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Carr, K.H. 1990. Adsorption/desorption studies of MON 13900 and Aerobic Soil Metabolites. Project Nos. MSL-8962; RD 1054. Unpublished study performed and submitted by Monsanto Agricultural Company, Chesterfield, MO.

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CONCLUSIONS:Mobility - Leaching and Adsorption/Desorption

1. This study is acceptable and fulfills EPA Data Requirements for Registering Pesticides by providing information on the mobility (batch equilibrium) of aged residues of oxazolidine ring-labeled [4-¹⁴C]MON 13900 and parent MON 13900 in loamy sand, sandy loam, silty clay loam, and silt loam soils. No additional information on the mobility of MON 13900 in soil is needed at this time.
2. Aged (30 days) residues of MON 13900 were very mobile in loamy sand, sandy loam, silty clay loam, and silt loam soils with Freundlich K_{ads} values of 0.79-3.50. Adsorption increased with soil clay content and CEC. Parent MON 13900 had Freundlich K_{ads} values of 0.60-3.72 and its major aerobic soil degradate, MON 13900 oxamic acid, had K_{ads} values of 0.65-3.21.

METHODOLOGY:

Samples (100 g, dry weight) of air-dried, sieved (2 mm) Sarpy sandy loam soil (59% sand, 31% silt, 10% clay, 0.8% organic matter, pH 8.0, CEC 10.3 meq/100 g) were placed in six flasks and adjusted to 85% of 0.33 bar moisture. The flasks were stoppered with foam plugs, then incubated at 25 ± 1 C in the dark for 3 days. Following the 3-day preincubation period, the soil samples were treated at 1.38 ppm with oxazolidine ring-labeled [4-¹⁴C]MON 13900 (radiochemical purity 98.12%, specific activity 27.6 mCi/mMol, Monsanto), dissolved in 50% aqueous methanol; after treatment, the soil moisture was readjusted to 85% of field capacity. Each flask was topped with a two-piece trapping tower (Figure 4) containing foam plugs to trap [¹⁴C]volatiles and Ascarite to trap evolved ¹⁴CO₂; the samples were then incubated at 25 ± 1 C in the dark for 30 days. The flasks

were weighed at 6- to 10-day intervals and water was added, as needed, to maintain the soil moisture at 65-85% of field capacity.

At 30 days posttreatment, the soil samples were separately extracted three times on a wrist-action shaker with 60% aqueous acetonitrile then once with 0.1 N ammonium hydroxide; extracts were separated from soil by centrifugation. Aqueous acetonitrile extracts from all six soil samples were pooled, as were the ammonium hydroxide extracts; aliquots of each pooled extract were analyzed for total radioactivity using LSC. The two pooled extracts were combined, and concentrated "to remove all organic solvent" by rotary evaporation (temperature not specified). The concentrated extract was analyzed for total radioactivity using LSC. Additional aliquots were analyzed by reverse phase HPLC using UV (254 nm) and radioactivity detection on a Brownlee RP-18 precolumn followed by a Beckman Altex Ultrasphere-ODS C-18 column eluted with a two-step gradient of acetonitrile and 0.002 M dibasic ammonium phosphate.

The combined extract was found to contain 0.945 ppm [^{14}C]MON 13900 residues; the calcium concentration of the combined extract was adjusted to 0.01 M using calcium sulfate. Subsamples of the combined extract were diluted with 0.01 M calcium sulfate solution to produce three additional solutions containing 0.050, 0.202, and 0.603 ppm [^{14}C]MON 13900 residues.

Air-dried; sieved (2 mm) loamy sand, sandy loam, silt loam, and silty clay loam soils (Table 2) were used to determine adsorption of the aged MON 13900 residues. A preliminary experiment to determine equilibration time was conducted using the solutions containing 0.202 and 0.945 ppm [^{14}C]MON 13900 residues and the four soils. Soil: solution slurries (1 g soil:5 g solution) were shaken in culture tubes for 1, 2, 3, 5, 21, 24, and 41 hours; an equilibration time of 21-24 hours was selected for the definitive study (Table 6).

For the definitive adsorption experiment, 1 g samples of each soil and 5 g of the calcium sulfate solutions containing 0.050, 0.202, 0.603, and 0.945 ppm [^{14}C]MON 13900 residues were transferred to screw-cap glass culture tubes. The soil:solution slurries were shaken at room temperature (not specified) for 21-24 hours. After the shaking period, the slurries were centrifuged. The supernatant was removed, weighed, and triplicate aliquots were analyzed for total radioactivity using LSC. Selected samples were analyzed for MON 13900 and its degradates by HPLC as described above.

Desorption of MON 13900 residues was determined by replacing the supernatant removed after adsorption with an equal volume (approximately 5 g) of pesticide-free 0.01 M calcium sulfate solution. The soil:solution slurries were shaken at room temperature for 21-24 hours. After shaking, the slurries were centrifuged and aliquots of the supernatant were analyzed by LSC and, if sufficient [^{14}C]MON 13900 residues were present, by HPLC. The supernatant was replaced with an equal volume of pesticide-free CaSO_4 solution, and the desorption procedure was repeated twice more. [^{14}C]MON 13900 residues remaining adsorbed to the soil following desorption were quantified by LSC following combustion.

DATA SUMMARY:

Based on batch equilibrium studies, aged (30 days) residues of oxazolidine ring-labeled [$4\text{-}^{14}\text{C}$]MON 13900 (radiochemical purity 98.1%), at 0.050, 0.202, 0.603, and 0.945 ppm, were determined to be very mobile in Spinks loamy sand, Sarpy

sandy loam, Sable silty clay loam, and Drummer silt loam soil:calcium sulfate solution slurries (1:5, w:w) that were equilibrated for 21-24 hours at room temperature. Freundlich K_{ads} values were 0.79 for the loamy sand soil, 1.70 for the sandy loam soil, 3.47 for the silty clay loam soil, and 3.50 for the silt loam soil; respective K_{oc} values were 71.3, 327.6, 213.0, and 247.2 (Table 13). Adsorption of [^{14}C]MON 13900 residues increased from 14.1-20.7% on the loamy sand soil, to 24.4-41.1% on the sandy loam soil, 44.3-61.4% on the silty clay loam soil, and 46.4-63.1% on the silt loam soil (Tables 7-10). Adsorption increased with increasing soil clay content and CEC. The K_{des} values were 0.50-1.08 for the loamy sand soil, 1.02-1.90 for the sandy loam soil, 1.72-4.22 for the silty clay loam soil, and 0.98-3.32 for the silt loam soil (Table 15). Material balances ranged from 85.0 to 111.5% of the applied (Tables 4 and 5).

Freundlich K_{ads} values for MON 13900 were determined to be 0.60 for the loamy sand soil, 1.73 for the sandy loam soil, 3.17 for the silty clay loam soil, and 3.72 for the silt loam soil; respective K_{oc} values were 55.7, 341.4, 224.0, and 289.9 (Table 13). The K_{des} values for MON 13900 were 1.98-4.98 for the sandy loam, silty clay loam, and silt loam soils; insufficient MON 13900 adsorbed to the loamy sand soil to calculate K_{des} values (Table 16).

Freundlich K_{ads} values for MON 13900 oxamic acid were 0.65 for the loamy sand soil, 0.84 for the sandy loam soil, 3.21 for the silty clay loam soil, and 0.87 for the silt loam soil; respective K_{oc} values were 97.4, 194.8, 95.0, and 60.1 (Table 14). Insufficient MON 13900 oxamic acid was detected in the desorption solutions to calculate K_{des} values.

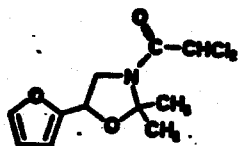
In the aged soil extract used for the adsorption experiments, parent MON 13900 comprised 80.5% of the total radioactivity in the extract and its major aerobic soil degradate 2-[5-(2-furanyl)-2,2-dimethyl-3-oxazolidinyl]-2-oxoacetic acid (MON 13900 oxamic acid, Fraction B) comprised 11.2%. HPLC analysis of solutions following adsorption and desorption was used to isolate and quantify parent MON 13900 and MON 13900 oxamic acid.

COMMENTS:

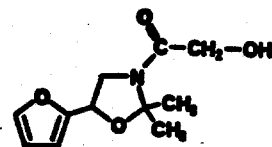
1. Typically, batch equilibrium studies are conducted using unaged pesticide and a study investigating the mobility of aged residues is conducted separately, usually using column leaching techniques. In this study, the pesticide was aged in sandy loam soil for 30 days, and extracted with aqueous acetonitrile and ammonium hydroxide; the resulting soil extract was used for the batch equilibrium experiments. Total [^{14}C]MON 13900 residues, parent MON 13900, and MON 13900 oxamic acid were determined to be very mobile in the loamy sand, sandy loam, silty clay loam, and silt loam soils used. Should the registrant believe that the results are not representative of the mobility of unaged MON 13900 and that aging of the pesticide may have affected its mobility (such as causing some interaction between the pesticide and its degradates that may have increased its mobility), then a mobility study (preferably batch equilibrium) using unaged MON 13900 can be submitted.
2. It was reported that the adsorption/desorption studies were conducted at room temperature; however, the temperature was not specified.
3. Four controls, which consisted of one culture tube containing only test solution at each concentration, were included with the soil:solution slurries in the

definitive adsorption experiment. It was reported by the study author that 2.2-5.3% of the applied radioactivity adsorbed to the glass culture tubes of the "no soil" controls.

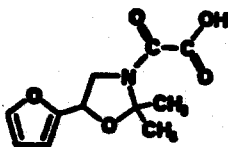
4. A stability experiment determined that MON 13900 did not significantly degrade during the batch equilibrium experiments. Soil:solution slurries (1 g soil:5 g solution) were prepared using each of the four soil types and 0.01 M calcium sulfate solution containing 0.976 ppm oxazolidine ring-labeled [4-¹⁴C]MON 13900 (radiochemical purity 97.2%). The soil:solution slurries were shaken for 40 hours, then centrifuged and the supernatants were analyzed by LSC and HPLC. After 40 hours of shaking, parent MON 13900 comprised 94.3-97.9% of the total radioactivity in the solution (Table 27).
5. To determine material balances for the aging portion of the study, volatile and bound [¹⁴C]residues were measured. The foam plugs in the trapping towers were collected and replaced at 10, 17, 24, and 30 days posttreatment and Ascarite was collected at 17 and 30 days posttreatment. Foam plugs from the trapping towers were placed in scintillation cocktail and analyzed for total radioactivity using LSC. Ascarite from the trapping towers was placed in a flask and dissolved in distilled water. The flask was immersed in ice; the adsorbed ¹⁴CO₂ was released from the Ascarite using concentrated sulfuric acid and trapped in phenethylamine solution. The trapping solution was analyzed for total radioactivity using LSC. [¹⁴C]Residues remaining in the extracted soil were quantified using LSC following combustion. Total ¹⁴CO₂ accounted for 13.4% of the applied radioactivity and bound [¹⁴C]residues were 14.5%; the material balance for the aging portion of this study was 90.8% of the applied (Table 3).
6. The registrant reported that MON 13900 [3-(dichloroacetyl)-5-(2-furanyl)-2,2-dimethyloxazolidine] is a safener intended for use with chloroacetanilide and sulfonylurea herbicides in corn and sorghum. The maximum projected use rate for MON 13900 is 0.4 lb/A.
7. The registrant reported that for studies conducted using radiolabeled MON 13900, the compound was synthesized with the radiolabel in the carbon atom adjacent to the nitrogen in the oxazolidine ring portion of the molecule. Studies were not conducted with the compound labeled in the furan ring portion of the molecule because degradation of the radiolabeled furan ring would result in radiolabeled ring fragments that would be natural products composed of low numbers of carbon, hydrogen, and oxygen atoms.



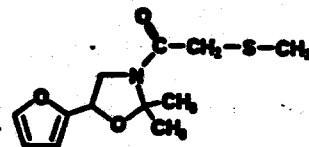
3-(Dichloroacetyl)-5-(2-furanyl)-2,2-dimethyloxazolidine
(NHN 13900)



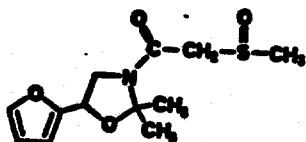
5-(2-Furanyl)-3-(hydroxyacetyl)-2,2-dimethyloxazolidine
(NHN 13900 Alcohol)



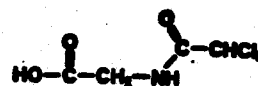
2-{5-(2-Furanyl)-2,2-dimethyl-3-oxazolidinyl}-2-oxoacetic acid
(NHN 13900 Oxamic acid)



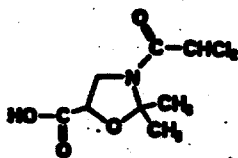
5-(2-Furanyl)-2,2-dimethyl-3-(methylthioacetyl)oxazolidine
(NHN 13900 Methyl sulfide)



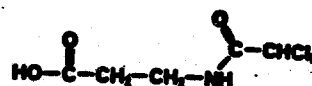
3-[(Methylsulfinyl)acetyl]-2,2-dimethyl-5-(2-furanyl)oxazolidine
(NHN 13900 Methyl sulfoxide)



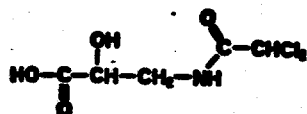
N-(Dichloroacetyl)glycine



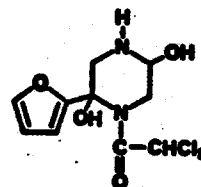
3-(Dichloroacetyl)-2,2-dimethyl-5-oxazolidinylcarboxylic acid
(NHN 13900 Oxazolidine acid)



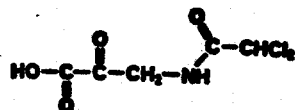
N-(Dichloroacetyl)-D-alanine



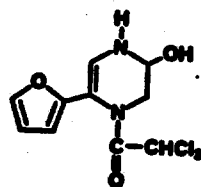
3-[(Dichloroacetyl)amino]-2-hydroxypropanoic acid



1-(Dichloroacetyl)-2-(2-furanyl)-2,5-piperazinediol



3-[(Dichloroacetyl)amino]-2-oxopropanoic acid



4-(Dichloroacetyl)-5-(2-furanyl)-1,2,3,4-tetrahydropyrazinol

Table 2: Physical Properties of Soils Used in the Adsorption/Desorption Studies of MON 13900 and Its Aerobic Soil Metabolites¹

Textural Classification Order ²	USDA Classification ³	Sable silty clay loam 4	Sarpy sandy loam Entisol mixed, mesic, Typic Udipsamment	Drummer silt loam Mollisol fine-silty, mixed, mesic, Typic Haplaquoll	Spinks loamy sand Alfisol sandy, mesic, mesic, Psammentic
Location		Monmouth, IL	New Bloomfield, MO	Decatur, IL	East Lansing, MI
% Sand		7	59	23	77
% Silt		62	31	53	19
% Clay		31	10	24	4
pH (1:1 soil:H ₂ O)		5.8	8	6.90	6.80
Cation Exchange Capacity (meq/100g)		22.9	10.3	22.10	6.30
% Moisture at 1/3 atm (Field Capacity)		29.50	12.99	27.10	9.48
% Moisture at 15 atm (Wilting Point)		15.67	6.60	14.16	4.95
Bulk Density (g/mL)		1.13	1.11	1.11	1.25
% Organic Matter ³		3.5	0.80	2.10	1.80
% Organic Carbon		2.0	0.58	1.78	1.15
% CaCO ₃		1.10	4.58	1.25	1.33

¹ Information not available.

² All data was generated (except where indicated) by A & L Agricultural Laboratories, 411 N. Third St., Memphis, TN; 1987 (Sable, 1989).

³ Information was obtained from Dr. Robert Held, soil scientist with the USDA Soil Conservation Service, Franklin, MO via phone communication, 1985. The

Drummer, Spinks, and Dupo USDA Classifications were obtained from a memo by W.R. Purdue to R.A. Conkin, 1980.

⁴ Determined colorimetrically.

Table 3: Mass Balance Data for the Aerobic Aging of MON 13900 in Sarpy Sandy Loam Soil

Sample	DPM	% of Applied DPM	% of Applied DPM
Acetonitrile/Water Extracts	109415940	59.9	
0.1 N NH ₄ OH	5214436	2.9	
Total Extractable	114630376		62.8
Bound Residues	26552756	14.5	14.5
Volatiles Day 10	48510	0.03	
Volatiles Day 17	46930	0.03	
Volatiles Day 24	31925	0.02	
Volatiles Day 30	30422	0.02	
Total Volatiles	157787		0.1
CO ₂ Day 10	10925444	6.0	
CO ₂ Day 24	10012270	5.5	
CO ₂ Day 30	3576004	2.0	
Total CO ₂	24513718		13.4
Total Recovery	165854637		90.8

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Table 4: Mass Balance Data for the Adsorption/Desorption Experiments with MON 13900 in Drummer Silt Loam and Sable Silty Clay Loam Soils

Soil	Replicate	Initial Sol'n (ppm)	MON 13900 Equivalents (μg)						Total Recovery (%)	
			AD Sol'n	D1 Sol'n	D2 Sol'n	D3 Sol'n	Soil ^a	Total Recovered		Total Applied
Drummer	A	0.050	0.09	0.05	0.03	0.02	0.03	0.22	0.24	90.3
Drummer	B	0.050	0.09	0.05	0.02	0.02	0.04	0.23	0.24	92.8
Drummer	A	0.202	0.35	0.17	0.11	0.07	0.11	0.81	0.96	85.0
Drummer	B	0.202	0.43	0.20	0.11	0.07	0.12	0.91	0.96	95.1
Drummer	A	0.603	1.45	0.62	0.32	0.20	0.23	2.82	2.87	98.3
Drummer	B	0.603	1.45	0.63	0.34	0.19	0.27	2.87	2.86	100.5
Drummer	A	0.945	2.39	0.98	0.46	0.30	0.55	4.69	4.47	104.9
Drummer	B	0.945	2.37	0.94	0.43	0.29	0.52	4.54	4.44	102.3
Mean										96.1
Std.Dev.										6.6
Sable	A	0.050	0.10	0.05	0.03	0.02	0.04	0.24	0.24	100.4
Sable	B	0.050	0.10	0.05	0.03	0.02	0.04	0.24	0.24	100.7
Sable	A	0.202	0.37	0.20	0.13	0.09	0.10	0.88	0.95	93.0
Sable	B	0.202	0.46	0.23	0.12	0.07	0.17	1.04	0.96	108.1
Sable	A	0.603	1.53	0.70	0.34	0.21	0.33	3.12	2.88	108.2
Sable	B	0.603	1.51	0.70	0.35	0.20	0.40	3.15	2.87	109.9
Sable	A	0.945	2.49	1.11	0.54	0.31	0.53	4.09	4.48	111.4
Sable	B	0.945	2.48	1.14	0.56	0.33	0.43	4.95	4.54	108.9
Mean										105.1
Std.Dev.										6.4

^aDetermined by combustion analysis.

Drummer = Drummer silt loam; Sable = Sable silt loam;

Table 5: Mass Balance Data for the Adsorption/Desorption Experiments with MON 13900 in Sarpy Sandy Loam and Spinks Loamy Sand Soils

Soil	Replicate	Initial Sol'n (ppm)	MON 13900 Equivalents (μ g)							Total Recovery (%)
			AD Sol'n	D1 Sol'n	D2 Sol'n	D3 Sol'n	Soil*	Total Recovered	Total Applied	
Sarpy	A	0.050	0.15	0.05	0.02	0.01	0.02	0.25	0.24	103.2
Sarpy	B	0.050	0.15	0.05	0.02	0.01	0.01	0.24	0.24	101.0
Sarpy	A	0.202	0.56	0.22	0.10	0.03	0.05	0.96	0.96	100.6
Sarpy	B	0.202	0.64	0.19	0.07	0.06	0.04	1.00	0.95	105.1
Sarpy	A	0.603	2.11	0.62	0.21	0.09	0.11	3.12	2.88	108.5
Sarpy	B	0.603	2.09	0.59	0.21	0.09	0.12	3.09	2.88	107.4
Sarpy	A	0.945	3.02	0.97	0.42	0.21	0.30	4.93	4.48	110.2
Sarpy	B	0.945	3.41	0.97	0.33	0.14	0.17	5.02	4.51	111.5
Mean										105.9
Std.Dev.										4.1
Spinks	A	0.050	0.19	0.04	0.01	0.00	0.01	0.25	0.24	103.4
Spinks	B	0.050	0.19	0.04	0.01	0.00	0.01	0.25	0.24	104.4
Spinks	A	0.202	0.79	0.14	0.03	0.01	0.04	1.00	0.96	105.0
Spinks	B	0.202	0.80	0.13	0.03	0.01	0.04	1.00	0.96	104.0
Spinks	A	0.603	2.45	0.42	0.09	0.03	0.08	3.06	2.85	107.3
Spinks	B	0.603	2.49	0.39	0.09	0.03	0.08	3.08	2.91	105.9
Spinks	A	0.945	3.88	0.63	0.13	0.04	0.12	4.81	4.53	106.0
Spinks	B	0.945	3.81	0.63	0.13	0.04	0.11	4.73	4.47	105.8
Mean										105.2
Std.Dev.										1.3

*Determined by combustion analysis.

Sarpy = Sarpy sandy loam; Spinks = Spinks loamy sand

Table 6: Summary of Data from Adsorption Kinetics Experiment with the MON 13900 and Soil Metabolite Mixture

Soil	Hours of Shaking	Sol'n Concentration (ppm)			
		0.202 ppm		0.945 ppm	
		A	B	A	B
Drummer	0	0.202	0.202	0.945	0.945
Drummer	1	0.110	0.108	0.600	0.592
Drummer	2	0.101	0.100	0.567	0.559
Drummer	3	0.098	0.098	0.555	0.550
Drummer	5	0.092	0.092	0.531	0.524
Drummer	21	0.084	0.078	0.484	0.476
Drummer	24	0.086	0.084	0.482	0.474
Drummer	41	0.160	0.143	0.461	0.448
Sable	0	0.202	0.202	0.945	0.945
Sable	1	0.111	0.110	0.581	0.596
Sable	2	0.105	0.102	0.562	0.567
Sable	3	0.102	0.132	0.548	0.557
Sable	5	0.097	0.096	0.523	0.528
Sable	21	0.088	0.087	0.477	0.481
Sable	24	0.087	0.085	0.472	0.474
Sable	41	0.082	0.081	0.456	0.455
Sarpy	0	0.202	0.202	0.945	0.945
Sarpy	1	0.155	0.153	0.774	0.676
Sarpy	2	0.150	0.150	0.763	0.678
Sarpy	3	0.148	0.148	0.753	0.679
Sarpy	5	0.144	0.142	0.729	0.670
Sarpy	21	0.133	0.132	0.682	0.644
Sarpy	24	0.134	0.133	0.685	0.649
Sarpy	41	0.126	0.122	0.645	0.604
Spinks	0	0.202	0.202	0.945	0.945
Spinks	1	0.178	0.180	0.860	0.861
Spinks	2	0.175	0.176	0.852	0.852
Spinks	3	0.172	0.174	0.840	0.848
Spinks	5	0.169	0.170	0.825	0.828
Spinks	21	0.162	0.162	0.789	0.789
Spinks	24	0.159	0.162	0.787	0.795
Spinks	41	0.291	0.194	1.467	1.599

1 g soil (dry weight) used with 5 g solution

Several of the 41-hour samples reflect higher concentrations than the 24-hour samples. This is probably due to the presence of soil particles in the 41-hour sample.

Table 7: Adsorption Data for the MON 13900 and Soil Metabolite Mixture on Drummer Silt Loam Soil

Initial Sol'n (ppm)	Rep	Sol'n Weight (g)				MON 13900 in AD Sol'n (ppm) (C_e)	MON 13900 Equivalents (μg)				MON 13900 Adsorbed to Soil (%)
		Dosing	Super-natant	Total Initial ^a	Sol'n in Soil ^b		Super-natant	Sol'n in Soil	Dosing Sol'n	Adsorbed to Soil (x)	
0.050	A	4.79	4.19	4.90	0.71	0.019	0.08	0.01	0.24	0.15	61.36
0.050	B	4.82	4.24	4.93	0.69	0.019	0.08	0.01	0.24	0.15	60.96
0.202	A	4.73	3.58	4.84	1.26	0.073	0.26	0.09	0.96	0.60	63.14
0.202	B	4.74	4.12	4.85	0.73	0.088	0.36	0.06	0.96	0.53	55.56
0.603	A	4.76	4.12	4.87	0.75	0.297	1.22	0.22	2.87	1.42	49.59
0.603	B	4.74	4.11	4.85	0.74	0.299	1.23	0.22	2.86	1.41	49.23
0.945	A	4.73	4.03	4.84	0.81	0.495	1.99	0.40	4.47	2.07	46.42
0.945	B	4.70	4.09	4.81	0.72	0.492	2.01	0.35	4.44	2.07	46.72

^aWeight of initial dosing solution + 0.11 g water in soil

^bSolution remaining in soil after supernatant removal.

Rep = Replicate

C_e = MON 13900 in Sol'n at Equilibrium (ppm)

x = MON 13900 in Soil at Equilibrium (μg)

m (soil dry weight) = 1.0 g for all samples

\bar{x} = MON 13900 Adsorbed to Soil (ppm)

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Table 8: Adsorption Data for the MON 13900 and Soil Metabolite Mixture on Sable Silty Clay Loam Soil

Initial Sol'n (ppm)	Rep	Sol'n Weight (g)		MON 13900 in AD Sol'n (ppm) (C _e)		MON 13900 Equivalents (μg)			MON 13900 Adsorbed to Soil (%)
		Dosing	Super-natant	Total Initial ^a	Sol'n in Soil ^b	Super-natant	Sol'n in Soil	Dosing Sol'n	
0.050	A	4.84	4.10	5.12	1.02	0.08	0.02	0.24	57.5
0.050	B	4.76	4.10	5.04	0.94	0.08	0.02	0.24	58.3
0.202	A	4.67	3.83	4.95	1.12	0.28	0.08	0.95	61.4
0.202	B	4.75	4.05	5.03	0.98	0.37	0.09	0.96	52.7
0.603	A	4.78	4.01	5.06	1.05	1.22	0.32	2.88	46.8
0.603	B	4.76	4.00	5.04	1.04	1.20	0.31	2.87	47.4
0.945	A	4.74	3.87	5.02	1.15	1.92	0.57	4.48	44.3
0.945	B	4.81	3.98	5.09	1.11	1.94	0.54	4.54	45.3

^aWeight of initial dosing solution + 0.28 g water in soil

^bSolution remaining in soil after supernatant removal.

Rep = Replicate

C_e = MON 13900 in Sol'n at Equilibrium (ppm)

x = MON 13900 in Soil at Equilibrium (μg)

m (soil dry weight) = 1.0 g for all samples

\bar{x} = MON 13900 Adsorbed to Soil (ppm)

Table 9: Adsorption Data for the MON 13900 and Soil Metabolite Mixture on Sarpy Sandy Loam Soil

Initial Sol'n (ppm)	Rep	Sol'n Weight (g)				MON 13900 in AD Sol'n (ppm) (C_e)	MON 13900 Equivalents (μg)				MON 13900 Adsorbed to Soil (%)
		Dosing	Super-natant	Total Initial ^a	Sol'n in Soil ^b		Super-natant	Sol'n in Soil	Dosing Sol'n	Adsorbed to Soil (x)	
0.050	A	4.72	4.24	4.81	0.57	0.031	0.13	0.02	0.24	0.09	37.4
0.050	B	4.79	4.33	4.88	0.55	0.031	0.14	0.02	0.24	0.09	36.8
0.202	A	4.72	4.18	4.81	0.63	0.117	0.49	0.07	0.96	0.39	41.1
0.202	B	4.69	4.22	4.78	0.56	0.135	0.57	0.08	0.95	0.30	32.1
0.603	A	4.77	4.12	4.86	0.74	0.433	1.78	0.32	2.88	0.77	26.8
0.603	B	4.77	4.14	4.86	0.72	0.430	1.78	0.31	2.88	0.79	27.3
0.945	A	4.74	4.10	4.83	0.73	0.626	2.56	0.46	4.48	1.46	32.5
0.945	B	4.77	4.13	4.86	0.73	0.701	2.90	0.51	4.51	1.10	24.4

^aWeight of initial dosing solution + 0.06 g water in soil

^bSolution remaining in soil after supernatant removal.

Rep = Replicate

C_e = MON 13900 in Sol'n at Equilibrium (ppm)

x = MON 13900 in Soil at Equilibrium (μg)

m (soil dry weight) = 1.0 g for all samples

μg = MON 13900 Adsorbed to Soil (ppm)

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Table 10: Adsorption Data for the MON 13900 and Soil Metabolite Mixture on Spinks Loamy Sand Soil

Initial Sol'n (ppm)	Rep	Sol'n Weight (g)				MON 13900 in AD Sol'n (ppm) (C_e)	MON 13900 Equivalents (μg)				MON 13900 Adsorbed to Soil (%)
		Dosing	Super-natant	Total Initial ^a	Sol'n in Soil ^b		Super-natant	Sol'n in Soil	Dosing Sol'n	Adsorbed to Soil (x)	
0.050	A	4.75	4.36	4.81	0.45	0.039	0.17	0.02	0.24	0.05	20.7
0.050	B	4.73	4.34	4.79	0.45	0.040	0.17	0.02	0.24	0.05	19.9
0.202	A	4.73	4.30	4.79	0.49	0.164	0.71	0.08	0.96	0.17	17.7
0.202	B	4.75	4.32	4.81	0.49	0.165	0.71	0.08	0.96	0.17	17.2
0.603	A	4.73	4.28	4.79	0.51	0.511	2.19	0.26	2.85	0.40	14.1
0.603	B	4.75	4.37	4.88	0.51	0.510	2.23	0.26	2.91	0.42	14.4
0.945	A	4.80	4.33	4.86	0.53	0.798	3.46	0.42	4.53	0.66	14.5
0.945	B	4.73	4.26	4.79	0.53	0.796	3.39	0.42	4.47	0.66	14.7

^aWeight of initial dosing solution + 0.09 g water in soil

^bSolution remaining in soil after supernatant removal.

Rep = Replicate

C_e = MON 13900 in Sol'n at Equilibrium (ppm)

x = MON 13900 in Soil at Equilibrium (μg)

m (soil dry weight) = 1.0 g for all samples

$\frac{x}{m}$ = MON 13900 Adsorbed to Soil (ppm)

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Table 13: Summary of Adsorption Coefficients for the Adsorption of the MON 13900 and Soil Metabolite Mixture and MON 13900

Compound	Soil	K	$\pm 95\%$ Conf Bound	$\frac{1}{n}$	$\pm 95\%$ Conf Bound
Mixture	Drummer	3.50	0.28	0.74	0.07
Mixture	Sable	3.47	0.35	0.77	0.10
Mixture	Sarpy	1.70	0.54	0.81	0.42
Mixture	Spinks	0.79	0.04	0.91	0.09
MON 13900	Drummer	3.72	0.40	0.72	0.08
MON 13900	Sable	3.17	0.40	0.69	0.10
MON 13900	Sarpy	1.73	0.85	0.83	0.52
MON 13900	Spinks	0.60	0.03	0.89	0.06
Compound	Soil	K_d	$\pm 95\%$ Conf Bound	K_{oc}	
Mixture	Drummer	4.40	0.42	247.2	
Mixture	Sable	4.26	0.37	213.0	
Mixture	Sarpy	1.90	0.32	327.6	
Mixture	Spinks	0.82	0.04	71.3	
MON 13900	Drummer	5.16	0.53	289.9	
MON 13900	Sable	4.48	0.54	224.0	
MON 13900	Sarpy	1.98	0.38	341.4	
MON 13900	Spinks	0.64	0.03	55.7	

Mixture = the MON 13900 and soil metabolite mixture.

MON 13900 = MON 13900 alone.

Table 14: Summary of Adsorption Coefficients for the Adsorption of MON 13900 Oxamic Acid II (see Figures 19 and 20 for graphs)

Soil	K	$\pm 95\%$ Conf Bound	$\frac{1}{n}$	$\pm 95\%$ Conf Bound
Drummer	0.87	0.51	0.92	0.22
Sable	3.21	0.50	1.19	0.06
Sarpy	0.84	0.77	0.89	0.34
Spinks	0.65	0.51	0.79	0.29
Soil	K_d	$\pm 95\%$ Conf Bound	K_{oc}	
Drummer	1.07	0.08	60.1	
Sable	1.90	0.10	95.0	
Sarpy	1.13	0.15	194.8	
Spinks	1.12	0.16	97.4	

Table 15: Summary of Freundlich Desorption Coefficients for the Desorption of the MON 13900 and Soil Metabolite Mixture

Soil	Initial Concentration (ppm)	K	$\pm 95\%$ Conf Bound	$\frac{1}{n}$	$\pm 95\%$ Conf Bound
Drummer	0.050	0.98	0.16	0.48	0.04
Drummer	0.202	1.93	1.28	0.49	0.21
Drummer	0.603	3.22	0.43	0.67	0.08
Drummer	0.945	3.32	0.36	0.65	0.08
Sable	0.050	1.72	0.53	0.64	0.07
Sable	0.202	3.05	2.48	0.69	0.28
Sable	0.603	4.01	0.87	0.90	0.14
Sable	0.945	4.22	0.97	1.02	0.23
Sarpy	0.050	1.02	0.28	0.71	0.07
Sarpy	0.202	1.48	1.22	0.70	0.34
Sarpy	0.603	1.90	0.61	1.06	0.34
Sarpy	0.945	1.89	1.41	1.00	1.20
Spinks	0.050	0.50	0.23	0.72	0.14
Spinks	0.202	0.84	0.24	0.90	0.15
Spinks	0.603	1.08	2.32	1.44	3.17
Spinks	0.945	0.96	0.08	1.69	0.33

Table 16: Summary of Freundlich Desorption Coefficients for the Desorption of MON 13900

Soil	Initial Concentration (ppm)	K	$\pm 95\%$ Conf Bound	$\frac{1}{n}$	$\pm 95\%$ Conf Bound
Drummer	0.202	1.98	6.44	0.48	1.04
Drummer	0.603	3.66	0.60	0.72	0.09
Drummer	0.945	3.63	0.41	0.69	0.08
Sable	0.202	3.08	12.77	0.66	1.36
Sable	0.603	4.98	1.46	1.01	0.17
Sable	0.945	4.81	1.46	1.13	0.27
Sarpy	0.202	2.23	7.72	0.85	1.37
Sarpy	0.603	3.54	3.10	1.71	0.83
Sarpy	0.945	2.25	4.25	1.14	2.43

Desorption coefficients could not be calculated for the 0.050 ppm concentration since the solutions were too dilute for HPLC/RAD analysis.

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Table 27: Summary of Stability Experiment with MON 13900 and Soil Metabolites

Sample	Replicate	MON 13900 % Distribution
Initial		97.2
Drummer	A	95.3
Drummer	B	94.9
Sable	A	97.9
Sable	B	97.3
Sarpy	A	96.4
Sarpy	B	96.7
Spinks	A	94.5
Spinks	B	94.3

MON 13900 quantified by HPLC/RAD analysis.

Initial Solution Concentration was 0.976 ppm

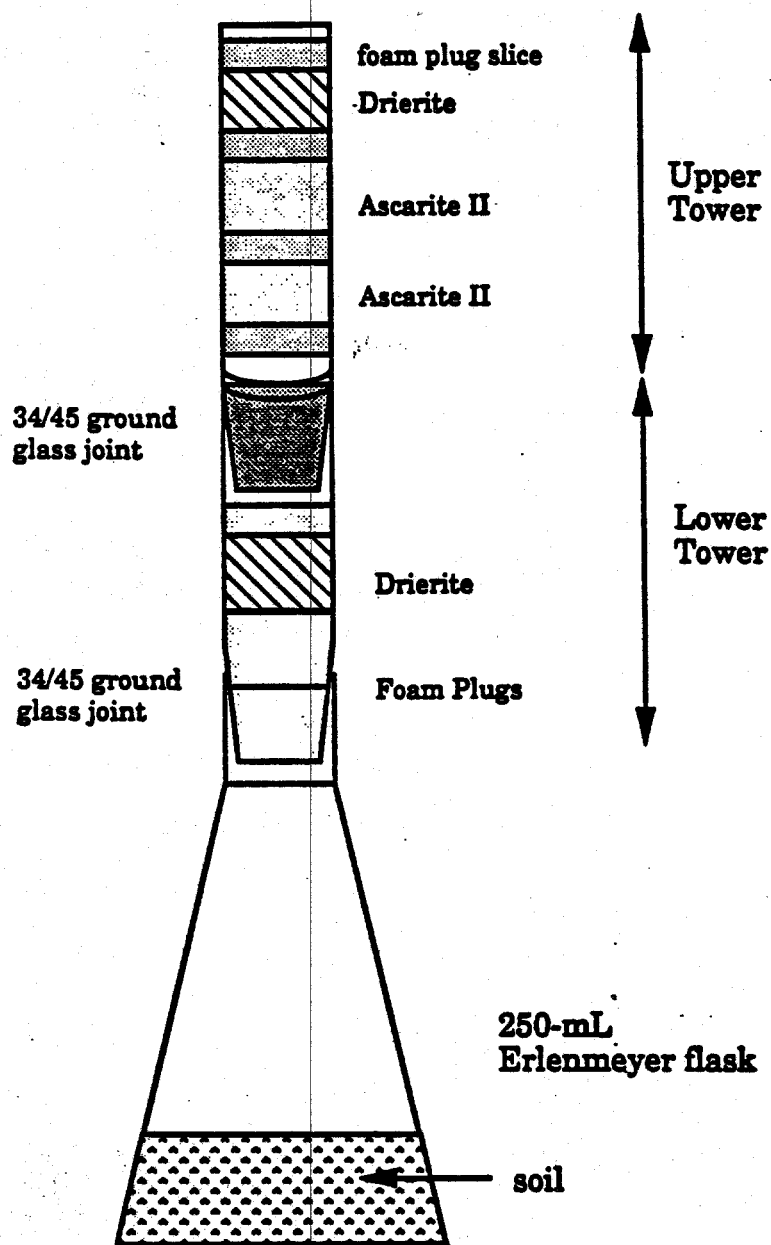
MON 13900 equivalents.

See Section 3.5.7 for a description
of this experiment.

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Figure 4: Apparatus Used in the MON 13900 Adsorption/Desorption Study; Aerobic Soil Incubation Portion



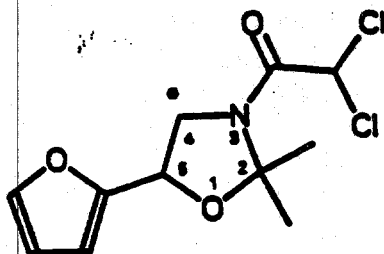
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STUDY AUTHOR(S)'S RESULTS AND/OR CONCLUSIONS

4 RESULTS & DISCUSSION

4.1 Study Design

This study was designed to provide adsorption/desorption data for MON 13900, I, and its aerobic soil metabolites. The protocol for this study (Monsanto Protocol Number 88-27-M25) was designed to satisfy U.S. EPA Pesticide Assessment Guidelines, Subdivision N, Guideline 163-1, Leaching and Adsorption/Desorption Studies. The MON 13900 that was used was labeled with ^{14}C in the oxazolidine ring. The use of the radiolabeled material enabled quantification of MON 13900 equivalents in solution and soil by liquid scintillation counting.



I, MON 13900

* -indicates position of ^{14}C -label

Several experiments were conducted within this study. They were: (1) the generation of the MON 13900 and aerobic soil metabolite mixture; (2) an adsorption kinetics experiment; (3) the adsorption/desorption experiment (batch equilibrium); and (4) a stability experiment. These are described in greater detail below.

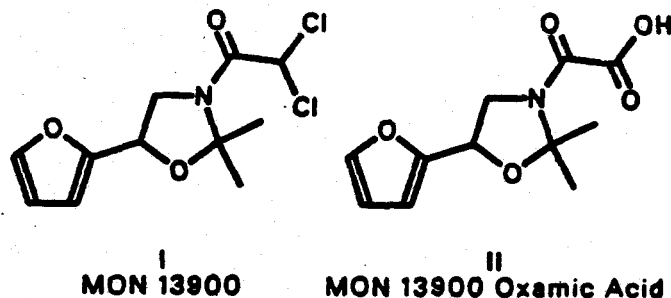
4.2 Generation of Aerobic Soil Metabolites

The EPA Guidelines^{8,9} indicate that the mixture of soil metabolites present after thirty days of aerobic soil metabolism should be used for the batch equilibrium studies. Sarpy sandy loam soil was chosen for the aerobic incubation since results from the MON 13900 Aerobic Soil Metabolism Study² indicated that fewer bound residues were formed in Sarpy sandy loam than in Sable silty clay loam (the second soil used in the Aerobic Soil Metabolism Study).

^{14}C -MON 13900 was applied to Sarpy sandy loam soil at a rate of 1.38 parts per million, based on soil dry weight. The soil samples were incubated in darkness for 30 days under aerobic conditions (25 °C, darkness) to generate a mixture of MON 13900 aerobic soil metabolites. After 30 days of incubation, the soil was exhaustively extracted (see Section 3.5.2, page 21) and a single pooled extract was prepared. Analysis of the pooled extract by liquid scintillation counting (LSC)

indicated that the extract contained 62.8% of the applied radioactivity (see Table 3, page 45).

The aged soil extract was concentrated to remove all organic solvent, and then further concentrated to a concentration of 0.945 ppm MON 13900 equivalents. HPLC/RAD analysis indicated that 80.5% of the distribution was parent MON 13900 (Figure 6, page 75). Three metabolite fractions (labeled Metabolite Fractions A, B, and C) were also observed, representing 5.3, 11.2, and 3.0% of the HPLC/RAD distribution, respectively. Fraction A was a mixture of polar metabolites. Fractions B and C were assigned structures based on HPLC retention time comparisons. Fraction B was assigned the structure of the MON 13900 oxamic acid II, based on HPLC retention time comparisons with an authentic standard. Fraction C was assigned the structure of a methyl sulfoxide derivative of MON 13900 based on HPLC retention time comparisons with a soil extract from the MON 13900 Aerobic Soil Metabolism Study.² Fractions A, B, and C were all observed in the aerobic soil metabolism study. No structures were assigned to the components in Fraction A.



The calcium content of the concentrated extract was determined by the Monsanto Physical Sciences Center to be 169 $\mu\text{g/mL}$ (see Section 3.5.4, page 21). Calcium sulfate was added to bring the calcium content to 0.01 M. Dosing solutions for the adsorption/desorption experiment were prepared at four concentrations of MON 13900 equivalents: 0.050 ppm, 0.202 ppm, 0.603 ppm, and 0.945 ppm.

Radiolabeled volatiles and CO_2 were trapped and quantified for the aerobic soil incubation as described in Section 3.6.3. The soil remaining after extraction was combusted to determine unextractable radioactivity. Table 3 (page 45) summarizes the distribution and total accountability of radioactivity during the aerobic aging portion of the study. Total recovery for this experiment was 90.8%, with bound residues totaling 14.5% of applied dpm.

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