

US EPA ARCHIVE DOCUMENT

DATA EVALUATION RECORD 1

GUIDELINE 161-1

STUDY ID 420197-13

Mislankar, S.G., and K.H. Carr. 1989b. Hydrolysis studies of MON 13900. - 911596
 Project Nos. MSL-8973; RD 1054. Unpublished study performed and submitted by
 Monsanto Agricultural Company, Chesterfield, MO.

REVIEWED BY:	L. Binari	TITLE:	Staff Scientist
EDITED BY:	L. Mickley	TITLE:	Staff Scientist
	L. Parsons		Staff Scientist
APPROVED BY:	W. Spangler	TITLE:	Project Manager
ORG:	Dynamac Corporation Rockville, MD		
APPROVED BY:	B. Conerly-Perks	<i>E. B. Conerly-Perks 6/30/93</i>	
TITLE:	Chemist		
ORG:	EFGWB/EFED/OPP		
SIGNATURE:			

CONCLUSIONS:Degradation - Hydrolysis

1. This study is acceptable and fulfills EPA Data Requirements for Registering Pesticides by providing information on the hydrolysis of oxazolidine ring-labeled [4-¹⁴C]MON 13900 at pH 5, 7, and 9. No additional data on the hydrolysis of MON 13900 are required at this time.
2. MON 13900 did not hydrolyze in sterile aqueous buffered solutions (pH 5, 7, and 9) that were incubated in the dark at 25 C.

METHODOLOGY:

Oxazolidine ring-labeled [4-¹³C/¹⁴C]MON 13900 (radiochemical purity >99%, specific activity 18.9 mCi/mMol, Monsanto) plus unlabeled MON 13900 (purity 100%, Monsanto), dissolved in acetonitrile, was added at 58.15-60.07 ppm to filter-sterilized (0.2 um) aqueous 0.01 M buffer solutions adjusted to pH 5 (sodium acetate), pH 7 (potassium phosphate), and pH 9 (boric acid); the final concentration of the cosolvent (acetonitrile) was 0.35%. Duplicate aliquots (300-600 mg) of the solutions were analyzed for total radioactivity using LSC. Additional aliquots (3 mL) of the solutions were transferred to 1-dram glass vials. The vials were sealed with Teflon-lined caps, then incubated at 25 ± 1 C in the dark. Duplicate vials of each pH solution were removed for analysis at 0, 7, 14, 21, and 28 days posttreatment.



Duplicate aliquots (150-600 mg) of each test solution were analyzed for total radioactivity using LSC. Additional aliquots (300-600 mg) were analyzed for MON 13900 and possible degradates by HPLC using UV (254 nm) and radioactivity detection on an RP-18 precolumn followed by a Spherisorb S5 Nitrile column eluted with an isocratic and linear gradient mobile phase of acetonitrile and 0.001 M dibasic ammonium phosphate. Radioactive compounds were identified by comparison to retention times of unlabeled reference standards. Selected samples were also analyzed using LC/MS.

DATA SUMMARY:

Oxazolidine ring-labeled [4-¹⁴C]MON 13900 (radiochemical purity >99%), at 58-60 ppm, was stable in sterile aqueous buffered solutions (pH 5, 7, and 9) that were incubated in the dark at 25 ± 1 C for 28 days. MON 13900 ranged from 57.4 to 60.7 ppm at all sampling intervals (Table 1). During the study, material balances ranged from 99.5 to 104.8% of the applied (Table 2).

COMMENTS:

1. The aqueous solubility of MON 13900 was reported to be approximately 214 ppm.
2. 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.
3. 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.

8 TABLES

Table 1: Quantification of MON 13900 in the Hydrolysis Experiments

Sampling Time (Days)	Replicate	% Distribution MON 13900 ^a	PPM ^b	PPM MON 13900 ^c
pH 5				
0	1	98.7	58.52	57.73
0	2	98.8	58.49	57.76
7	1	98.4	58.27	57.35
7	2	98.9	58.31	57.59
14	1	100.0	57.97	57.97
14	2	99.0	58.47	57.91
21	1	99.3	60.95	60.52
21	2	98.4	58.28	57.56
28	1	100.0	58.76	58.76
28	2	99.3	57.89	57.60
Average		99.1	58.58	58.05
Std.Dev.		0.6	0.87	0.95
pH 7				
0	1	98.4	58.53	57.58
0	2	98.6	59.02	58.18
7	1	99.0	58.66	58.05
7	2	98.6	58.71	57.89
14	1	98.7	58.88	58.12
14	2	99.5	58.87	58.58
21	1	99.3	58.82	58.42
21	2	100.0	58.68	58.68
28	1	99.3	58.78	58.39
28	2	99.3	59.16	58.74
Average		99.1	58.81	58.28
Std.Dev.		0.5	0.18	0.37
pH 9				
0	1	98.0	60.67	59.44
0	2	98.5	60.68	59.79
7	1	98.4	59.84	58.90
7	2	99.0	60.86	60.28
14	1	100.0	60.72	60.72
14	2	99.3	60.57	59.94
21	1	99.5	60.47	60.15
21	2	99.3	60.31	59.87
28	1	99.1	60.36	59.83
28	2	100.0	60.66	60.66
Average		99.1	60.49	59.96
Std.Dev.		0.7	0.29	0.54

^a Percent distribution of MON 13900 determined by HPLC/RAD.
 Data from the Monsanto Automated Chromatography System (MACS).
^b PPM is expressed as MON 13900 equivalents, and was determined from liquid scintillation counting of duplicate aliquots of the solution.
^c PPM of MON 13900 in solution, calculated from the percent distribution of MON 13900 times the PPM of the solution.

CONTAINS TRADE SECRET OR
 OTHERWISE CONFIDENTIAL
 INFORMATION OF MONSANTO
 COMPANY

Table 2: Total Recoveries of ¹⁴C-Radioactivity for the MON 13900 Hydrolysis Experiments

Sampling Time (Days)	Replicate	PPM ^a	Recovery (%) ^b
pH 5			
0	1	58.52	100.6
0	2	58.49	100.6
7	1	58.27	100.2
7	2	58.21	100.1
14	1	57.97	99.7
14	2	58.47	100.6
21	1	60.95	104.8
21	2	58.28	100.2
28	1	58.76	101.0
28	2	57.89	99.5
Average		58.58	100.7
Std.Dev.		0.87	1.5
pH 7			
0	1	58.53	100.6
0	2	59.02	101.4
7	1	58.66	100.8
7	2	58.71	100.9
14	1	58.88	101.2
14	2	58.87	101.2
21	1	58.82	101.1
21	2	58.68	100.8
28	1	58.78	101.0
28	2	59.16	101.7
Average		58.81	101.1
Std.Dev.		0.18	0.3
pH 9			
0	1	60.67	101.0
0	2	60.68	101.0
7	1	59.84	99.6
7	2	60.86	101.3
14	1	60.72	101.1
14	2	60.37	100.5
21	1	60.47	100.7
21	2	60.31	100.4
28	1	60.36	100.5
28	2	60.66	101.0
Average		60.49	100.7
Std.Dev.		0.29	0.5

CONTAINS TRADE SECRET OR OTHERWISE CONFIDENTIAL INFORMATION OF MONSANTO COMPANY

^a PPM is expressed as MON 13900 equivalents, and was determined from liquid scintillation counting of duplicate aliquots of the solution.

^b Recovery is expressed as percent of initial concentration of MON 13900 in the stock buffer solution (pH 5: 58.15 ppm; pH 7: 58.19 ppm; pH 9: 60.07 ppm).