

TEXT SEARCHABLE DOCUMENT - 2010

Data Evaluation Record on the adsorption-desorption of dimethyl disulfide [DMDS] in soil

PMRA Submission Number {.....}

EPA MRID Number 46917015

Data Requirement: PMRA Data Code:
EPA DP Barcode: D332939
OECD Data Point:
EPA Guideline: 163-1

Test material:

Common name: Dimethyl disulfide.
Chemical name:
IUPAC name: Dimethyl disulfide.
CAS name: Not reported.
CAS No.: 624-92-0.
Synonyms: Dimethyldisulfide; DMDS; 2,3-dithiabutane; methyl disulfide;
(methyldithio)methane; (methylidisulfanyl)methane; methyldithion ethane.
Smiles string: S(SC)C (EPI Suite, v3.12 SMILES String).

Primary Reviewer: Amy Barnes
Cambridge Environmental

Signature:
Date: 3/5/07


Secondary Reviewer: Joan Harlin
Cambridge Environmental

Signature:
Date: 3/5/07

QC/QA Manager: Joan Gaidos
Cambridge Environmental

Signature:
Date: 3/5/07

Final Reviewer: Gabe Rothman
EPA Reviewer

Signature: ~~8/21/08~~ 
Date: 5/12/10

Company Code:
Active Code:
Use Site Category:
EPA PC Code: 029088

CITATION: Völkel, W. 2006. Adsorption/desorption of DMDS on soils. Unpublished study performed by RCC Ltd, Itingen, Switzerland; sponsored by Arkema, Paris, France, and Cerexagri S.A., Plaisir, France; and submitted by Cerexagri, Inc., King of Prussia, Pennsylvania. RCC Study Number 856203. Experimental start date November 19, 2004, and completion date November 7, 2005 (p. 10). Final report issued June 19, 2006.



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EXECUTIVE SUMMARY

The adsorption/desorption characteristics of [¹⁴C]dimethyl disulfide (DMDS) were studied in a sandy loam soil [Speyer 2.2, pH 5.6, organic carbon 2.3%] and a loam soil [Mechtildshausen, pH 7.4, organic carbon 1.28%], each from Germany, a clay loam soil [Mussig, pH 7.6, organic carbon 2.98%] and a silt loam soil [Bretagne 1b, pH 5.4, organic carbon 2.0%], each from France, in a batch equilibrium experiment. The experiment was conducted in accordance with USEPA Subdivision N, Chemistry: Environmental Fate, Section 163-1: Leaching and Adsorption/Desorption Studies. This study was conducted in compliance with the Swiss Ordinance relating to Good Laboratory Practice. The adsorption phase of the study was carried out by equilibrating gamma irradiated air-dried soil with [¹⁴C]dimethyl disulfide at nominal test concentrations of 0.001, 0.002, 0.011, 0.021, and 0.102 mg a.i./kg soil, in the dark at 20 ± 2°C for 24 hours. The equilibrating solution used was 0.01M CaCl₂ solution purged with helium. The soil solution ratio was 1:1 (w:v). The desorption phase of the study was carried out by replacing the adsorption solution with an equivalent volume of 0.01M CaCl₂ solution and equilibrating in the dark at 20 ± 2°C for 44 hours. A single desorption step was performed for each test soil.

The supernatant solutions after adsorption and the desorption step were separated by centrifugation, and were analyzed for total radioactivity using LSC. Aliquots of the adsorption and desorption supernatants were analyzed for [¹⁴C]dimethyl disulfide using HPLC.

The experimental temperature employed during the study was reported to be maintained at 20 ± 2°C; supporting data were not provided. The pH of the control solution without soil was 6.03. The pH of the soils after equilibration with 0.01M CaCl₂ solution ranged from 5.81-7.30. Based on HPLC analysis of the adsorption supernatants, [¹⁴C]dimethyl disulfide was not completely stable, comprising 74.5-94.1% of the recovered radioactivity. Based on HPLC analysis of the desorption supernatants, [¹⁴C]dimethyl disulfide was completely degraded in the Mechtildshausen loam and Mussig clay loam soils and was slightly degraded in the Speyer 2.2 sandy loam and Bretagne 1b silt loam soils, comprising 75.28-85.64% of the recovered radioactivity. Based on HPLC analysis of the application solution and the supernatant of the control solution after 24 hours of shaking, the radiochemical purity of the test substance was 98.1% and 98.4%, respectively. Mass balances could not be determined from the definitive study.

After 24 hours of equilibration, the study author reported 39.6 – 24.7% of the applied [¹⁴C]dimethyl disulfide was adsorbed to the sandy loam soil (registrant-calculated). Registrant-calculated Freundlich adsorption K values were 0.532, 0.257, 0.257, and 0.828; Freundlich adsorption K_{oc} values are 23, 20, 9, and 41 for Speyer sandy loam, Mechtildshausen loam, Mussig clay loam, and Bretagne silt loam soils respectively. Registrant-calculated adsorption K and K_{oc} values are not reported. The reviewer-calculated Freundlich adsorption K values are 0.719, 0.297, 0.300, and 1.355; Freundlich K_{oc} values are 31, 23, 10, and 68 for the Speyer sandy loam, Mechtildshausen loam, Mussig Clay loam, and Bretagne silt loam soils, respectively. and the Freundlich K_{oc} value is 89. The reviewer-calculated adsorption K values are 0.679, 0.597,

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0.554, 0.860; adsorption K_{oc} values 30, 46, 19, and 43 for the Speyer sandy loam, Mechtildshausen loam, Mussig Clay loam, and Betagne silt loam soils, respectively.

In the desorption kinetic experiment, a constant decrease of radioactivity in the supernatant was observed. The sandy loam soil averaged 34.0% of the adsorbed after 4 hours, decreased to 20.9% after 24 hours, and was -3.5% after 44 hours. The registrant-calculated Freundlich desorption K values are 0.923 and 0.652; Freundlich K_{oc} values are 40 and 33 for the Speyer sandy loam and Betagne silt loam soils, respectively. The registrant-calculated desorption K and K_{oc} values were not reported. Reviewer-calculated Freundlich desorption K values are 2.53 and 1.89; Freundlich desorption K_{oc} values are 147 and 159 for the Speyer sandy loam and Betagne silt loam soils, respectively. The reviewer-calculated Freundlich desorption K and K_{oc} values were not determined. In the desorption kinetic experiment, a slow decrease of radioactivity in the supernatants of the Speyer 2.2 sandy loam and Bretagne 1b silt loam soils was observed. Radioactivity in the desorption supernatants of the Speyer 2.2 sandy loam soil averaged 43.2% of the adsorbed after 4 hours, decreased to 32.1% after 24 hours, and was 2.4% after 44 hours; corresponding values for the Bretagne 1b silt loam soil were 45.9%, 39.4%, and 2.3%. Radioactivity in the desorption supernatants for the Mechtildshausen loam and Mussig clay loam soil rapidly decreased over time. Radioactivity in the desorption supernatants of the Mechtildshausen loam soil averaged 29.8% of the adsorbed after 4 hours, decreased to 6.6% after 24 hours, and was -9.0% after 44 hours; corresponding values for the Mussig clay loam soil were 29.3%, -46.8%, and -23.0%.

Results Synopsis:

Soil type:	Speyer 2.2 Sandy loam.
Amount adsorbed:	27.4-30.3% of the applied.
Adsorption K_d :	0.679 (reviewer-calculated)
Adsorption K_{oc} :	30 (reviewer-calculated)
Freundlich adsorption K :	0.719 (reviewer-calculated)
Freundlich adsorption K_{oc} :	31 (reviewer-calculated)
Amount desorbed:	21.4 – 25% of the adsorbed
Desorption K_d :	3.38 (reviewer-calculated)
Desorption K_{oc} :	147 (reviewer-calculated)
Freundlich desorption K :	2.53 (reviewer-calculated)
Freundlich desorption K_{oc} :	110 (reviewer-calculated)

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Soil type: Mechtildshausen Loam.
Amount adsorbed: 25.6-38.8% of the applied.
Adsorption K_d : 0.597 (reviewer-calculated)
Adsorption K_{oc} : 46 (reviewer-calculated)
Freundlich adsorption K: 0.297 (reviewer-calculated)
Freundlich adsorption K_{oc} : 23 (reviewer-calculated)
Amount desorbed: Not reported.
Desorption K_d : Not reported.
Desorption K_{oc} : Not reported.
Freundlich desorption K_d : Not determined...
Freundlich desorption K_{oc} : Not determined..

Soil type: Mussig Clay loam.
Amount adsorbed: 24.7-39.6% of the applied.
Adsorption K_d : 0.554 (reviewer-calculated)
Adsorption K_{oc} : 19 (reviewer-calculated)
Freundlich adsorption K: 0.300 (reviewer-calculated)
Freundlich adsorption K_{oc} : 10 (reviewer-calculated)
Amount desorbed: Not determined.
Desorption K: Not reported.
Desorption K_{oc} : Not reported.
Freundlich desorption K: Not determined.
Freundlich desorption K_{oc} : Not determined.

Soil type: Bretagne 1b Silt loam.
Amount adsorbed: 25.7-32.9% of the applied.
Adsorption K_d : 0.860 (reviewer-calculated)
Adsorption K_{oc} : 43 (reviewer-calculated)
Freundlich adsorption K: 1.355 (reviewer-calculated)
Freundlich adsorption K_{oc} : 68 (reviewer-calculated)
Amount desorbed: 16.2 – 27.3% of the adsorbed
Desorption K: 3.18 (reviewer-calculated)
Desorption K_{oc} : 159 (reviewer-calculated)
Freundlich desorption K: 1.890 (reviewer-calculated)
Freundlich desorption K_{oc} : 95 (reviewer-calculated)

Study Acceptability: This study is classified as Acceptable. Volatile residues were not trapped in the experimental design. However, material balances exceeded 90 percent in the preliminary experiment in all cases.

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I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with OECD Guideline for Testing of Chemicals No. 106: "Adsorption/Desorption" (2000); and under consideration of European Community Commission Directive 95/36/EC (1995) and Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 163-1: Leaching and Adsorption/Desorption Studies (1982; p. 11). The following significant deviations from the objectives of Subdivision N guidelines were noted:

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

COMPLIANCE: This study was conducted in compliance with the Swiss Ordinance relating to Good Laboratory Practice (2000; p. 3). Signed and dated No Data Confidentiality, GLP, Quality Assurance statements were provided (pp. 1-3, 5). A Certificate of Authenticity was not provided.

A. MATERIALS:

1. Test Material [¹⁴C]Dimethyl disulfide (DMDS; p. 16).

Chemical Structure: See DER Attachment 1.

Description: Pale yellow liquid; Technical grade (radiolabeled test material, p. 16).

Purity:
Radiolabeled Radiochemical purity: Batch I: >99%; Batch II: 98.7% (p. 16).
Lot/Batch No.: Batch I: 040401 (RCC No. 156096/A);
Batch II: 49520-1-4C (RCC No. 162945/A).
Analytical purity: Not reported.
Specific radioactivity: Batch I: 14.5 MBq/mg; Batch II: 8.96 MBq/mg.
Location of the label: Labeled on both carbons of the molecule.

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Storage conditions of test chemicals:

Radiolabeled test substance was stored at *ca.* -20°C at RCC and at <0°C at the sponsor facility (p. 16).

Physico-chemical properties of dimethyl disulfide:

Parameter	Value	Comment
Molecular weight	Not reported.	
Molecular formula	C ₂ H ₆ S ₂	
Water Solubility	Not reported.	
Vapor Pressure/Volatility	28.6 mm Hg (DMDS)/121.26 mm Hg (hexane)	At 25°C.
UV Absorption	Not reported.	
pKa	Not reported.	
K _{ow} /log K _{ow}	Not reported.	
log P _{ow}	1.77	
Stability of compound at room temperature, if provided	Stable under normal conditions.	

Data were obtained from pp. 16-17 of the study report.

2. Soil Characteristics

Table 1: Description of soil collection and storage.

Description	Sandy loam	Loam	Clay loam	Silt loam
Geographic location	Speyer; Rhineland-Palatine, Germany.	Mechtildshausen, Hesse, Germany.	Mussig, Alsace, France.	St. Yves, Bretagne, France.
Coordinates	49°18'N, 8°26'W	50°02'N, 8°18'E	48°14'N, 7°31'E	47°55'N, 3°11'W
Pesticide use history at the collection site	No fertilization or treatment with pesticides for ≥12 months prior to sampling.			
Collection procedures	Not reported.			
Sampling depth (cm)	Top 20 cm.			
Storage conditions	Not reported.			
Storage length ¹	<i>ca.</i> 24 months.	<i>ca.</i> 19 months.	<i>ca.</i> 44 months.	<i>ca.</i> 40-44 months.
Soil preparation	Air-dried and sieved (2 mm).			

Data were obtained from p. 17 of the study report.

¹ Storage length was determined by reviewer as the interval between the field sampling date (January 2003 for Speyer 2.2 sandy loam, June 2003 for Mechtildshausen loam, July 2001 for Mussig clay loam, and July and October 2001 for Bretagne 1b silt loam soil) and the experimental study initiation (November 2004).

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Table 2: Properties of the soils.

Property	Speyer 2.2	Mechtildshausen	Mussig	Bretagne 1a	Bretagne 1b
Soil texture (USDA)	Sandy loam	Loam	Clay loam	Silt loam	Silt loam
% Sand (> 0.05 mm)	75.3	45.31	21.52	19.34	17.37
% Silt (0.002-0.05 mm)	16.6	37.12	44.32	61.24	65.23
% Clay (< 0.002 mm)	8.1	17.57	34.15	19.42	17.40
pH (0.01M CaCl ₂)	5.6	7.4	7.6	5.8	5.4
Organic carbon (g/100 g soil)%	2.3	1.28	2.98	1.97	2.0
Organic matter (%)	3.97	2.21	5.14	3.40	3.45
CEC (mmol/100 g soil)	11	11.4	36.8	8.5	12.9
Bulk density (g/cm ³)	0.96	1.04	1.03	1.06	1.15
Soil Taxonomic Classification	Cambisol	Luvic Phaeozem	Dystric Cambisol	Dystric Cambisol	Dystric Cambisol
CaCO ₃ (%)	Not reported.				
Moisture at 1/3 atm (%)	Not reported.				
Bulk density (g/cm ³)	Not reported.				
Biomass (mg microbial C/100 g or CFU or other)	Not reported.				
Soil mapping unit (for EPA)	Not reported.				

Data were obtained from Table 1, p. 35 of the study report.

Soil bulk density and taxonomic classification were obtained from registrant clarification e-mail.

C. STUDY DESIGN:

1. Preliminary study: Preliminary experiments were conducted to determine the appropriate soil:solution ratio and equilibrium times and adsorption of the test material to the test vessels, and to assure the stability of the test compound during selected exposure time to be used in the definitive study (p. 18).

Prior to study initiation, stock solutions were prepared for the preliminary studies by mixing [¹⁴C]dimethyl disulfide (in hexane) with ethanol (p. 19). Aliquots were analyzed for total radioactivity using LSC.

To determine the adsorption equilibration time, 3 x 4-15 g of Mussig clay loam soil and Bretagne 1a silt loam soil were added into headspace vials and suspended in *ca.* 14.5 – 20.0 ml of 0.01M CaCl₂ solution to make soil:solution ratios of 1:5, 1:2.5, and 1:1 (w:v; pp. 18-19). The samples were pre-equilibrated by shaking for ≥ 12 hours in the dark at 20 ± 2°C. Following pre-equilibration, the samples were treated with *ca.* 48 - 66-μL aliquot of [¹⁴C]dimethyl disulfide stock solution at a nominal test concentration of *ca.* 0.06 mg/L, sealed with crimp-caps with septa, and shaken for 48 hours (p. 22). Following shaking, the samples were centrifuged and duplicate aliquots of the supernatants were analyzed for total radioactivity using LSC. Aliquots of the supernatants were analyzed using HPLC. Selected samples at the 1:2.5 (w:v) soil:solution

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ratio were analyzed for mass balance. The soil was extracted three times with acetonitrile (*ca.* 10 mL; p. 23). The extracts were combined and quantified by LSC. Following extraction, the samples were combusted. After 48 hours, adsorption averaged 86.3%, 82.0%, and 36.3% for the Mussig clay loam soil at soil:solution ratios of 1:1, 1:2.5, and 1:5 (w:v), respectively; corresponding values for the Bretagne 1a silt loam soil are 80.1%, 65.7%, and 14.0% (p. 29; Table 2, p. 36). Mass balances determined for duplicate soils at a soil:solution ratio of 1:2.5 (w:v) following the adsorption phase averaged 98.1% (range 97.8-98.3%) and 98.9% (range 98.7-99.1%) of the applied for the Mussig clay loam and Bretagne 1a silt loam soil, respectively (Table 3, p. 37).

Treated aqueous samples without soil were exposed for 48 hours and analyzed by LSC to determine glass adsorption (p. 21). It was determined that adsorption to the surface of the test vessels was very low, with [¹⁴C]dimethyl disulfide accounting for 98.5-100.6% of the applied after 48 hours (p. 30; Table 2, p. 36).

To determine the adsorption equilibration time, (2 x 5.4 g) of Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam soil, and Bretagne 1a silt loam soil were added into headspace vials and suspended in *ca.* 18.9 mL of 0.01M CaCl₂ solution to make a soil:solution ratio of 1:3.5 (w:v; pp. 20, 22). The samples were pre-equilibrated by shaking for ≥ 12 hours in the dark at 20 ± 2°C. Following pre-equilibration, the samples were treated with 100-μL aliquot of [¹⁴C]dimethyl disulfide stock solution at a nominal test concentration of 0.012 mg/L (p. 21). The samples were sealed with crimp-caps with septa and shaken for 2, 5, 24, and 48 hours. Following each sampling interval, the samples were centrifuged and duplicate aliquots of the supernatants were analyzed for total radioactivity using LSC. Controls (treated aqueous samples without soil) were assayed the same way as the treated samples. Aliquots of the supernatants were analyzed using HPLC. Selected samples were analyzed for mass balance. The soil was extracted three times with acetonitrile (*ca.* 10 mL; p. 23). The extracts were combined and quantified by LSC. Following extraction, the samples were combusted. Duplicate samples of Speyer 2.2 sandy loam and Mechtildshausen loam soils were additionally extracted with methanol/water at 3N HCl. No equilibrium was reached. After 24 hours, adsorption averaged 26.4%, 26.1%, 64.8%, and 14.0% of the applied for the Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam soil, and Bretagne 1a silt loam soil, respectively; corresponding values after 48 hours are 45.1%, 50.0%, 69.3%, and 21.0% of the applied (p. 30; Table 4, p. 38). Mass balances determined for duplicate soils after 48 hours following the adsorption phase averaged 95.1% (range 94.9-95.3%), 95.3% (range 94.9-95.7%), 96.7% (range 96.3-97.2%), and 102.1% (range 100.5-103.7%) of the applied for the Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam soil, and Bretagne 1a silt loam soil, respectively (Table 5, p. 39). HPLC analysis of the supernatants showed that the test item was not stable (Figure 8, p. 60).

The adsorption test was repeated with Speyer 2.2 sandy loam soil at a soil:solution ratio of 1:3.5 (w:v) and a nominal concentration of 0.019 mg/L, with the 0.01M CaCl₂ solution purged with helium for 30 minutes (pp. 19-20). The above procedure was followed; no mass balance test was performed. No equilibrium was reached. Adsorption averaged 62.1% and 76.7% of the applied after 24 and 48 hours, respectively (p. 30; Table 6, p. 40). The instability of the test item was

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observed by the degradation in the supernatants and the high adsorption. According to its polarity, dimethyl disulfide should not be readily adsorbed.

The test was repeated using soil samples that were sterilized by gamma irradiation. The test was repeated using the same four soils and procedure as listed above but with a soil:solution ratio of 1:2.5 (w:v) and a nominal concentration of 0.1 mg/L (pp. 19, 21-22). An equilibrium was reached between 5-24 hours (p. 30; Figure 1, p. 52). After 24 hours, adsorption averaged 11.6%, 11.5%, 12.5%, and 16.9% for the Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam soil, and Bretagne 1a silt loam soil, respectively (Table 7, p. 41). Mass balances determined for duplicate soils after 48 hours following the adsorption phase averaged 101.3% (range 100.6-102.1%), 100.7% (range 100.3-101.1%), 102.1% (range 102.0-102.1%), and 101.6% (range 101.5-101.7%) of the applied for the Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam soil, and Bretagne 1a silt loam soil, respectively (Table 8, p. 42). Registrant-calculated Freundlich adsorption K values averaged 0.5, 0.6, 0.4, and 0.8 for the Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam soil, and Bretagne 1a silt loam soil, respectively; corresponding Freundlich K_{oc} values were 23, 47, 15, and 42 (p. 31; Table 9, p. 43). Registrant-calculated adsorption K and K_{oc} values were not reported. Based on HPLC analysis, dimethyl disulfide accounted for 86.0-96.8% of the radioactivity in the supernatant solutions; the soil extracts showed only dimethyl disulfide (Figures 10-11, pp. 62-63). The control solution showed 100% dimethyl disulfide (Figure 9, p. 61). It was determined that adsorption to the surface of the test vessels was very low, with [14 C]dimethyl disulfide accounting for 99.4-100.5% of the applied after 48 hours (Table 7, p. 41; Figure 2, p. 53).

Based on the results of the preliminary studies, it was determined that the definitive study would be conducted using an equilibration time of 24 hours and soil:solution ratios of 1:1 (w:v) for all test soils (p. 31). It was also determined to sterilize the test soils for the definitive study using gamma radiation due to instability of the test substance.

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2. Definitive study experimental conditions:

Table 3: Study design for the adsorption phase.

Parameters		Speyer 2.2 Sandy loam	Mechtildshausen Loam	Mussig Clay loam	Bretagne 1b Silt loam
Condition of soil (air dried/fresh)		Air-dried; sterilized using gamma radiation. ¹			
Have these soils been used for other laboratory studies? (specify which)					
Soil (g/replicate)		14.5			
Equilibrium solution used (eg: 0.01N CaCl ₂)		0.01M CaCl ₂ , purged with helium gas.			
Control used (with salt solution only) (Yes/No)		Yes.			
Test material concentrations ²	Nominal application rates (mg a.i./kg soil)	0.001, 0.002, 0.011, 0.021, 0.102			
	Analytically measured concentrations (mg a.i./kg soil)	Not reported.			
Identity and concentration of co-solvent, if any		Ethanol, concentration not reported.			
Soil:solution ratio (w:v)		1:1			
Initial pH of the equilibration solution, if provided		6.03			
No. of replications	Controls	Duplicate.			
	Treatments	Duplicate.			
Equilibration	Time (hours)	24			
	Temperature (°C)	20 ± 2°C			
	Darkness (Yes/No)	Yes.			
	Shaking method	Rotary shaker.			
	Shaking time (hours)	24			
Method of separation of supernatant (eg., centrifugation)		Centrifugation.			
Centrifugation	Speed (rpm)	2800			
	Duration (min)	10			
	Method of separation of soil and solution	Not reported.			

Data were obtained from pp. 18-22 and Table 16, p. 51 of the study report.

1 The test soils were equilibrated with CaCl₂ solution, purged with helium, for ≥ 12 hours prior to use.

2 Test material concentrations were calculated by the reviewer by converting mg/L to mg a.i./kg using the following equation: [test concentration (mg/L) × total volume of test material (mL)] ÷ amount of soil (g); eg. For the Speyer 2.2 sandy loam soil, highest concentration, nominal application rate: [0.102 mg/L × 14.5 mL] ÷ 14.5 g = 0.102 mg a.i./kg soil.

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Table 4: Study design for the desorption phase.

Parameters		Speyer 2.2 Sandy loam	Mechtildshausen Loam	Mussig Clay loam	Bretagne 1b Silt Loam
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption		Yes.			
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.001	0.0003	0.0004	0.0004	0.0003
	0.002	0.0006	0.0008	0.0007	0.0005
	0.011	0.0031	0.0035	0.0031	0.0031
	0.021	0.0057	0.0061	0.0067	0.0065
	0.102	0.0308	0.0260	0.0252	0.0335
No. of desorption steps		1			
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M CaCl ₂)		0.01M CaCl ₂ ; ca. 14.5 mL.			
Soil:solution ratio (w:v)		1:1			
Replications	Controls	Duplicate.			
	Treatments	Duplicate.			
Desorption equilibration	Time (hours)	44			
	Temperature (°C)	20 ± 2°C			
	Darkness	Yes.			
	Shaking method	Rotary shaker.			
	Shaking time (hours)	44			
Centrifugation	Speed (rpm)	2800			
	Duration (min)	10			
	Method of separation of soil and solution	Not reported.			

Data were obtained from pp. 18-23 and Table 10, pp. 44-45 of the study report.

Desorption Kinetics: The desorption kinetic experiment was carried out for all four soils at a soil:solution ratio of 1:1 (w:v) for all test concentrations (0.001, 0.002, 0.011, 0.021, and 0.102 mg/kg soil). Following 24 hours of adsorption, the supernatant was removed and replaced with an equivalent volume of CaCl₂ solution that had been purged with helium, and a desorption phase was conducted (p. 23). After 4, 24, and 44 hours of desorption, duplicate aliquots were analyzed by LSC. Aliquots of the supernatants were analyzed using HPLC after 44 hours to check stability.

3. Description of analytical procedures:

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

Total ¹⁴C measurement: Following the adsorption and desorption phases, aliquots of the supernatants were analyzed for total radioactivity using LSC (pp. 21, 23). The amount of the test

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item absorbed was determined from the difference between the initial and final amount in the aqueous phase (p. 21).

Non-extractable residues, if any: No non-extractable residues were determined in this study.

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

Identification and quantification of parent compound: Aliquots of the adsorption and desorption supernatants were analyzed for [¹⁴C]dimethyl disulfide using HPLC under the following conditions (pp. 24-25): Merck Lichrospher 100 RP 18 pre-column (4 x 4 mm; 5 µm particle size), Nucleosil C-18 column (4.6 x 250 mm; 5 µm particle size), mobile phase combining (Solvent A) water and (Solvent B) acetonitrile [percent A:B (v:v) at 0 min., 75:25; 15 min., 0:100; 20 min., 0:100; 20.1 min., 75:25; and 35 min., 75:25], flow rate of 1 mL/minute, using a FLO-ONE Beta A500 or 500TR detector.

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

Detection limits (LOD, LOQ) for the parent compound: For LSC analysis, the Limits of Detection (LOD) were 0.15%, 0.13%, and 0.15% of the applied for the aqueous phase, soil extracts, and combustion non-extractables, respectively (corresponding to 0.003 µg, 0.0020 µg, and 0.003 µg parent equivalents; Appendix I, pp. 68-69). The corresponding LSC Limits of Quantification (LOQ) were 0.23%, 0.19%, and 0.22% of the applied (corresponding to 0.004 µg, 0.003 µg, and 0.004 µg parent equivalents). For HPLC analysis, the LOQ was 1.1% of the applied. The LOD was not reported.

Detection limits (LOD, LOQ) for the transformation products, if appropriate: Samples were not analyzed for transformation products of dimethyl disulfide.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The experimental temperature employed during the study was reported to be maintained at $20 \pm 2^\circ\text{C}$; supporting data were not provided (p. 18). The pH of the control solution without soil was 6.03 (Table 16, p. 51). The pH of the soils after equilibration with 0.01M CaCl₂ solution ranged from 5.81-7.30. Based on HPLC analysis of the adsorption supernatants, [¹⁴C]dimethyl disulfide was not completely stable, comprising 74.5-94.1% of the recovered radioactivity (p. 31; Figure 13, p. 65). Based on HPLC analysis of the desorption supernatants, [¹⁴C]dimethyl disulfide was completely degraded in the Mechtildshausen loam and Mussig clay loam soils and was slightly degraded in the Speyer 2.2 sandy loam and Bretagne lb silt loam soils, comprising 75.28-85.64% of the recovered radioactivity (p. 32; Figure 14, p. 66). Based on HPLC analysis of the application solution and the supernatant of the control solution after 24 hours of shaking, the radiochemical purity of the test substance was 98.1% and 98.4%, respectively (Figure 12, p. 64).

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B. MASS BALANCE: Mass balances were not determined in the definitive study. .

Table 5: Recovery of [¹⁴C]dimethyl disulfide, expressed as percentage of applied radioactivity, in soil after adsorption/desorption (mean ± s.d.)¹.

Matrices	Speyer 2.2 Sandy loam	Mechtildshausen Loam	Mussig Clay loam	Bretagne 1b Silt loam
At the end of the adsorption phase				
Supernatant solution				
Solid phase (extracted)				
Non-extractable residues in soil, if measured				
Total recovery				
At the end of the desorption phase				
Supernatant solution				
Solid phase (total ¹⁴ C)				
Non-extractable residues in soil, if measured				
Total recovery				

¹ Mass balances were not determined in the definitive experiment.

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Table 6: Concentration of [¹⁴C]dimethyl disulfide in the solid and liquid phases at the end of adsorption equilibration period (mean; n = 2).

Concentration (mg a.i./kg soil)	Speyer 2.2 Sandy loam			Mechtildshausen Loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed
0.001	0.0003	0.0006	28.5	0.0004	0.0006	38.8
0.002	0.0006	0.0013	27.6	0.0008	0.0012	37.9
0.011	0.0031	0.0062	29.5	0.0035	0.0066	32.7
0.021	0.0057	0.0125	27.4	0.0061	0.0137	29.2
0.102	0.0308	0.0587	30.3	0.0260	0.0703	25.6

Concentration (mg a.i./kg soil)	Mussig Clay loam			Bretagne 1b Silt loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% adsorbed
0.001	0.0004	0.0006	39.6	0.0003	0.0006	27.1
0.002	0.0007	0.0013	34.4	0.0005	0.0012	25.7
0.011	0.0031	0.0070	29.4	0.0031	0.0055	29.6
0.021	0.0067	0.0133	32.3	0.0065	0.0107	31.1
0.102	0.0252	0.0721	24.7	0.0335	0.0509	32.9

1 Data were obtained from Table 10, pp. 44-45 of the study report. Means were determined by the study author.

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Table 7: Concentration of [¹⁴C]dimethyl disulfide in the solid and liquid phases at the end of the desorption step (mean, n = 2).

Concentration (mg a.i./kg soil)	Speyer 2.2 Sandy loam			Mechtildshausen Loam ¹		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed
0.001	0.0003	0.0002	21.4	ND	ND	ND
0.002	0.0006	0.0005	21.8	ND	ND	ND
0.011	0.0028	0.0026	24.3	ND	ND	ND
0.021	0.0047	0.0052	25.0	ND	ND	ND
0.102	0.0284	0.0221	21.7	ND	ND	ND

Concentration (mg a.i./kg soil)	Mussig Clay loam ¹			Bretagne 1b Silt loam		
	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed	on soil (mg a.i./kg)	in solution (µg a.i./mL)	% desorbed as % of the adsorbed
0.001	ND	ND	ND	0.0004	0.0002	16.2
0.002	ND	ND	ND	0.0006	0.0005	21.6
0.011	ND	ND	ND	0.0031	0.0027	25.3
0.021	ND	ND	ND	0.0058	0.0057	27.3
0.102	ND	ND	ND	0.0312	0.0246	24.1

Data were obtained from Table 14, p. 49 of the study report. Means were determined by the study author. ND= Not determined.

¹ [¹⁴C]Dimethyl disulfide was completely degraded in the Mechtildshausen loam and Mussig clay loam soils after 44 hours of desorption (p. 32).

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Table 8: Reviewer calculated adsorption and desorption constants of [¹⁴C]dimethyl disulfide in the soils.

Soil	Adsorption						Desorption					
	K _d	K _f	1/n	r ²	K _{oc}	K _{foc}	K _d	K _f	1/n	r ²	K _{oc}	K _{foc}
Speyer 2.2 Sandy loam	0.679	0.719	1.01	0.999	30	31	3.38	2.53	0.95	0.99	147	110
Mechtildshausen Loam ²	0.597	0.297	0.87	0.999	46	23	NR	ND	ND	ND	ND	ND
Mussig Clay loam ²	0.554	0.300	0.88	0.997	19	10	NR	ND	ND	ND	ND	ND
Bretagne 1b Silt loam	0.860	1.355	1.09	0.998	43	68	3.18	1.89	0.92	0.99	159	95

K_d - Adsorption and desorption coefficients; K_f - Freundlich adsorption and desorption coefficients; 1/n - Slope of Freundlich adsorption/desorption isotherms.

K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).

r² - Regression coefficient of Freundlich equation.

NR = Not reported; ND = Not determined.

1 [¹⁴C]Dimethyl disulfide was completely degraded in the Mechtildshausen loam and Mussig clay loam soils after 44 hours of desorption (p. 32).

Table 9: Registrant calculated adsorption and desorption constants of [¹⁴C]dimethyl disulfide in the soils.

Soil	Adsorption						Desorption					
	K _d	K _f	1/n	r ²	K _{oc}	K _{foc}	K _d	K _f	1/n	r ²	K _{oc}	K _{foc}
Speyer 2.2 Sandy loam	NR	0.532	1.02	0.9992	21	23	NR	0.923	0.96	0.9925	NR	40
Mechtildshausen Loam ²	NR	0.257	0.86	0.9997	42	20	NR	ND	ND	ND	NR	ND
Mussig Clay loam ²	NR	0.257	0.87	0.9970	17	9	NR	ND	ND	ND	NR	ND
Bretagne 1b Silt loam	NR	0.828	1.07	0.9994	28	41	NR	0.652	0.88	0.9847	NR	33

K_{oc} values for each soil were determined based on the mean of K_{oc} values for each sample in Table 10, pp. 44-45.

All other data were obtained from pp. 32-33; Tables 12, 15, pp. 47, 50; and Figures 3-4, 6-7, pp. 54-56, 58-59 of the study report.

K_d - Adsorption and desorption coefficients; K_f - Freundlich adsorption and desorption coefficients; 1/n - Slope of Freundlich adsorption/desorption isotherms.

K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon).

r² - Regression coefficient of Freundlich equation.

NR = Not reported; ND = Not determined.

1 Freundlich K_f values were calculated by the study author using the following equation (pp. 26-28):

$$\log C_s = \log K_f + (1/n) \log (C_{aq}), \text{ where}$$

C_s = soil concentration after adsorption or desorption (μg/g);

C_{aq} = concentration of supernatant after adsorption or desorption (μg/g);

1/n = exponential constant or slope; and

K_f = Freundlich sorption constant.

2 [¹⁴C]Dimethyl disulfide was completely degraded in the Mechtildshausen loam and Mussig clay loam soils after 44 hours of desorption (p. 32).

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C. ADSORPTION: After 24 hours of equilibration, 27.4-30.3%, 25.6-38.8%, 24.7-39.6%, and 25.7-32.9% of the applied [¹⁴C]dimethyl disulfide was adsorbed to the Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam, and Bretagne 1b silt loam soils, respectively (p. 31; Table 10, pp. 44-45). Registrant-calculated Freundlich adsorption K values were 0.532, 0.257, 0.257, and 0.828 for the Speyer 2.2 sandy loam, Mechtildshausen loam, Mussig clay loam, and Bretagne 1b silt loam soils, respectively; corresponding Freundlich K_{oc} values were 23, 20, 9, and 41 (pp. 32-33; Table 12, p. 47; Figures 3-4, pp. 54-56). Registrant-calculated adsorption K and K_{oc} values were not reported.

The reviewer calculated Freundlich K and K_d values for both the adsorption and desorption phases. The below equations show the calculations of K_f and K_d and subsequent K_{foc} and K_{oc} values.

Freundlich Adsorption and Desorption K_f Value Calculation:

$$K_f = \frac{C_o V_o - C_{eq} V_o}{m} \div C_{eq}^{1/n}$$

Adsorption and Desorption K_d Value Calculation:

$$K_d = \frac{C_o V_o - C_{eq} V_o}{m} \div C_{eq}$$

Freundlich Adsorption K_f Value Normalized to Organic Carbon Content (K_{foc}) Calculation:

$$K_{foc} = \frac{K_f}{\%OC}$$

Adsorption K_d Value Normalized to Organic Carbon Content (K_{oc}) Calculation:

$$K_{oc} = \frac{K_d}{\%OC}$$

where

C_o = the concentration in the water before sorption (µg/mL);;

V_o = the total water volume in the batch system (ml);

m = the dry mass of sorbent (g);

% OC = percent organic carbon in the soil; and

1/n = exponent of the Freundlich isotherm.

The reviewer calculated values values were similar to the registrant's provided values for all partition coefficients. The equations shown in II.C were used for these calculations. Registrant-calculated Freundlich adsorption K values were 0.532, 0.257, 0.257, and 0.828; Freundlich adsorption K_{oc} values are 23, 20, 9, and 41 for Speyer sandy loam, Mechtildshausen loam, Mussig clay loam, and Bretagne silt loam soils respectively. Registrant-calculated adsorption K and K_{oc} values are not reported. The reviewer-calculated Freundlich adsorption K

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values are 0.719, 0.297, 0.300, and 1.355; Freundlich K_{oc} values are 31, 23, 10, and 68 for the Speyer sandy loam, Mechtildshausen loam, Mussig Clay loam, and Betagne silt loam soils, respectively. and the Freundlich K_{oc} value is 89. The reviewer-calculated adsorption K values are 0.679, 0.597, 0.554, 0.860; adsorption K_{oc} values 30, 46, 19, and 43 for the Speyer sandy loam, Mechtildshausen loam, Mussig Clay loam, and Betagne silt loam soils, respectively.

The reviewer-calculated r² value for K_{ads} vs. % organic carbon was 0.1441, K_{ads} vs. pH was 4 x 10⁻⁵, and K_{ads} vs. % clay was 2 x 10⁻⁵. The statistical analysis included the average K_{ads} values and site-specific data for the Speyer, Germany Loam; Mechtildshausen, Germany Loam; Mussig, France Loam; Bretagne, France Silt Loam (MRID 46917015) soil studies and California Sandy Loam soil study (MRID 46917014).

D. DESORPTION: Registrant-calculated Freundlich desorption K values were 0.923 and 0.652 for the Speyer 2.2 sandy loam and Bretagne 1b soils, respectively; corresponding Freundlich desorption K_{oc} values were 40 and 33 (pp. 32-33; Table 15, p. 50; Figures 6-7, pp. 58-59). [¹⁴C]Dimethyl disulfide was completely degraded in the desorption supernatants of the Mechtildshausen loam and Mussig clay loam soils (Figure 14, p. 66). Therefore, Freundlich values could not be determined. Registrant-calculated desorption K and K_{oc} values were not reported. In the desorption kinetic experiment, a slow decrease of radioactivity in the supernatants of the Speyer 2.2 sandy loam and Bretagne 1b silt loam soils was observed. Radioactivity in the desorption supernatants of the Speyer 2.2 sandy loam soil averaged 43.2% of the adsorbed after 4 hours, decreased to 32.1% after 24 hours, and was 2.4% after 44 hours; corresponding values for the Bretagne 1b silt loam soil were 45.9%, 39.4%, and 2.3% (Table 13, p. 48; Figure 5, p. 57).

The reviewer calculated Freundlich adsorption K values values were similar to the registrant's provided values.. The equations shown in II.C were used for these calculations. The registrant-calculated Freundlich desorption K values are 0.923 and 0.652; Freundlich K_{oc} values are 40 and 33 for the Speyer sandy loam and Betagne silt loam soils, respectively. The registrant-calculated desorption K and K_{oc} values were not reported. Reviewer-calculated Freundlich desorption K values are 2.53 and 1.89; Freundlich desorption K_{oc} values are 147 and 159 for the Speyer sandy loam and Betagne silt loam soils, respectively. The reviewer-calculated Freundlich desorption K and K_{oc} values were not determined.

Radioactivity in the desorption supernatants for the Mechtildshausen loam and Mussig clay loam soil rapidly decreased over time. Radioactivity in the desorption supernatants of the Mechtildshausen loam soil averaged 29.8% of the adsorbed after 4 hours, decreased to 6.6% after 24 hours, and was -9.0% after 44 hours; corresponding values for the Mussig clay loam soil were 29.3%, -46.8%, and -23.0%.

III. STUDY DEFICIENCIES

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1. Volatile residues were not trapped in the experimental design.
2. Material balances were not determined.

IV. REVIEWER'S COMMENTS

1. The reviewer calculated Freundlich $1/n$ values for the adsorption phase were below 0.9 for the Mechtildshausen loam and Mussig clay loam soils. The registrant calculated Freundlich $1/n$ values for the desorption phase were below 0.9 in the Bretagne 1b silt loam soil. Freundlich $1/n$ values under idealized conditions should be in the range of 0.9 to 1.1.
2. The study author reported incorrectly reported that for the preliminary and screening tests, the aqueous supernatant and the combined extracts of each tube were submitted to HPLC analysis after 24 hours of adsorption (Section 2.3.7, p. 23). The HPLC analyses were conducted after 48 hours of adsorption, based on Tables 3 and 8 of the study report (pp. 37, 42).
3. The maximum field application rate for dimethyl disulfide was not reported. Subdivision N guidelines specify that one test concentration should be roughly equivalent to the maximum proposed or registered field application rate of the parent compound.
4. Registrant values for the indirectly determined concentrations of [^{14}C] DMDS in soil after equilibrium $[(C_oV_o - C_{aq}V_o)/m]$ do not match the reviewer's calculated values.
5. None of the test soils had an organic matter content of $\leq 1\%$, as recommended by Subdivision N guidelines.
6. FAO soil classifications were provided by the registrant. The Speyer, Germany, Mussig, France, and Bretagne, France soils are all classified as cambisols which are equivalent to Inceptisols in the U.S. Taxonomic Classification system. The Mechtildshausen, Germany soil is classified as Luvic Phaeozem which is equivalent to the Chernozemic soils in the U.S. Taxonomic Classification system. 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 163-1. Mobility 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.

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

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Attachment 1: Structures of Parent Compound and Transformation Products

Data Evaluation Record on the adsorption-desorption of dimethyl disulfide [DMDS] in soil

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Dimethyl disulfide [dimethyldisulfide; DMDS; 2,3-dithiabutane; methyl disulfide; (methyldithio)methane; (methylsulfanyl)methane; methyldithion ethane]

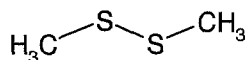
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CAS Name: Not reported.

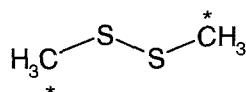
CAS Number: 624-92-0

SMILES String: S(SC)C (EPI Suite, v3.12 SMILES String).

Unlabeled



[¹⁴C]dimethyl disulfide



* = Location of the radiolabel.

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Identified Compounds

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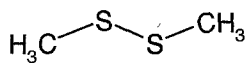
Dimethyl disulfide [dimethyldisulfide; DMDS; 2,3-dithiabutane; methyl disulfide; (methyldithio)methane; (methyldisulfanyl)methane; methyldithion ethane]

IUPAC Name: Dimethyl disulfide.

CAS Name: Not reported.

CAS Number: 624-92-0

SMILES String: S(SC)C (EPI Suite, v3.12 SMILES String).



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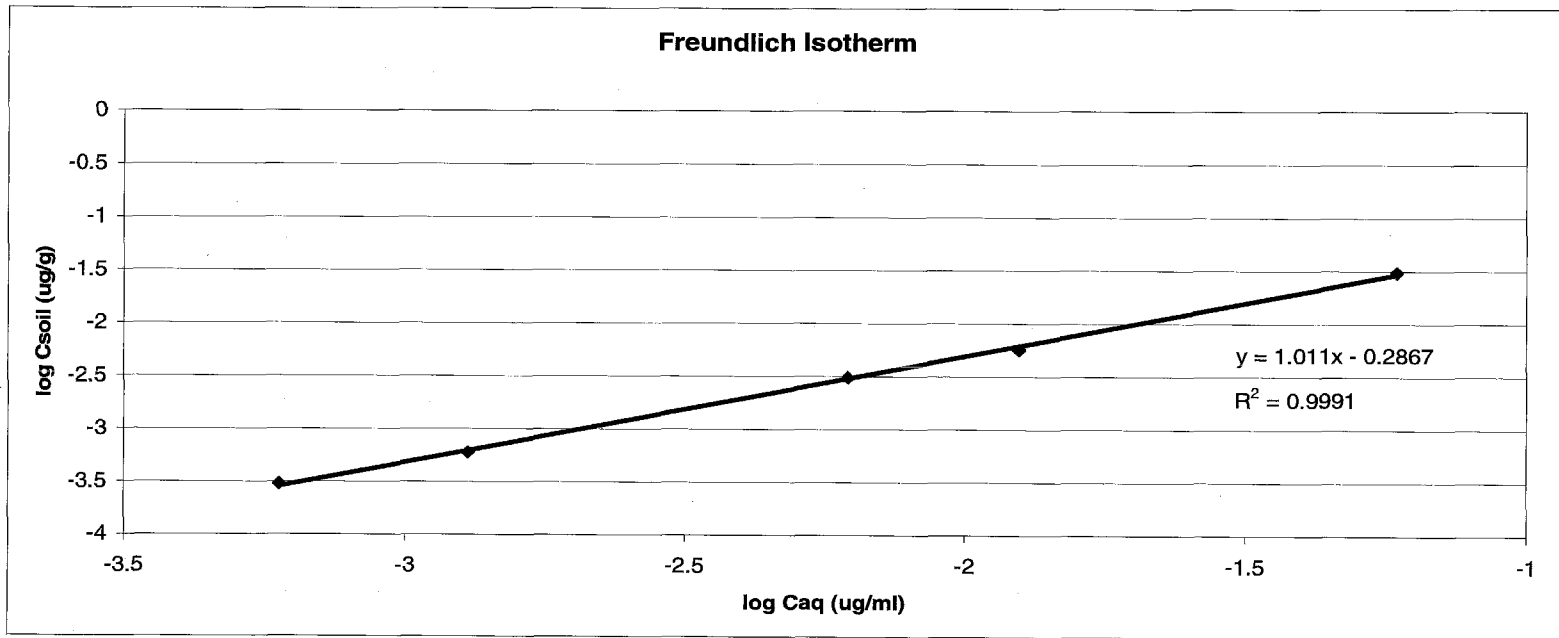
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Attachment 2: Excel Spreadsheets

Figure 2-1. Calculation of adsorption soil – water partition coefficients Kd, Koc, Kf, and Kfoc for Speyer, Germany Sandy Loam Soil.

C _o Initial Solution Conc. (µg/ml)	C _{soil} Conc. in soil after equilibrium (µg/g)	C _{aq} Conc. in solution after equilibrium (µg/ml)	V _o Volume of Solution (ml)	m Dry mass of sorbent (g)	(C _o V _o - C _{aq} V _o)/m	Kd (ml/g)	OC (%)	Koc (ml/g)	log C _{soil}	log C _{aq}	1/n	Kf (ml/g)	Kfoc (ml/g)
0.102	0.0308	0.0587	14.5	14.5	0.0433	0.737649	0.023	32.0717	-1.511449	-1.231362	1.011	0.761018	33.08773
0.021	0.0057	0.0125	14.5	14.5	0.0085	0.68	0.023	29.56522	-2.244125	-1.90309	1.011	0.71358	31.02523
0.011	0.0031	0.0062	14.5	14.5	0.0048	0.774194	0.023	33.66059	-2.508638	-2.207608	1.011	0.818716	35.59634
0.002	0.0006	0.0013	14.5	14.5	0.0007	0.538462	0.023	23.41137	-3.221849	-2.886057	1.011	0.579297	25.18683
0.001	0.0003	0.0006	14.5	14.5	0.0004	0.666667	0.023	28.98551	-3.522879	-3.221849	1.011	0.723351	31.45004
					Σ/n	0.679394		29.53888				0.719192	31.26924

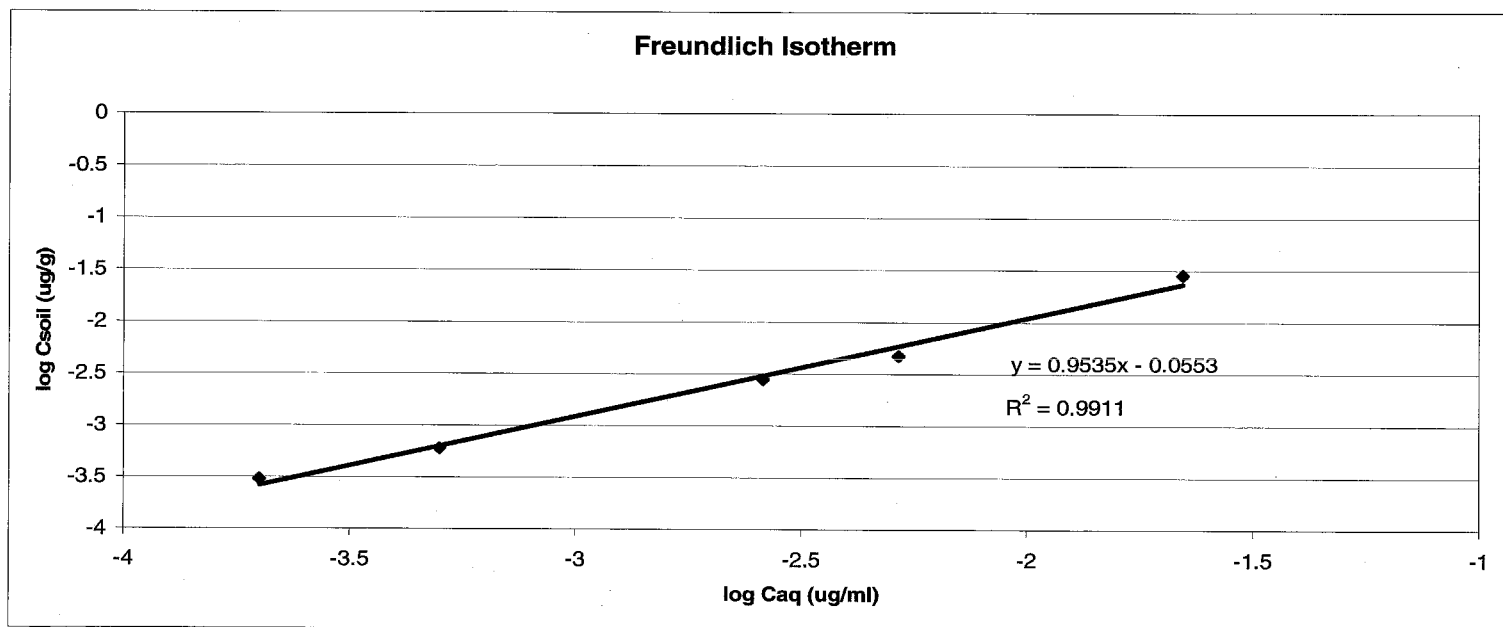


Notes:

1. Data obtained from Table 10, pp. 44-45.
2. C_{soil} and C_{aq} based on registrant-reported mean of two replicates.
3. Registrant only reported the mean C_{soil} and C_{aq} values, but not for individual replicates. Therefore, the C_{soil} and C_{aq} values could not be verified.
4. Registrant reported values of [¹⁴C] DMDS concentrations in soil after equilibrium (shown as C_{soil} above) do not match the calculated values [shown as C_oV_o-C_{aq}V_o/m above].

Figure 2-2. Calculation of desorption soil – water partition coefficients Kd, Koc, Kf, and Kfoc for Speyer, Germany Sandy Loam Soil.

C _o Initial Solution Conc. (µg/ml)	C _{soil} Conc. in soil after equilibrium (µg/g)	C _{aq} Conc. in solution after equilibrium (µg/ml)	V _o Volume of Solution (ml)	m Dry mass of sorbent (g)	(C _o V _o - C _{aq} V _o)/m	Kd (ml/g)	OC (%)	Koc (ml/g)	log C _{soil}	log C _{aq}	1/n	Kf (ml/g)	Kfoc (ml/g)
0.102	0.0284	0.0221	14.5	14.5	0.0799	3.615385	0.023	157.1906	-1.546682	-1.655608	0.9535	3.02809	131.6561
0.021	0.0047	0.0052	14.5	14.5	0.0158	3.038462	0.023	132.107	-2.327902	-2.283997	0.9535	2.379293	103.4475
0.011	0.0028	0.0026	14.5	14.5	0.0084	3.230769	0.023	140.4682	-2.552842	-2.585027	0.9535	2.44964	106.5061
0.002	0.0006	0.0005	14.5	14.5	0.0015	3	0.023	130.4348	-3.221849	-3.30103	0.9535	2.1068	91.60001
0.001	0.0003	0.0002	14.5	14.5	0.0008	4	0.023	173.913	-3.522879	-3.69897	0.9535	2.691894	117.0389
					Σ/n	3.376923		146.8227				2.531143	110.0497

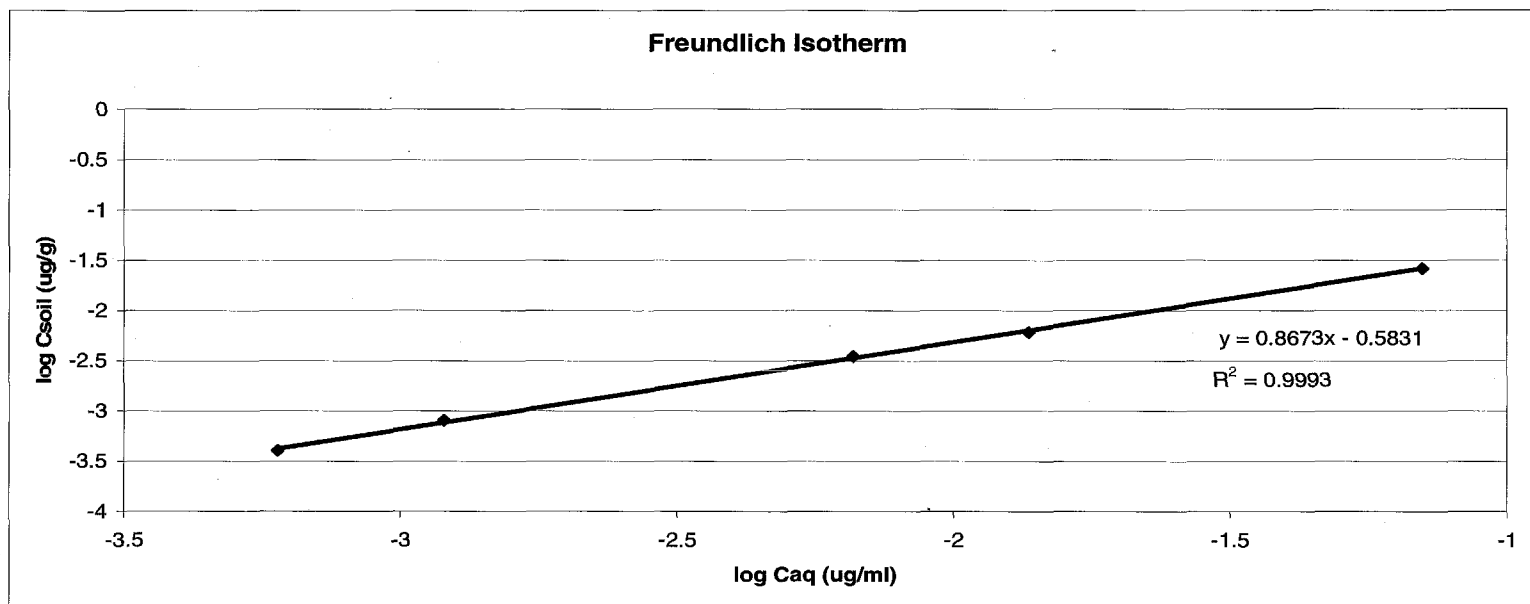


Notes:

1. Data obtained from Table 14, p. 49.
2. C_{soil} and C_{aq} based on registrant-reported mean of two replicates.
3. Registrant only reported the mean C_{soil} and C_{aq} values, but not for individual replicates. Therefore, the C_{soil} and C_{aq} values could not be verified.
4. Registrant reported values of [¹⁴C] DMDS concentrations in soil after equilibrium (shown as C_{soil} above) do not match the calculated values [shown as C_oV_o-C_{aq}V_o/m above].

Figure 2-3. Calculation of adsorption soil – water partition coefficients Kd, Koc, Kf, and Kfoc for Mechtildshausen, Germany Sandy Loam Soil.

C _o Initial Solution Conc. (µg/ml)	C _{soil} Conc. in soil after equilibrium (µg/g)	C _{aq} Conc. in solution after equilibrium (µg/ml)	V _o Volume of Solution (ml)	m Dry mass of sorbent (g)	(C _o V _o - C _{aq} V _o)/m	Kd (ml/g)	OC (%)	Koc (ml/g)	log C _{soil}	log C _{aq}	1/n	Kf (ml/g)	Kfoc (ml/g)
0.102	0.026	0.0703	14.5	14.5	0.0317	0.450925	0.0128	35.22849	-1.585027	-1.153045	0.8673	0.317026	24.76766
0.021	0.0061	0.0137	14.5	14.5	0.0073	0.532847	0.0128	41.62865	-2.21467	-1.863279	0.8673	0.30154	23.55782
0.011	0.0035	0.0066	14.5	14.5	0.0044	0.666667	0.0128	52.08333	-2.455932	-2.180456	0.8673	0.342422	26.75175
0.002	0.0008	0.0012	14.5	14.5	0.0008	0.666667	0.0128	52.08333	-3.09691	-2.920819	0.8673	0.273096	21.33566
0.001	0.0004	0.0006	14.5	14.5	0.0004	0.666667	0.0128	52.08333	-3.39794	-3.221849	0.8673	0.249098	19.46074
					Σ/n	0.596754		46.62143				0.296637	23.17473

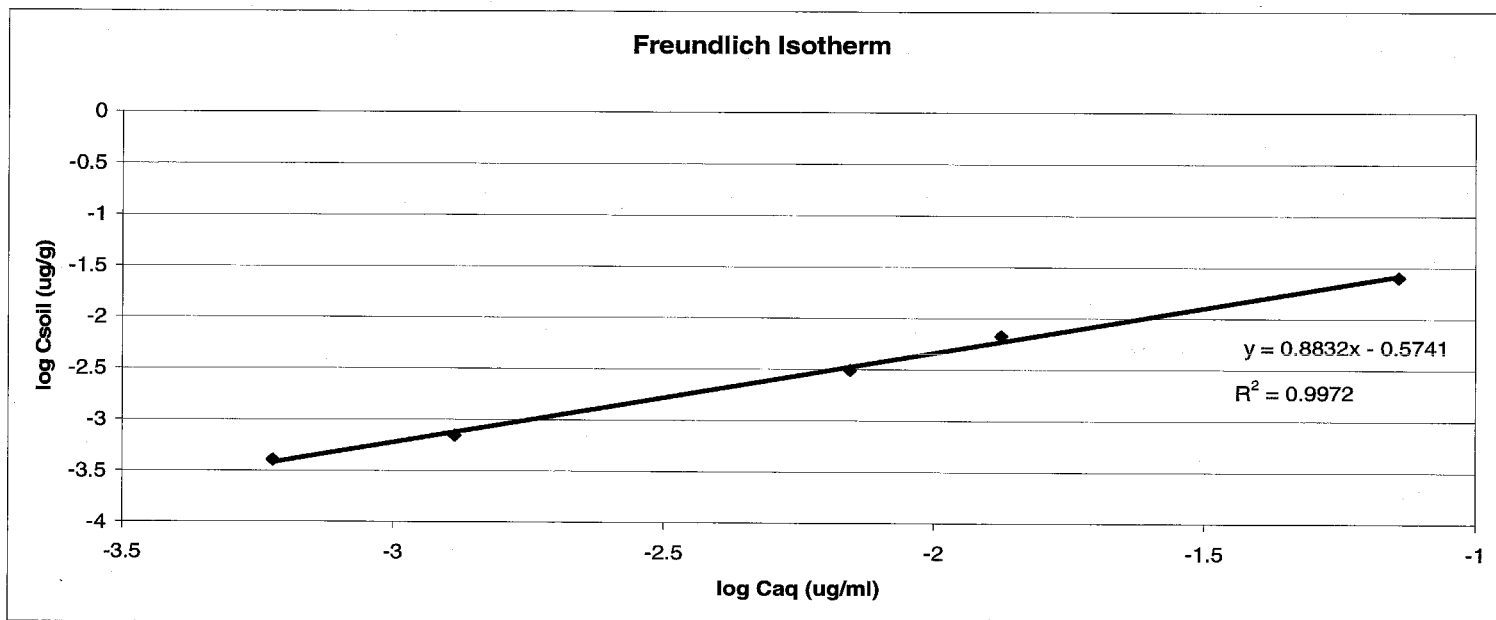


Notes:

1. Data obtained from Table 10, pp. 44-45.
2. C_{soil} and C_{aq} based on registrant-reported mean of two replicates.
3. Registrant only reported the mean C_{soil} and C_{aq} values, but not for individual replicates. Therefore, the C_{soil} and C_{aq} values could not be verified.
4. Registrant reported values of [¹⁴C] DMDS concentrations in soil after equilibrium (shown as C_{soil} above) do not match the calculated values[shown as CoVo-CaqVo)/m above].

Figure 2-4. Calculation of adsorption soil – water partition coefficients Kd, Koc, Kf, and Kfoc for Mussig, France Clay Loam soil.

C _o Initial Solution Conc. (µg/ml)	C _{soil} Conc. in soil after equilibrium (µg/g)	C _{aq} Conc. in solution after equilibrium (µg/ml)	V _o Volume of Solution (ml)	m Dry mass of sorbent (g)	(C _o V _o - C _{aq} V _o)/m	Kd (ml/g)	OC (%)	Koc (ml/g)	log C _{soil}	log C _{aq}	1/n	Kf (ml/g)	Kfoc (ml/g)
0.102	0.0252	0.0721	14.5	14.5	0.0299	0.414702	0.0298	13.91617	-1.598599	-1.142065	0.8832	0.30503	10.23591
0.021	0.0067	0.0133	14.5	14.5	0.0077	0.578947	0.0298	19.42776	-2.173925	-1.876148	0.8832	0.349546	11.72975
0.011	0.0031	0.007	14.5	14.5	0.004	0.571429	0.0298	19.17546	-2.508638	-2.154902	0.8832	0.320088	10.74121
0.002	0.0007	0.0013	14.5	14.5	0.0007	0.538462	0.0298	18.06918	-3.154902	-2.886057	0.8832	0.247778	8.314708
0.001	0.0004	0.0006	14.5	14.5	0.0004	0.666667	0.0298	22.37136	-3.39794	-3.221849	0.8832	0.280283	9.405471
					Σ/n	0.554041		18.59199				0.300545	10.08541

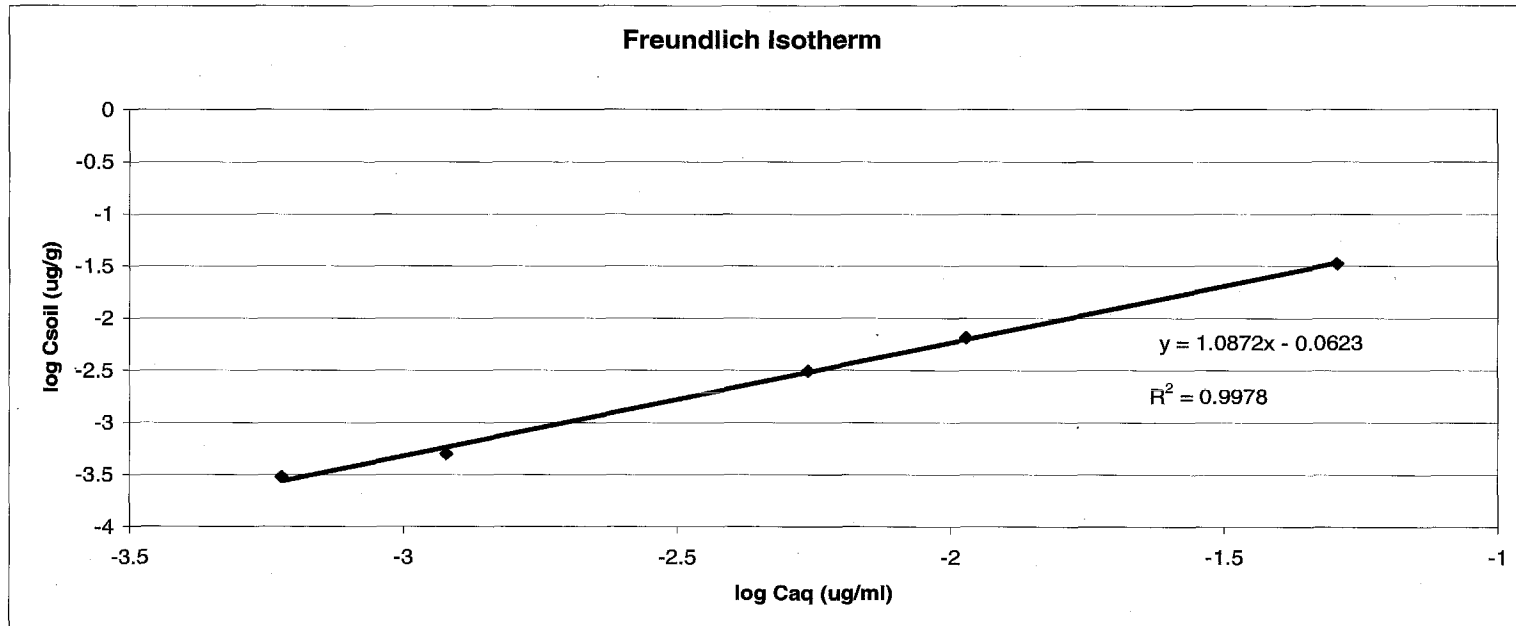


Notes:

1. Data obtained from Table 10, pp. 44-45.
2. C_{soil} and C_{aq} based on registrant-reported mean of two replicates.
3. Registrant only reported the mean C_{soil} and C_{aq} values, but not for individual replicates. Therefore, the C_{soil} and C_{aq} values could not be verified.
4. Registrant reported values of [¹⁴C] DMDS concentrations in soil after equilibrium (shown as C_{soil} above) do not match the calculated values [shown as C_oV_o-C_{aq}V_o/m above].

Figure 2-5. Calculation of adsorption soil – water partition coefficients Kd, Koc, Kf, and Kfoc Bretagne, FR Silt Loam soil.

C _o Initial Solution Conc. (µg/ml)	C _{soil} Conc. in soil after equilibrium (µg/g)	C _{aq} Conc. in solution after equilibrium (µg/ml)	V _o Volume of Solution (ml)	m Dry mass of sorbent (g)	(C _o V _o - C _{aq} V _o)/m	Kd (ml/g)	OC (%)	Koc (ml/g)	log C _{soil}	log C _{aq}	1/n	Kf (ml/g)	Kfoc (ml/g)
0.102	0.0335	0.0509	14.5	14.5	0.0511	1.003929	0.02	50.19646	-1.474955	-1.293282	1.0872	1.301599	65.07997
0.021	0.0065	0.0107	14.5	14.5	0.0103	0.962617	0.02	48.13084	-2.187087	-1.970616	1.0872	1.429852	71.49262
0.011	0.0031	0.0055	14.5	14.5	0.0055	1	0.02	50	-2.508638	-2.259637	1.0872	1.574129	78.70646
0.002	0.0005	0.0012	14.5	14.5	0.0008	0.666667	0.02	33.33333	-3.30103	-2.920819	1.0872	1.198406	59.92032
0.001	0.0003	0.0006	14.5	14.5	0.0004	0.666667	0.02	33.33333	-3.522879	-3.221849	1.0872	1.273075	63.65374
					Σ/n	0.859976		42.99879				1.355412	67.77062

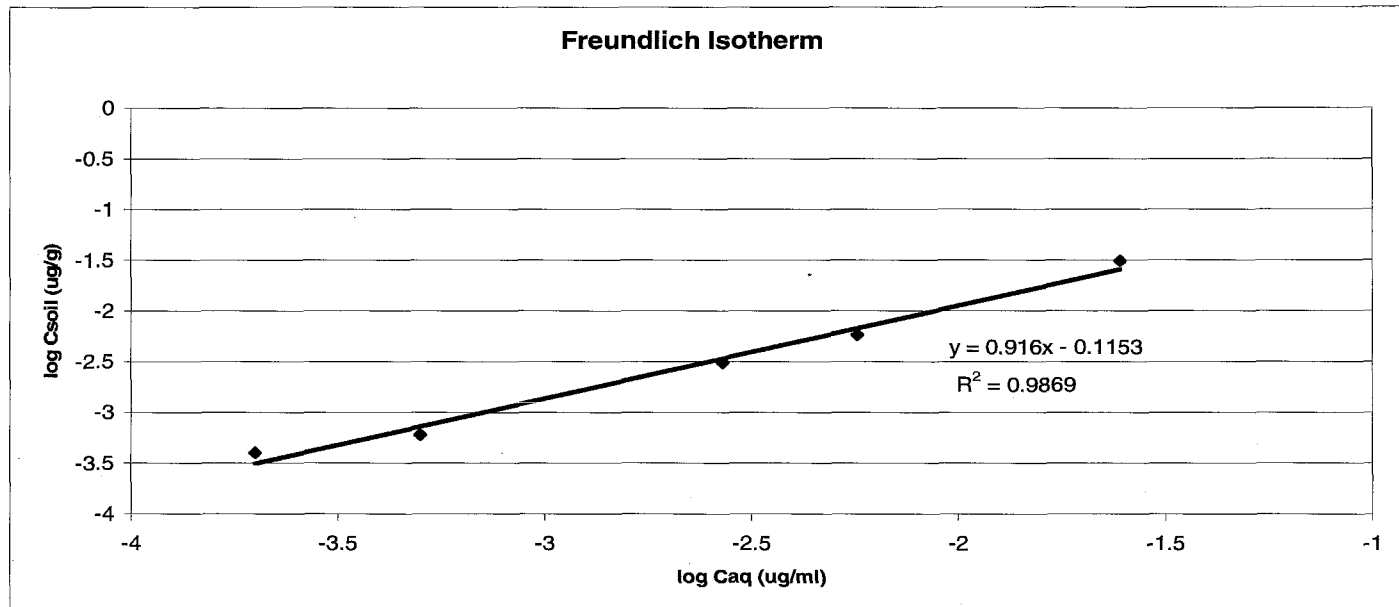


Notes:

1. Data obtained from Table 10, pp. 44-45.
2. C_{soil} and C_{aq} based on registrant-reported mean of two replicates.
3. Registrant only reported the mean C_{soil} and C_{aq} values, but not for individual replicates. Therefore, the C_{soil} and C_{aq} values could not be verified.
4. Registrant reported values of [¹⁴C] DMDS concentrations in soil after equilibrium (shown as C_{soil} above) do not match the calculated values [shown as CoVo-CaqVo)/m above].

Figure 2-6. Calculation of desorption soil – water partition coefficients Kd, Koc, Kf, and Kfoc Bretagne, FR Silt Loam soil.

C _o Initial Solution Conc. (µg/ml)	C _{soil} Conc. in soil after equilibrium (µg/g)	C _{aq} Conc. in solution after equilibrium (µg/ml)	V _o Volume of Solution (ml)	m Dry mass of sorbent (g)	(C _o V _o - C _{aq} V _o)/m	Kd (ml/g)	OC (%)	Koc (ml/g)	log Csoil	log Caq	1/n	Kf (ml/g)	Kfoc (ml/g)
0.102	0.0312	0.0246	14.5	14.5	0.0774	3.146341	0.02	157.3171	-1.505845	-1.6090649	0.916	2.304859	115.243
0.021	0.0058	0.0057	14.5	14.5	0.0153	2.684211	0.02	134.2105	-2.236572	-2.2441251	0.916	1.739042	86.9521
0.011	0.0031	0.0027	14.5	14.5	0.0083	3.074074	0.02	153.7037	-2.508638	-2.5686362	0.916	1.870462	93.5231
0.002	0.0006	0.0005	14.5	14.5	0.0015	3	0.02	150	-3.221849	-3.30103	0.916	1.58429	79.21451
0.001	0.0004	0.0002	14.5	14.5	0.0008	4	0.02	200	-3.39794	-3.69897	0.916	1.955899	97.79497
					Σ/n	3.180925		159.0463				1.890911	94.54553

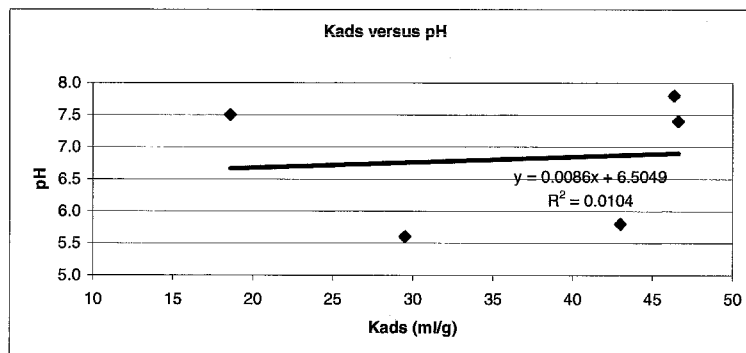
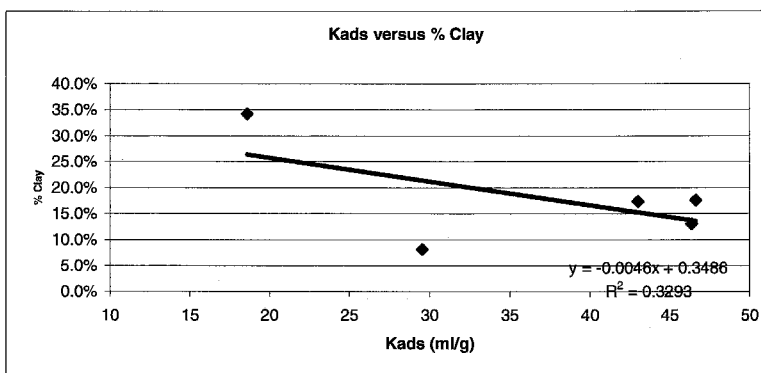
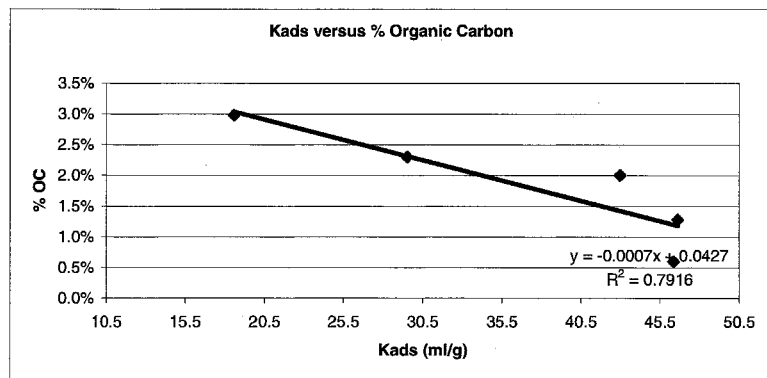


Notes:

1. Data obtained from Table 14, p. 49.
2. Csoil and Caq based on registrant-reported mean of two replicates.
3. Registrant only reported the mean Csoil and Caq values, but not for individual replicates. Therefore, the Csoil and Caq values could not be verified.
4. Registrant reported values of [¹⁴C] DMDS concentrations in soil after equilibrium (shown as C_{soil} above) do not match the calculated values [shown as C_oV_o-C_{aq}V_o/m above].

Figure 2-7. Statistical regression analysis of Kads versus site-specific % organic matter, % clay, and pH from California Sandy Loam; Speyer, Germany Loam; Mechtildshausen, Germany Loam; Mussig, France Loam; and Bretagne, France Silt Loam soil studies.

Soil	Kd (ml/g)	% OC	% Clay	pH
CA Sandy Loam ¹	46.36591	0.006	0.130	7.8
Speyer, GM Sandy Loam ²	29.53888	0.023	0.081	5.6
Mechtildshausen, GM Loam ²	46.62143	0.0128	0.176	7.4
Mussig, FR Clay Loam ²	18.59199	0.0298	0.342	7.5
Bretagne, FR Silt Loam ²	42.99879	0.02	0.174	5.8
Σ/n	36.8234			



Notes:

1. Data were obtained from Table 1, p. 33. Kads values were reviewer-calculated via the direct method using data obtained from Table 11, pp. 43 of the study report (MRID 46917014).
2. Data were obtained from Table 1, p. 35. Kads values were reviewer-calculated via the direct method using data obtained from Table 10, pp. 44-45 of the study report (MRID 46917015).