DATA EVALUATION RECORD

STUDY 13

CHEM 122990	Mesotrione	§163-1

CAS No. 104206-82-8
FORMULATION--00--ACTIVE INGREDIENT

STUDY ID 44505204
Rowe, D. and M. C. G. Lane. 1997. ZA1296: Adsorption properties in 13 soils. Laboratory Project ID: 97JH176. Unpublished study performed by ZENECA Limited, Bracknell, Berkshire, UK; and submitted by ZENECA Inc., Wilmington, DE.

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CONCLUSIONS

Mobility - Leaching & Adsorption/Desorption

1. This study is scientifically valid **(acceptable)** and provides valuable information on the soil mobility (batch equilibrium) of mesotrione (ZA1296) in 13 U.S. soils. However, because the test compound was equilibrated at only one concentration, Freundlich K_{ads} and K_{oc} values could not be calculated. Instead, only simple K_d's were reported. Desorption of the test compound was not studied.

   In combination with other mobility studies, EPA Subdivision N Guideline requirements for soil mobility (batch equilibrium) are ***satisfied***. However, the registrant should consider the critical elements in the Comments section of this report, as these may affect the validity and consequent acceptability of future study submissions.

2. This study was designed to complement other batch equilibrium submissions by providing additional, simple adsorption data for mesotrione in soils with a variety of different properties. Among the soil variables, pHs ranged systematically from approximately 4.6 to 7.5. The data show that for the acidic mesotrione (pKa = 3.1) there is a strong inverse correlation between Koc and pH in the range tested. Results show that at pHs typical of agricultural soils mesotrione has high potential mobility.

3. The mobility of uniformly phenyl ring-labeled [^{14}C]mesotrione, at a nominal concentration of 0.2 µg/mL, was determined in Champaign (low pH; 4.6-5.0), Danville, Breeze, Martinsville, and Delavan silt loam; Valley Springs, New Holland, Clarence, and Champaign (high pH; 7.3-7.5) silty clay loam; Noblesville and Elk City loam; Osceola loamy sand; and Land O' Lakes clay loam soil:solution slurries that were equilibrated for 24 hours at **20 ± 2°C**. Freundlich K_{ads}, K_{oc}, and 1/N values could not be determined because the test compound was equilibrated at only one concentration; therefore, simple K_d and K_{oc} values were calculated. Simple K_d values were 2.3 for Osceola loamy sand (1.0% o.m.), 5.0 for Champaign (low pH) silt loam, 3.4 for Noblesville loam, 4.4 for Valley Springs silty clay loam, 1.1 for Elk City loam, 1.3 for New Holland silty clay loam, 1.6 for Danville silt loam, 1.0 for Breeze silt loam, 0.68 for Martinsville silt loam, 0.74 for Delavan silt loam, 0.63 for Clarence silty clay loam, 0.82 for Land O' Lakes clay loam (3.8% o.m.), and 0.61 for Champaign (high pH) silty clay loam. The following respectively derived sorption **K_{oc} values and corresponding soil pH values** (Table 3, p. 18) clearly show a strong inverse correlation between the two variables, and that mesotrione has high potential mobility in typical agricultural soils:

Koc(mL/g):	**390**	**240**	**250**	**210**	**110**	**73**	**98**	**120**	**90**	**70**	**60**	**37**	**29**
pH (in water):	**4.6**	**5.0**	**5.0**	**5.1**	**5.3**	**5.3**	**5.6**	**5.5**	**6.0**	**6.0**	**6.4**	**6.6**	**7.5**

   The reviewer-calculated linear regression correlation coefficient for the relationship pH *vs.* ln (Koc) is -0.92, with a coefficient of determination (r^2) of 0.85. For the relationship pH *vs.* Koc, the inverse correlation coefficient is -0.79 (r^2 = 0.63). Poor correlation for the relationships K_d *vs.* organic matter, K_d *vs.* pH, and K_d *vs.* percentage clay content is indicated by reviewer-calculated r^2 values of 0.12, 0.43 and 0.001, respectively. Additional correlations (or multiple correlations) among the soil variables would be interesting to explore.

METHODOLOGY

Based on the results of a previous study (MRID 44505203) of the adsorption of uniformly phenyl ring-labeled [^{14}C]mesotrione {ZA1296; 2-(4-methyl-2-nitrobenzoyl)cyclohexane-1,3-dione; radiochemical purity >95%, specific activity 1.12 GBq/mmol; pp. 12, 13}, an adsorption equilibration period of 24 hours was chosen (p. 9). In a previous study (MRID 44505203), adsorption of the test compound to the Teflon centrifuge tubes was not observed (p. 10).

Aliquots (19 mL) of 0.01 M $CaCl_2$ solution were added to centrifuge tubes containing subsamples (10 g) of sterilized, air-dried, sieved (2 mm) Champaign (low pH; 4.6-5.0), Danville, Breeze, Martinsville, and Delavan silt loam; Valley Springs, New Holland, Clarence, and Champaign (high pH; 7.3-7.5) silty clay loam; Noblesville and Elk City loam; Osceola loamy sand; and Land O' Lakes clay loam soils (Table 1, p. 11) and the samples were pre-equilibrated overnight on a shaker (pp. 9-10). The centrifuge tubes containing the soil:solution slurries were treated with uniformly phenyl ring-labeled [^{14}C]mesotrione, dissolved in toluene and 0.01 M $CaCl_2$ solution (1 mL), at a nominal concentration of 0.2 μg/mL (pp. 12-13). Duplicate tubes were prepared for each soil type; additional tubes of 0.01 M $CaCl_2$ solution with soil were prepared as controls. The soil:solution slurries (1:2, w:v) were equilibrated by shaking for 24 hours at **20 ± 2°C**; light conditions were not reported. Following the equilibration period, soil:solution slurries were centrifuged and the supernatants decanted (p. 14). Aliquots of each supernatant were analyzed for total radioactivity by LSC; the detection limit was not reported. The remaining supernatant was stored frozen (-20 ± 5°C; duration not reported) until further analysis.

To determine compound stability during the equilibration period, supernatants (individual replicates) were thawed and concentrated to dryness (p. 15). Residues were resuspended in acetonitrile, sonicated, and analyzed by TLC using Sorbsil-C_{30} silica plates developed in chloroform:methanol:ammonia (69:27:4, v:v:v; p. 16); radioactivity on TLC plates was quantified using radioimage scanning. Samples were co-chromatographed with nonradiolabeled (method of visualization not reported) and radiolabeled reference standards.

To determine compound stability during the adsorption phase, soil samples (individual replicates) were extracted three times by shaking with methanol:0.5% concentrated hydrochloric acid (9:1, v:v), centrifuged, and the supernatant decanted (p. 15). Triplicate aliquots of the combined supernatants were analyzed for total radioactivity by LSC. Aliquots of soil extracts were placed in separating funnels with deionized water and partitioned three times into dichloromethane. The organic phase was concentrated and analyzed by TLC as described previously for the supernatants.

Triplicate subsamples of dried, post-extracted soils were analyzed for total radioactivity by LSC following combustion (p. 16); data were corrected for combustion efficiency.

DATA SUMMARY

The mobility of uniformly phenyl ring-labeled [^{14}C]mesotrione (radiochemical purity >95%), at a nominal concentration of 0.2 µg/mL, was determined in Champaign (low pH; 4.6-5.0), Danville, Breeze, Martinsville, and Delavan silt loam; Valley Springs, New Holland, Clarence, and Champaign (high pH; 7.3-7.5) silty clay loam; Noblesville and Elk City loam; Osceola loamy sand; and Land O' Lakes clay loam soil:solution slurries that were equilibrated for 24 hours at 20 ± 2°C. Freundlich K_{ads}, K_{oc}, and 1/N values could not be determined because the test compound was equilibrated at only one concentration; therefore, simple K_d and K_{oc} values were calculated. Simple K_d values were 2.3 for Osceola loamy sand (1.0% o.m.), 5.0 for Champaign (low pH) silt loam, 3.4 for Noblesville loam, 4.4 for Valley Springs silty clay loam, 1.1 for Elk City loam, 1.3 for New Holland silty clay loam, 1.6 for Danville silt loam, 1.0 for Breeze silt loam, 0.68 for Martinsville silt loam, 0.74 for Delavan silt loam, 0.63 for Clarence silty clay loam, 0.82 for Land O' Lakes clay loam (3.8% o.m.), and 0.61 for Champaign (high pH) silty clay loam (Table 3, p. 18); corresponding K_{oc} values were 390, 240, 250, 210, 110, 73, 98, 120, 90, 70, 60, 37, and 29 mL/g. The reviewer-calculated coefficient of determination (r^2) values for the relationships K_d *vs.* organic matter, K_d *vs.* pH and K_d *vs.* percentage clay content were 0.12, 0.43 and 0.001, respectively.

Data indicating the percentages of the applied radioactivity adsorbed to the 13 soils were not reported. Concentration data for adsorption of the test compound to all soils were provided (Table 5, p. 26).

Stability data (TLC) were reported for the parent compound in the supernatants and soil extracts following adsorption (Table 6, p. 28; see Comment #5). Recoveries of the parent compound from the supernatants were 92.2-99.1% for all soils. Recoveries of parent compound from the soil extracts were 60.6-96.5% (7 of 13 samples <90%) for all soils.

Material balances (across all soil types) were 88-97% of the applied radioactivity (Table 4, p. 24).

COMMENTS

1. Freundlich K_{ads}, K_{oc}, and 1/N values could not be determined because the test compound was equilibrated at only one concentration (0.2 µg/mL). Instead, only simple K_d's were reported. A minimum of four concentrations of the test compound in the soil:solution slurries are needed to calculate valid Freundlich K_{ads} values. However, this study was submitted as a supplemental study, and was designed to provide additional adsorption data for mesotrione.

2. The desorption of the test compound was not studied and K_{des} values were not reported.

3. The study authors stated that all test soils were sterilized by gamma irradiation prior to use to inhibit microbial degradation of the parent compound (p. 9). Sterilized soils may have significantly altered physical and chemical properties, which may affect the adsorption of pesticides by the soils. If the registrant chooses to use sterilized soil to study mobility, the batch equilibrium studies must include data for reference chemicals of known mobility. Results from batch equilibrium studies including reference chemicals of known mobility were not submitted.

4. Method detection limits were not reported. Both method detection limits and limits of quantitation should be reported to allow the reviewer to evaluate the adequacy of the method.

5. The test compound was stable (>90%) in the supernatants of all soils and in the soil extracts of six soils. The stability of the test compound in the soil extracts of the remaining seven soils was questionable. Recoveries of the test compound from the soil extracts were 88.6%, 60.6%, 81.3%, 61.9%, 87.2%, 80.6% and 89.1% for Noblesville loam, Valley Springs silty clay loam, Breeze silt loam, Elk City loam, Martinsville silt loam, New Holland silty clay loam and Clarence silty clay loam soils, respectively (Table 6, p. 28). The study authors stated that the main degradate observed on the TLC plates appeared to be 4-(methylsulfonyl)-2-nitrobenzoic acid (MNBA) which probably resulted from the instability of mesotrione during extraction (p. 17). The study authors further stated that it is believed that this degradation did not occur during the equilibration period. The adsorption coefficients reported by the registrant were calculated assuming that all radioactivity was present as parent (p. 18).

6. The study authors stated that the adsorption of mesotrione is inversely related to pH and directly related to soil organic matter content (p. 7). The reviewer-calculated coefficient of determination (r^2) values for the relationships K_d *vs.* organic matter and K_d *vs.* pH were 0.12 and 0.43, respectively. The study authors stated that "in more acidic soils a greater proportion of the chemical will be in the associated form leading to greater lypophilicity, and as a result a greater affinity for soil organic matter" (p. 7); the pKa of mesotrione is 3.1.

7. Data indicating the percentages of the applied radioactivity adsorbed to the soils were not provided. Generally, batch equilibrium studies include percentage of the applied radioactivity data for adsorption, desorption, and nonextractables.

8. The study authors stated (p. 9) that all 13 soils utilized in this study were the same type of soils used in an aerobic soil metabolism study (MRID 44505129).

9. The soil series names of the soils were not reported. Instead, the soils were referred to by their geographic locations or descriptions of their location (Table 1, p. 11).

10. The solubility of mesotrione in water or in the test solution was not reported.

MRID# 44505204

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Pages 7 through 13 are not included in this copy.

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