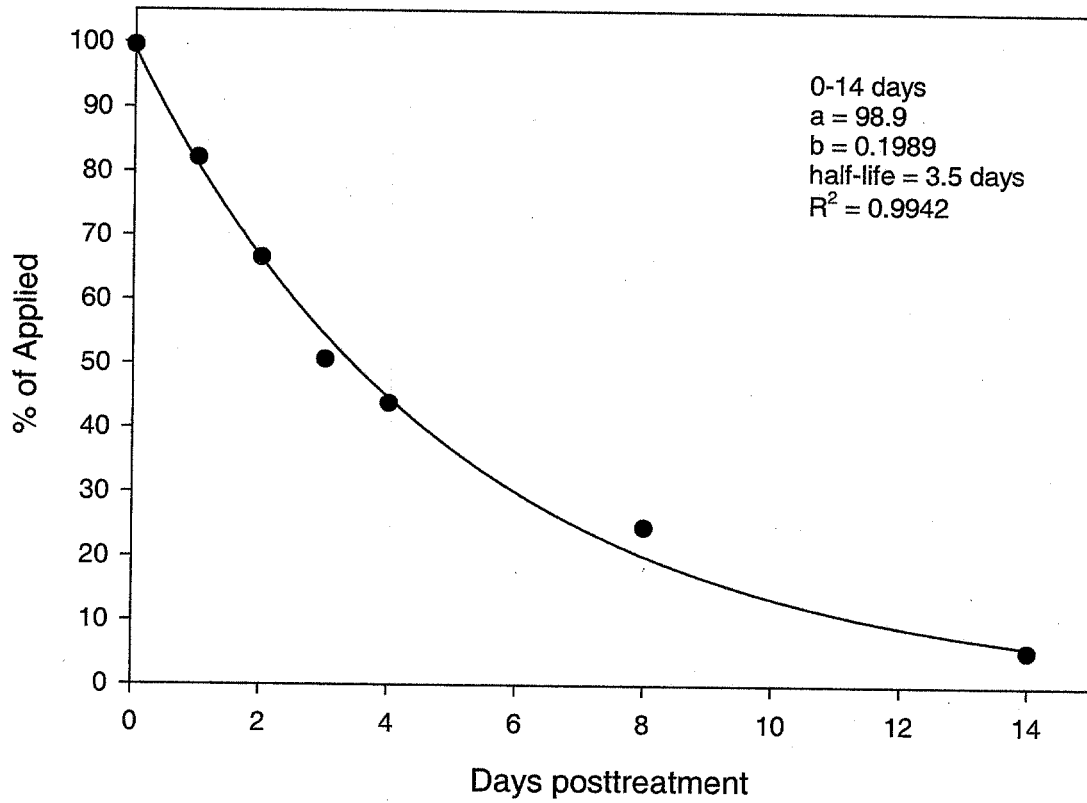
0-14 days
a = 98.9
b = 0.1989
half-life = 3.5 days
R^2 = 0.9942

% of Applied

Days posttreatment

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052819
Guideline: 162-1
California loamy sand: diffusion
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: 98.8698}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 0.198866}}
[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 = 0.99708369   Rsqr = 0.99417589   Adj Rsqr = 0.99301107

Standard Error of Estimate = 2.7193

	Coefficient	Std. Error	t	P
a	98.8698	2.1969	45.0036	<0.0001
b	0.1989	0.0105	18.8548	<0.0001

Analysis of Variance:

	DF	SS	MS	F	P
Regression	1	6311.3603	6311.3603	853.5001	<0.0001
Residual	5	36.9734	7.3947		
Total	6	6348.3337	1058.0556		

PRESS = 70.5751

Durbin-Watson Statistic = 2.1416

Normality Test: K-S Statistic = 0.2279   Significance Level = 0.8076

Constant Variance Test: Passed   (P = 0.7200)

Power of performed test with alpha = 0.0500: 1.0000

Chemical: Dimethyl disulfide
PC: 029088
MRID 47052819
Guideline: 162-1
California loamy sand: diffusion
bis-[methyl-^{14}C]-label
Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	98.8698	0.6502	0.2391	0.4057	0.3690
2	81.0396	1.0504	0.3863	0.4506	0.4115
3	66.4249	0.1151	0.0423	0.0472	0.0422
4	54.4458	-3.7958	-1.3959	-1.5915	-2.0266
5	44.6270	-0.8170	-0.3005	-0.3547	-0.3213
6	20.1434	4.4666	1.6425	1.9405	3.4934
7	6.1085	-0.6385	-0.2348	-0.2463	-0.2216

Influence Diagnostics:

Row	Cook'sDist	Leverage	DFFITS
1	0.1547	0.6527	0.5059
2	0.0366	0.2652	0.2472
3	0.0003	0.1944	0.0207
4	0.3800	0.2308	-1.1100
5	0.0247	0.2823	-0.2015
6	0.7451	0.2835	2.1976
7	0.0030	0.0911	-0.0702

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	98.8698	93.2224	104.5172	89.8833	107.8562
2	81.0396	77.4399	84.6393	73.1770	88.9022
3	66.4249	63.3426	69.5072	58.7853	74.0645
4	54.4458	51.0878	57.8039	46.6908	62.2008
5	44.6270	40.9130	48.3411	36.7114	52.5427
6	20.1434	16.4212	23.8656	12.2239	28.0629
7	6.1085	3.9990	8.2180	-1.1931	13.4101

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052819
Guideline: 162-1

Aerobic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in four soils.
Summations (material balances) and determination of means/standard deviations for applied radioactivity.
California loamy sand soil.

Day	Soil						Volatiles		Material	Tentative	Unided
	Extractable								balance	MSA[1]	extractable
	ACN	H2O 1	NaOCl	H2O 2	Total	Nonext.	KOH	CT			
	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	% AR	% AR	% AR
0	0.47	0.16	0.00	0.00	0.63	0.02	0.58	94.34	95.57	0.49	0.14
1	0.75	0.53	0.05	0.03	1.36	0.05	3.78	82.80	87.99	1.06	0.31
7	0.79	0.98	0.19	0.07	2.03	0.12	7.95	86.76	96.86	1.53	0.50
14	0.78	1.17	0.26	0.07	2.28	0.10	6.83	87.19	96.40	1.72	0.56
21	0.71	1.43	0.19	0.10	2.43	0.09	7.42	90.96	100.90	1.93	0.50
62	0.83	2.42	0.22	0.14	3.61	0.15	8.35	82.03	94.14	3.00	0.61
120	0.54	2.88	0.33	0.11	3.86	0.13	8.31	79.15	91.45	3.26	0.60

1 Quantitative results for MSA were not reported; study authors estimated
    ca. 70% of residues in the ACN extract, plus all radioactivity
    in H2O 1 extract was MSA (p. 22).
CT = solid sorbent trap, residues of which were identified as parent DMDS.

Overall	94.76
std. dev.	3.83
maximum	100.90
minimum	87.99
n =	7

"Passive" diffusion of [^{14}C]dimethyl disulfide from loamy sand (CA) soil.

Day	DMDS measured diffusion		
	Rep1	Rep 2	Mean
	%AR	%AR	% AR
0	0.46	0.50	0.48
1	18.27	17.55	17.91
2	34.89	32.04	33.47
3	48.65	50.05	49.35
4	56.94	55.45	56.20
8	75.52	75.27	75.40
14	93.94	95.11	94.53

Results from Appendix 1, pp. 48-49 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: 47052819
Guideline: 162-1

Aerobic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in four soils.
Summations (material balances) and determination of means/standard deviations for applied radioactivity.
Florida sand soil.

	Soil						Volatiles		Material	Tentative	Unided
	Extractable										
	ACN	H2O 1	NaOCl	H2O 2	Total	Nonext.	KOH	CT	balance	MSA[1]	extractable
Day	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	% AR	% AR	% AR
0	1.16	0.27	0.08	0.00	1.51	0.09	0.72	90.77	93.09	0.85	0.66
1	1.86	0.70	0.26	0.10	2.92	0.31	3.80	87.07	94.10	1.63	1.29
4	2.16	1.20	0.46	0.11	3.93	0.79	6.29	80.13	91.14	2.28	1.65
7	1.92	1.78	0.57	0.13	4.40	1.06	7.46	84.35	97.27	2.74	1.66
14	1.16	1.99	0.60	0.14	3.89	0.68	6.16	79.08	89.81	2.57	1.32
21	1.04	2.80	0.77	0.16	4.77	0.71	8.08	79.74	93.30	3.32	1.45
60	0.49	3.70	0.93	0.20	5.32	0.68	7.94	76.40	90.34	3.95	1.38
120	0.36	4.77	1.28	0.20	6.61	0.55	8.30	73.24	88.70	4.95	1.66

1 Quantitative results for MSA were not reported; study authors estimated
   ca. 50% of residues in the ACN extract, plus all radioactivity
   in H2O 1 extract was MSA (pp. 22-23).
CT = solid sorbent trap, residues of which were identified as parent DMDS.
Results from Appendix 1, p. 50 of the study report.

Overall	92.22
std. dev.	2.59
maximum	97.27
minimum	88.70
n =	8

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

Chemical: Dimethyl disulfide
PC: 029088
MRID: 47052819
Guideline: 162-1

Aerobic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in four soils.
Summations (material balances) and determination of means/standard deviations for applied radioactivity.
France clay loam soil.

	Soil						Volatiles				Material	Tentative	Unided
	Extractable							Volatile organics			balance	MSA[2]	extractable
	ACN	H2O 1	NaOCl	H2O 2	Total	Nonext.	KOH	CT 1[1]	CT 2	Total			
Day	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	% AR	% AR	% AR
0	0.86	0.59	0.08	0.02	1.55	0.06	0.57	0.00	90.47	90.47	92.65	1.45	0.10
1	2.16	4.01	0.63	0.23	7.03	0.54	9.99	10.01	64.90	74.91	92.47	6.17	0.86
4	8.07	13.61	2.28	0.81	24.77	1.59	11.47	28.61	26.85	55.46	93.29	21.68	3.09
7	10.66	18.44	4.58	1.42	35.10	2.78	9.92	35.12	10.55	45.67	93.47	29.10	6.00
11	10.65	21.85	4.24	1.59	38.33	1.70	9.67	37.60	3.66	41.26	90.96	32.50	5.83
14	11.11	22.06	4.25	1.64	39.06	2.39	9.52	37.29	1.51	38.80	89.77	33.17	5.89
21	10.40	22.57	4.02	1.47	38.46	3.40	11.04	38.60	0.22	38.82	91.72	32.97	5.49
59	0.32	1.70	3.12	1.69	6.83	4.26	30.81	35.27	0.03	35.30	77.20	2.02	4.81

Overall	90.19
std. dev.	5.04
maximum	93.47
minimum	77.20
n =	8

1 **CT 1** = "DMDS Measured Diffusion", **CT 2** = "DMDS Measured Sweep";
   (**CT** = solid sorbent trap, residues of which were identified as parent DMDS).
2 Quantitative results for MSA were not reported; study authors estimated all of radioactivity
   in the ACN and H2O 1 extracts was MSA (pp. 20-21).
3 Study authors subtracted "DMDS Measured Diffusion" result for day 1 clay loam (French) soil from total
   "DMDS Measured Sweep" of clay (Swiss) soil, so primary reviewer "added the amount back";
   69.12% + 10.01% = 79.13%
Results from Appendix 1, p. 47 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: 47052819
Guideline: 162-1

Aerobic metabolism of *bis*-[methyl-^{14}C]dimethyl disulfide in four soils.
Summations (material balances) and determination of means/standard deviations for applied radioactivity.
Switzerland clay soil.

	Soil						Volatiles				Material	Tentative	Unided
	Extractable					Nonext.	KOH	Volatile organics			balance	MSA[2]	extractable
	ACN	H2O 1	NaOCl	H2O 2	Total			CT 1[1]	CT 2	Total			
Day	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	%AR	% AR	% AR	% AR
0	0.89	0.53	0.18	0.00	1.60	0.25	0.61	0.00	89.16	89.16	91.62	1.42	0.18
1[3]	2.63	5.46	0.58	0.22	8.89	0.88	12.02	0.00	79.13	79.13	100.92	8.09	0.80
4	4.66	12.81	1.30	0.54	19.31	2.02	10.53	27.25	34.43	61.68	93.54	17.47	1.84
7	8.46	17.21	2.10	0.70	28.47	2.76	10.14	35.73	18.92	54.65	96.02	25.67	2.80
11	9.14	21.20	2.31	0.96	33.61	3.75	10.03	40.30	6.45	46.75	94.14	30.34	3.27
14	9.36	22.80	2.44	1.00	35.60	4.17	10.46	43.66	2.43	46.09	96.32	32.16	3.44
21	7.98	24.88	2.46	1.00	36.32	4.10	10.85	43.69	0.05	43.74	95.01	32.86	3.46
59	5.20	21.60	1.99	0.89	29.68	3.62	14.05	42.04	0.06	42.10	89.45	26.80	2.88
120	0.99	4.77	1.53	0.92	8.21	7.25	27.24	38.60	0.22	38.82	81.52	5.76	2.45

Overall	93.17
std. dev.	5.10
maximum	100.92
minimum	81.52
n =	9

1 **CT 1** = "DMDS Measured Diffusion", **CT 2** = "DMDS Measured Sweep";
    (**CT** = solid sorbent trap, residues of which were identified as parent DMDS).
2 Quantitative results for MSA were not reported; study authors estimated all of radioactivity
    in the ACN and H2O 1 extracts was MSA (pp. 20-21).
3 Study authors subtracted "DMDS Measured Diffusion" result for day 1 clay loam (French) soil from total
    "DMDS Measured Sweep" of clay (Swiss) soil, so primary reviewer "added the amount back";
    69.12% + 10.01% = 79.13%
Results from Appendix 1, p. 46 of the study report.
Means and standard deviations calculated using Microsoft program functions @average(A1:A2) and @stdevp(A1:A2).

Attachment 3

Excel and Sigmaplot Spreadsheets – DMDS Estimated Soil Degradation/Dissipation Plots and Statistics

Figure 3-1. DMDS 3-parameter exponential decay model plot and statistics for Switzerland clay soil (DMDS degradation contributing to total major degradate loads).

DMDS Concentration vs. Time
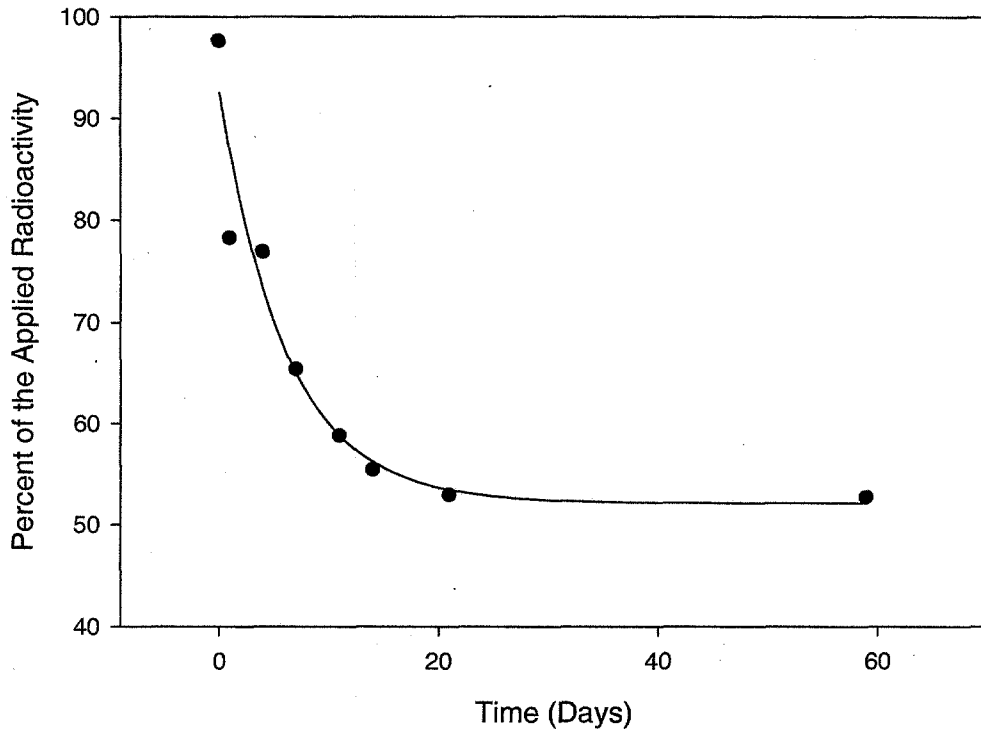
Nonlinear Regression

Data Source: Copy of Data 3 in 4_1_10.JNB
Equation: Exponential Decay, Single, 3 Parameter
f=y0+a*exp(-b*x)

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9690	0.9389	0.9145	4.6452

	Coefficient	Std. Error	t	P	VIF
y0	52.1281	3.5099	14.8518	<0.0001	4.5674<
a	40.3939	4.6772	8.6363	0.0003	2.1590
b	0.1638	0.0499	3.2831	0.0219	2.9600

Analysis of Variance:

Uncorrected for the mean of the observations:

	DF	SS	MS
Regression	3	37778.9324	12592.9775
Residual	5	107.8889	21.5778
Total	8	37886.8213	4735.8527

Corrected for the mean of the observations:

	DF	SS	MS	F	P
Regression	2	1658.9321	829.4661	38.4408	0.0009
Residual	5	107.8889	21.5778		
Total	7	1766.8210	252.4030		

Statistical Tests:

PRESS   408.9861

Durbin-Watson Statistic   3.0639   Failed

Normality Test   Passed   (P = 0.4412)

K-S Statistic = 0.2899   Significance Level = 0.4412

Constant Variance Test   Passed   (P = 0.0860)

Power of performed test with alpha = 0.0500: 0.9963

Regression Diagnostics:

Row	Std. Res.	Stud. Res.	Stud. Del. Res.
1	1.0803	1.8461	2.9263<
2	-1.7670	-2.1906<	-9.7612<
3	0.8022	0.9844	0.9807
4	0.0842	0.1039	0.0930
5	-0.0088	-0.0100	-0.0090
6	-0.1816	-0.2035	-0.1828
7	-0.1211	-0.1454	-0.1303
8	0.1118	0.1703	0.1528

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	2.1817	0.6576	4.0554<
2	0.8589	0.3494	-7.1528
3	0.1634	0.3359	0.6975
4	0.0019	0.3435	0.0673
5	1.0318E-005	0.2352	-0.0050
6	0.0035	0.2034	-0.0923
7	0.0031	0.3061	-0.0866
8	0.0128	0.5691	0.1755

95% Confidence:

Row	Predicted	95% Conf-L	95% Conf-U	95% Pred-L	95% Pred-U
1	92.5220	82.8389	102.2050	77.1485	107.8955
2	86.4178	79.3600	93.4757	72.5471	100.2885
3	73.1034	66.1828	80.0240	59.3020	86.9048
4	64.9589	57.9609	71.9569	51.1185	78.7993
5	58.7908	52.9998	64.5817	45.5198	72.0617
6	56.2037	50.8189	61.5885	43.1049	69.3026
7	53.4227	46.8168	60.0286	39.7764	67.0690
8	52.1307	43.1230	61.1384	37.1733	67.0880

Fit Equation Description:

[Variables]
x = col(1)
y = col(2)
reciprocal_y=1/abs(y)
reciprocal_ysquare=1/y^2
'Automatic Initial Parameter Estimates
yhat(q)=q[size(q)]
[Parameters]
y0 = yhat(y) "Auto {{previous: 52.1281}}
a = max(y)-yhat(y) "Auto {{previous: 40.3939}}
b = if(x50(x,y-yhat(y))=0, 1, -ln(.5)/x50(x,y-yhat(y))) "Auto {{previous: 0.163833}}
[Equation]
f=y0+a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
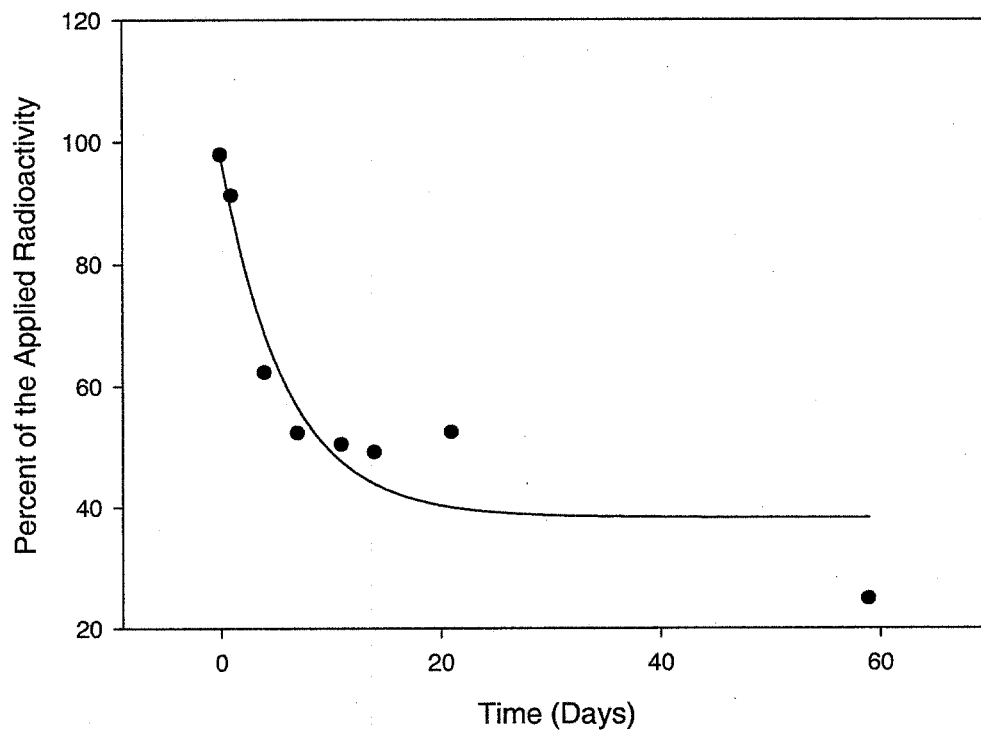[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 7

Figure 3-2. DMDS 3-parameter exponential decay model plot and statistics for France clay loam soil (DMDS degradation contributing to total major degradate loads).

DMDS Concentration vs. Time

Nonlinear Regression

Data Source: Data 6 in 4_1_10.JNB
Equation: Exponential Decay, Single, 3 Parameter
f=y0+a*exp(-b*x)

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9440	0.8911	0.8476	9.3056

	Coefficient	Std. Error	t	P	VIF
y0	38.3049	6.9310	5.5266	0.0027	4.4381<
a	58.9309	9.3349	6.3129	0.0015	2.1154
b	0.1686	0.0706	2.3882	0.0625	2.9130

Analysis of Variance:

Uncorrected for the mean of the observations:

	DF	SS	MS
Regression	3	32319.6747	10773.2249
Residual	5	432.9719	86.5944
Total	8	32752.6466	4094.0808

Corrected for the mean of the observations:

	DF	SS	MS	F	P
Regression	2	3543.6697	1771.8349	20.4613	0.0039
Residual	5	432.9719	86.5944		
Total	7	3976.6416	568.0917		

Statistical Tests:

PRESS   1439.1416

Durbin-Watson Statistic   1.9988   Passed

Normality Test   Passed   (P = 0.9833)

K-S Statistic = 0.1546   Significance Level = 0.9833

Constant Variance Test   Failed   (P = 0.0212)

Power of performed test with alpha = 0.0500: 0.9776

Regression Diagnostics:

Row	Std. Res.	Stud. Res.	Stud. Del. Res.
1	0.0628	0.1082	0.0969
2	0.3273	0.4057	0.3690
3	-0.6622	-0.8187	-0.7869
4	-0.4528	-0.5599	-0.5172
5	0.2975	0.3393	0.3070
6	0.5545	0.6207	0.5779
7	1.3223	1.5911	2.0255<
8	-1.4494	-2.1687<	-7.9639<

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.0077	0.6635	0.1361
2	0.0294	0.3491	0.2702
3	0.1181	0.3458	-0.5721
4	0.0552	0.3458	-0.3761
5	0.0115	0.2312	0.1684
6	0.0325	0.2019	0.2907
7	0.3779	0.3093	1.3555
8	1.9422	0.5533	-8.8640

95% Confidence:

Row	Predicted	95% Conf-L	95% Conf-U	95% Pred-L	95% Pred-U
1	97.2358	77.7510	116.7207	66.3835	128.0882
2	88.0942	73.9615	102.2269	60.3104	115.8780
3	68.3320	54.2652	82.3988	40.5817	96.0824
4	56.4138	42.3463	70.4812	28.6631	84.1644
5	47.5319	36.0297	59.0342	20.9894	74.0745
6	43.8696	33.1206	54.6185	17.6447	70.0945
7	40.0149	26.7110	53.3188	12.6434	67.3864
8	38.3078	20.5139	56.1016	8.4945	68.1210

Fit Equation Description:
[Variables]
x = col(1)
y = col(2)
reciprocal_y=1/abs(y)
reciprocal_ysquare=1/y^2
'Automatic Initial Parameter Estimates
yhat(q)=q[size(q)]
[Parameters]
y0 = yhat(y) "Auto {{previous: 38.3049}}
a = max(y)-yhat(y) "Auto {{previous: 58.9309}}
b = if(x50(x,y-yhat(y))=0, 1, -ln(.5)/x50(x,y-yhat(y))) "Auto {{previous: 0.168566}}
[Equation]
f=y0+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]
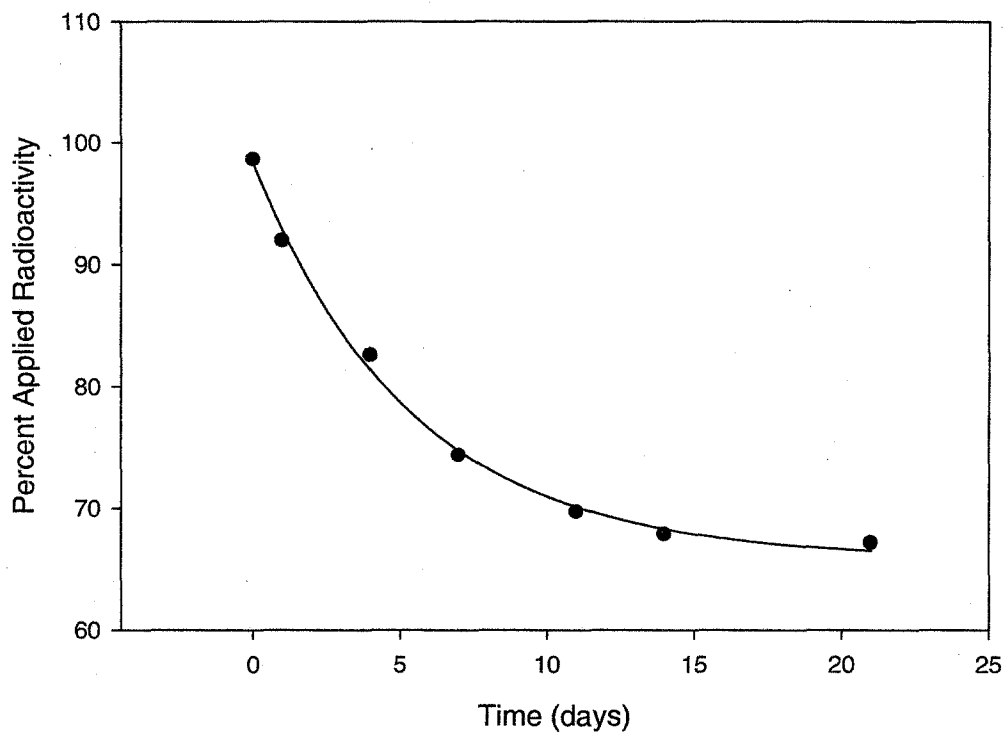b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 26

Figure 3-3. DMDS 3-parameter exponential decay model plot and statistics for Switzerland clay soil (DMDS degradation contributing to methanesulfonic acid loads in soil only).

DMDS Concentration versus Time

Nonlinear Regression

Data Source: Data 3 in Notebook1
Equation: Exponential Decay, Single, 3 Parameter
f=y0+a*exp(-b*x)

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9983	0.9965	0.9948	0.9045

	Coefficient	Std. Error	t	P	VIF
y0	65.8673	0.9114	72.2694	<0.0001	7.1071<
a	32.3842	1.0363	31.2497	<0.0001	2.6462
b	0.1851	0.0170	10.9024	0.0004	4.1927<

Analysis of Variance:

Uncorrected for the mean of the observations:

	DF	SS	MS
Regression	3	44460.9025	14820.3008
Residual	4	3.2726	0.8182
Total	7	44464.1751	6352.0250

Corrected for the mean of the observations:

	DF	SS	MS	F	P
Regression	2	933.3367	466.6684	570.3891	<0.0001
Residual	4	3.2726	0.8182		
Total	6	936.6094	156.1016		

Statistical Tests:

PRESS   11.3880

Durbin-Watson Statistic   2.9157   Failed

Normality Test   Passed   (P = 0.5786)

K-S Statistic = 0.2775   Significance Level = 0.5786

Constant Variance Test   Passed   (P = 0.7200)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Std. Res.	Stud. Res.	Stud. Del. Res.
1	0.3632	0.6670	0.6127
2	-0.9606	-1.1931	-1.2875
3	1.3474	1.7938	3.5128<
4	-0.4425	-0.5554	-0.5007
5	-0.4798	-0.5485	-0.4939
6	-0.5007	-0.5936	-0.5384
7	0.6731	1.0926	1.1297

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	0.3518	0.7035	0.9438
2	0.2575	0.3518	-0.9484
3	0.8285	0.4358	3.0874<
4	0.0592	0.3653	-0.3799
5	0.0307	0.2347	-0.2735
6	0.0476	0.2885	-0.3428
7	0.6504	0.6204	1.4442

95% Confidence:

Row	Predicted	95% Conf-L	95% Conf-U	95% Pred-L	95% Pred-U
1	98.2515	96.1451	100.3579	94.9737	101.5293
2	92.7789	91.2894	94.2684	89.8591	95.6987
3	81.3113	79.6534	82.9692	78.3020	84.3205
4	74.7303	73.2124	76.2481	71.7958	77.6647
5	70.0940	68.8774	71.3106	67.3035	72.8845
6	68.2929	66.9439	69.6419	65.4422	71.1436
7	66.5311	64.5530	68.5092	63.3343	69.7280

Fit Equation Description:

[Variables]
x = col(1)
y = col(2)
reciprocal_y=1/abs(y)
reciprocal_ysquare=1/y^2
'Automatic Initial Parameter Estimates
yhat(q)=q[size(q)]
[Parameters]
y0 = yhat(y) "Auto {{previous: 65.8673}}
a = max(y)-yhat(y) "Auto {{previous: 32.3842}}
b = if(x50(x,y-yhat(y))=0, 1, -ln(.5)/x50(x,y-yhat(y))) "Auto {{previous: 0.185113}}
[Equation]
f=y0+a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
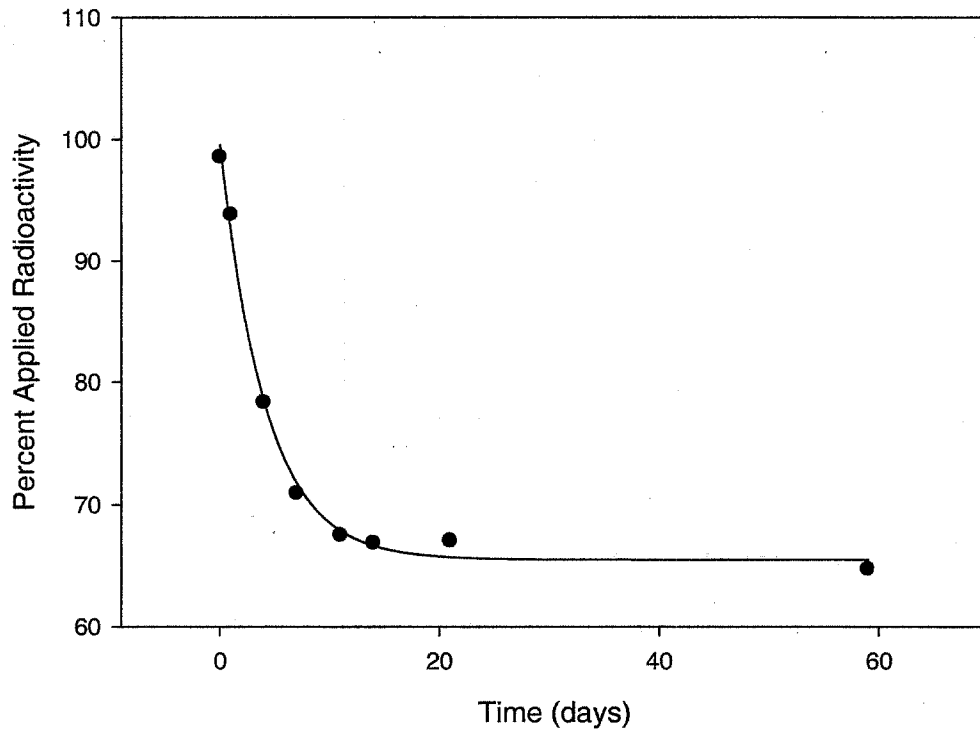[Constraints]
b>0
[Options]
tolerance=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 8

Figure 3-4. DMDS 3-parameter exponential decay model plot and statistics for France clay loam soil (DMDS degradation contributing to methanesulfonic acid loads in soil only).

DMDS Concentration vs. Time

Nonlinear Regression

Data Source: Data 4 in Notebook1
Equation: Exponential Decay, Single, 3 Parameter
f=y0+a*exp(-b*x)

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9972	0.9944	0.9921	1.1709

	Coefficient	Std. Error	t	P	VIF
y0	65.4818	0.7254	90.2648	<0.0001	3.0710
a	34.1053	1.1456	29.7718	<0.0001	1.7227
b	0.2422	0.0225	10.7630	0.0001	2.3187

Analysis of Variance:

Uncorrected for the mean of the observations:

	DF	SS	MS
Regression	3	47371.7590	15790.5863
Residual	5	6.8546	1.3709
Total	8	47378.6136	5922.3267

Corrected for the mean of the observations:

	DF	SS	MS	F	P
Regression	2	1215.4245	607.7123	443.2861	<0.0001
Residual	5	6.8546	1.3709		
Total	7	1222.2791	174.6113		

Statistical Tests:

PRESS   29.3561

Durbin-Watson Statistic   2.4151   Passed

Normality Test   Passed   (P = 0.9591)

K-S Statistic = 0.1698   Significance Level = 0.9591

Constant Variance Test   Passed   (P = 0.5779)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Std. Res.	Stud. Res.	Stud. Del. Res.
1	-0.8857	-1.7399	-2.4774<
2	1.3496	1.6828	2.2855<
3	-0.0887	-0.1228	-0.1100
4	-0.7166	-0.8743	-0.8496
5	-0.3043	-0.3376	-0.3054
6	0.1710	0.1920	0.1724
7	1.1424	1.3830	1.5741
8	-0.6677	-0.8506	-0.8227

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	2.8844	0.7408	-4.1886
2	0.5236	0.3568	1.7023
3	0.0046	0.4784	-0.1053
4	0.1244	0.3281	-0.5937
5	0.0088	0.1876	-0.1467
6	0.0032	0.2068	0.0880
7	0.2968	0.3176	1.0740
8	0.1503	0.3839	-0.6493

95% Confidence:

Row	Predicted	95% Conf-L	95% Conf-U	95% Pred-L	95% Pred-U
1	99.5871	96.9965	102.1777	95.6159	103.5582
2	92.2498	90.4520	94.0477	88.7440	95.7557
3	78.4238	76.3421	80.5056	74.7642	82.0834
4	71.7391	70.0150	73.4632	68.2705	75.2077
5	67.8562	66.5527	69.1597	64.5763	71.1362
6	66.6298	65.2610	67.9985	63.3234	69.9362
7	65.6924	63.9961	67.3887	62.2375	69.1473
8	65.4818	63.6170	67.3465	61.9411	69.0224

Fit Equation Description:
[Variables]
x = col(1)
y = col(2)
reciprocal_y=1/abs(y)
reciprocal_ysquare=1/y^2
'Automatic Initial Parameter Estimates
yhat(q)=q[size(q)]
[Parameters]
y0 = yhat(y) "Auto {{previous: 65.4818}}
a = max(y)-yhat(y) "Auto {{previous: 34.1053}}
b = if(x50(x,y-yhat(y))=0, 1, -ln(.5)/x50(x,y-yhat(y))) "Auto {{previous: 0.242243}}
[Equation]
f=y0+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=1e-10
stepsize=1
iterations=200

Number of Iterations Performed = 7

Attachment 4

Transformation Pathway Presented by Registrant and Illustration of Test System

Figure 10   Proposed metabolic Pathway
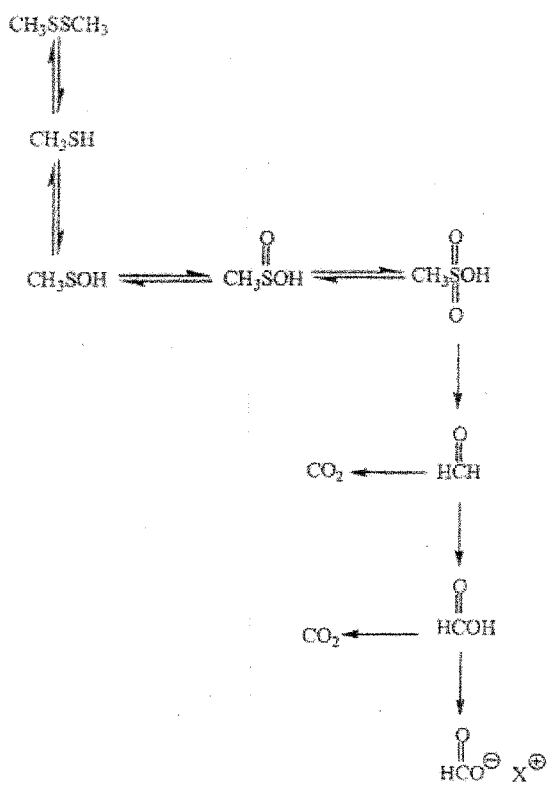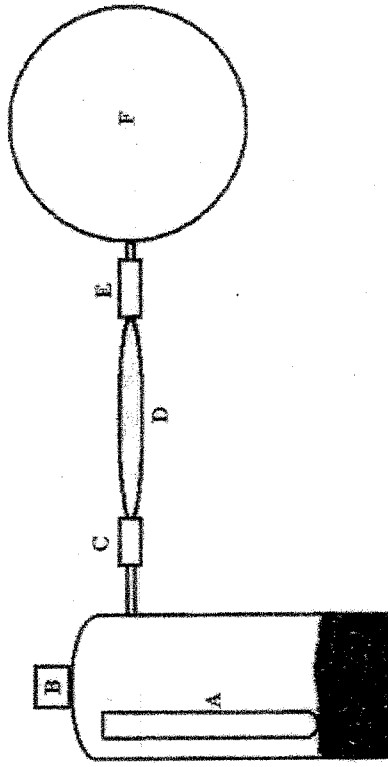
Dimethyl Disulfide Aerobic Soil Metabolism

Figure 1   Test Apparatus

A: Open tube containing 10 mL 1-N aqueous KOH
B: PTFE-lined septum cap
C: PTFE connecting tube
D: Draeger tube containing activated charcoal
E: Tygon® connecting tube
F: Gas-impermeable bag filled with oxygen