

DATA EVALUATION RECORD 6

5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole
§163-1

FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 43588009

Burr, C.M. and S.E. Newby. November 25, 1993. RPA 201772:
Adsorption/Desorption to and from Four Soils and an Aquatic Sediment.
Laboratory Report No. P93/085. Unpublished study performed by Rhone
Poulenc Agriculture, Limited, Essex, England, and submitted by Rhone
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CONCLUSIONS:

Unaged Mobility - Leaching and Adsorption/Desorption

1. The unaged batch equilibrium study in this review satisfies the unaged portion of the 163-1 data requirement.
2. Isoxaflutole [5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole] was very mobile in sand and sandy loam soils, moderately mobile in sandy loam soil, and essentially immobile in silty clay soil and loam sediment. Adsorption was shown to be reversible in all the soils studied with adsorption and desorption values that were comparable. Freundlich K_{ads} values were 0.51 for sand soil (0.5 % OC), 1.2 for the sandy loam (0.9 % OC), 2.2

for the loam soil (2.4 % OC), 9.3 for the silty clay soil (7.5 % OC), and 14.4 for the loam sediment (8.7 % OC). Adsorption increased with increasing soil organic carbon content. A Freundlich K_{des} value could not be calculated for the sand soil since all of the adsorbed material desorbed in one step. Freundlich K_{des} values were 2.6 for the sandy loam (0.9 % OC), 2.0 for the loam soil (2.4 % OC), 13.4 for the silty clay soil (7.5 % OC), and 10.4 for the loam sediment (8.7 % OC). Freundlich K_{oc} values were 101, 131, 93, 123, and 165 for adsorption and (none for sand soil), 284, 82, 179, and 119, respectively. The $1/N$ values were 1.0, 0.90, 0.94, 0.95, and 0.92 for adsorption and (none for sand soil), 0.93, 1.02, 0.95, and 0.90 for desorption, respectively.

3. There was significant degradation of parent isoxaflutole in the sand and loam soils, which had higher pH's (6.9-7.2) than the other soils (4.8-5.8). This degradation occurred when the soils were shaken for longer than the equilibrium time of 4 hours in the preliminary study. However, only minor degradation was observed after 4 hours of shaking for both adsorption and desorption, and the isotherms were still linear. The main degradate formed was RPA-202248 (**isoxaflutole with the isoxazole-ring opened**). RPA-202248 was a significant degradate in both the hydrolysis (MRID 43573254) and aerobic soil metabolism (MRID 43588006) studies in this review, and formed more rapidly as the pH increased.

METHODOLOGY:

Benzyl-labeled ^{14}C -isoxaflutole [5-cyclopropyl-4-(2-methanesulphonyl-4-trifluoromethylbenzoyl)isoxazole] (RPA 201772; radiochemical purity 98.5%; specific activity 679 MBQ/mmol [18.35 mCi/mMol, Rhone Poulenc, dissolved in acetonitrile at <1 %], was made into CaCl_2 solutions with a concentration of 1.5 mg/L, which is less than the 3.5 mg/L water solubility of isoxaflutole. This solution was further diluted to 0.015 mg/L, 0.15 mg/L, and 0.75 mg/L.

Preliminary Study-Glass Adsorption

To determine adsorption to glass, the registrant put 75 ml of 1.5 mg/L into 2 tubes, shook them for 24 hours, and analyzed an aliquot from each tube using LSC.

Preliminary Study-Equilibrium Time for Adsorption

The registrant added 15 g of sandy loam soil (oven-dried basis) to 12 tubes. After that, 75 ml of 1.5 mg/L solution was put into each tube. Two randomly-selected tubes were removed after shaking in darkness for 1, 2, 4, 8, 24, or 48 hours. Following removal, the tubes were centrifuged and supernatants were removed and weighed. Aliquots of the supernatants were analyzed for total radioactivity using LSC. HPLC was also used to characterize the radioactivity.

After centrifugation and removal of supernatants, the soil pellets were extracted twice with methylene cyanide:H₂O, centrifuged, and the supernatants were removed. Aliquots of the combined supernatants were analyzed using LSC. Following extraction, the soil pellets were allowed to dry and combusted to determine the amount of radioactivity remaining on the soil.

Preliminary Study-Equilibrium time for Desorption

The registrant added 15 g of soil (oven-dried basis) to 12 tubes. After that, 75 ml of 1.5 mg/L isoxaflutole were put into each tube. All tubes were removed after 4 hours of shaking and two randomly-selected tubes were removed after shaking in darkness for 1, 2, 4, 6.5, 24, or 48 hours. Following removal, the tubes were centrifuged and supernatants were removed and weighed. CaCl₂ (0.01 M, 75 ml) with no pesticide was added to each tube, the soil pellet was resuspended, and the triplicate aliquots of the supernatants were analyzed for total radioactivity using LSC. HPLC was also used to characterize the radioactivity.

After centrifugation and removal of supernatants, the soil pellets were extracted twice with methylene cyanide:H₂O, centrifuged, and the extraction supernatants were removed. Aliquots of the combined supernatants were analyzed using LSC and HPLC. Following extraction, the soil pellets were allowed to dry and combusted to determine the amount of radioactivity remaining on the soil.

Definitive Study

Triplicate tubes of 15 g soil (oven-dry basis) were put into tubes except for the sediment, which was added at 14 g (oven-dry basis). To the soil in the tubes was added 75 ml of dose solution at either 0.015, 0.15, 0.75, or 1.5 mg/L isoxaflutole. The exception was the sediment, which was treated with 70 ml of each solution. After weighing, the soil/solutions were transferred to an end-over-end shaker and shaken for 4 hours at 22 °C. After centrifuging and decanting the supernatant, fresh 0.01 M CaCl₂ with no added pesticide was added to each tube and the tubes were again shaken for 4 hours. The desorption cycle was repeated 4 additional times. Triplicate aliquots of supernatant were then removed and analyzed using LSC. As in the preliminary study, the soil pellets following desorption were extracted twice with methylene cyanide:H₂O, centrifuged, and the supernatants were removed. Aliquots of the combined supernatants were analyzed using LSC and HPLC. Following extraction, the soil pellets were allowed to dry and combusted to determine the amount of radioactivity remaining on the soil. HPLC/MS was also used for confirmation of chemical identities. Further details about the analytical methodology for both the preliminary and definitive studies may be seen in the attached Materials and Methods from the study. Also, the exact soil and sediment characteristics may be seen in the comments section of this DER.

DATA SUMMARY:

Based on the results of preliminary batch equilibrium experiments, it was found that binding to glass was minimal (<4 %). It was also found by using the sand soil, that an equilibration period of 4 hours was the most practical for the definitive study. The time was chosen because the isoxaflutole is both hydrolytically and metabolically unstable. After 4 hours in both the adsorption and desorption, there was only minimal degradation of parent isoxaflutole.

Based on batch equilibrium experiments, [^{14}C]isoxaflutole was very mobile in sand and sandy loam soils, moderately mobile in sandy loam soil, and essentially immobile in silty clay soil and loam sediment. Adsorption was shown to be reversible in all the soils studied with adsorption and desorption values that were comparable for each individual soil. Freundlich K_{ads} values were 0.51 for sand soil (0.5 % OC), 1.2 for the sandy loam (0.9 % OC), 2.2 for the loam soil (2.4 % OC), 9.3 for the silty clay soil (7.5 % OC), and 14.4 for the loam sediment (8.7 % OC). Adsorption increased with increasing soil organic carbon content. A Freundlich K_{des} value could not be calculated for the sand soil since all of the adsorbed material desorbed in one step. Freundlich K_{des} values were 2.6 for the sandy loam (0.9 % OC), 2.0 for the loam soil (2.4 % OC), 13.4 for the silty clay soil (7.5 % OC), and 10.4 for the loam sediment (8.7 % OC). Freundlich K_{oc} values were 101, 131, 93, 123, and 165 for adsorption and (none for sand soil), 284, 82, 179, and 119, respectively. The $1/N$ values were 1.0, 0.90, 0.94, 0.95, and 0.92 for adsorption and (none for sand soil), 0.93, 1.02, 0.95, and 0.90 for desorption, respectively.

At the termination of the experiment, material balances for the soil:solution slurries ranged from 98.23 to 104.26% of the applied. There was significant degradation of parent isoxaflutole in the sand and loam soils, which had higher pH's (6.9-7.2) than the other soils (4.8-5.8). This degradation occurred when the soils were shaken for longer than the equilibrium time of 4 hours in the preliminary studies. However, only minor degradation was observed after 4 hours of shaking for both adsorption and desorption, and the isotherms were still linear. The main degradate formed was RPA-202248 (isoxaflutole with the isoxazole-ring opened). RPA-202248 was a significant degradate in both the hydrolysis and aerobic soil metabolism studies in this review, and formed more rapidly as the pH increased.

COMMENTS:

1. The use of HPLC to characterize the radioactivity was vital, since isoxaflutole is both hydrolytically and metabolically unstable.

2. There was significant degradation of parent isoxaflutole in the sand and loam soils, which had higher pH's (6.9-7.2) than the other soils (4.8-5.8). This degradation occurred when the soils were shaken for longer than the equilibrium time of 4 hours. However, only minor degradation was observed after 4 hours of shaking for both adsorption and desorption, and the isotherms were still linear. The main degradate formed was RPA-202248 (**isoxaflutole with the isoxazole-ring opened**). RPA-202248 was a significant degradate in both the hydrolysis (MRID 43573254) and aerobic soil metabolism (MRID 43588006) studies in this review, and formed more rapidly as the pH increased.
3. In the definitive desorption study, all of the adsorbed pesticide desorbed from the andy soil in the first attempt. Therefore, no desorption isotherm was calculated for the sandy soil.

4. The chemical and physical characteristics of the soils and sediment used in this study follow in the Table.

Property	Soil				
Particle Size Distribution	93/7*	93/24	93/30	93/32	93/31 (Aquatic sediment)
Sand (%)	70	97.7	34	13	38
Silt (%)	24	0.9	44	44	47
Clay (%)	6	1.4	22	43	15
Textural Class					
USDA	Sandy loam	Sand	Loam	Silty clay	Loam
ADAS	Sandy loam	Sand	Clay loam	Silty clay	Sandy silty clay
Organic Carbon	0.9	0.5	2.4	7.5	8.7
Organic Matter (% OC *1.69)**	1.5	0.8	4.1	12.7	14.7
pH (0.01 M CaCl ₂)	5.6	7.2	6.9	4.8	5.8
Cation Exchange (CEC, meq/100g)	4.9	5.4	12.2	15.7	13.0
Bulk Density	1.54	1.71	1.2	0.8	0.9
Moisture Content when Collected	8.9	1.3	16.0	30.3	51.8

- * 93/7-American Agricultural Services Inc., Lucama, North Carolina, U.S.
 93/24-Hurdle Drove Farm, Hurdle Drove, West Row, Fenbury, St. Edmonds, Suffolk, U.K.
 93/30-Boarded Barns Farms, Ongar, Essex, U.K.
 93/32-Cooper Shaw Road, West Tilbury Marshes, Essex, U.K.
 93/31-Aldhams Far, Dead Lane, Lawford, Manningtree, Essex, U.K.

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In this study, the registrant used a factor of 1.69 to convert organic carbon to organic matter. In general, a factor of 1.72 is used to convert organic carbon to organic matter.

ISOXAFLUTOLE

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