DATA EVALUATION RECORD

I. Study Type: Batch Equilibrium

II. Citation:

Rowe, D. and M.C.G. Lane. 1995. ICIA5504: Adsorption and Desorption Properties in Soil of R402173, a Major Soil Metabolite. Performed by Zeneca Agrochemicals (Zeneca Limited), Berkshire, U.K. Submitted by Zeneca Agricultural Products (Zeneca Inc.), Wilmington, Delaware. MRID 43678180.

III. Reviewer:

Name: James A. Hetrick, Ph.D. James A. Hetrick
Title: Soil Chemist 30 JUL 1996
Organization: EFGWB/EFED/OPP

IV. Approved by:

Name: Paul J. Mastradone, Ph.D. Paul J. Mastradone
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V. Conclusions:

The study provides acceptable data on 2-[6-(2-cyanophenoxy) pyrimidin-4-yloxy]phenyl}acetate (R402173) partitioning in mineral soils. These data in conjunction with batch equilibrium data (MRID 43678179 and 43678177) fulfill the aged portion of the 163-1 data requirement. No additional data are needed at this time.

Radiolabelled R402173, at 0.03 to 2.0 µg/ml, had Freundlich adsorption partitioning coefficients of 0.74 ml/g (K_{oc}=25) in a Kenny sandy loam soil, 2.0 ml/g (K_{oc}=86) in a Wisborough Green silty clay loam soil, 0.27 ml/g (K_{oc}=93) in a ERTC loamy sand soil, 4.2 ml/g (K_{oc}=200) in a NRTC silty clay loam soil, 0.65 ml/g (K_{oc}=37) in the Hyde Farm sandy clay loam soil, and 2.9 ml/g (K_{oc}=110) in the Pickett Piece clay loam soil.

The reported data indicate R402173 is expected to be mobile to very mobile in terrestrial and aquatic environments.

VI. Materials and Methods:

The test soil from the United Kingdom are described as a Hyde Farm, Pickett Piece, Kenny Hill, and Wisborough Green. The test soil from the United States soils are described as ERTC and NRTC. Physicochemical properties of the test soils are shown in Table 2. The test soils were passed through a 2 mm sieve and then sterilized with gamma radiation.

Preliminary Study

A subsample (10g) of Hyde Farm test soil was placed into each of 12 Teflon centrifuge tubes, suspended in 19 ml of sterile pesticide-free 0.1M $CaCl_2$, and then mechanically shaken for 16 hours. After pre-equilibration, ten samples of each soil type were amended with radiolabeled R402173 (cyanophenyl labeled; SA=2.32 GBq $mmol^{-1}$; radiopurity = >98%) to yield a nominal concentration of 0.17 µg/ml. The remaining two samples of each soil type were not amended with R402173 to serve as a treatment controls. Two soilless samples of 0.01M $CaCl_2$ with radiolabeled R402173 concentration of 0.17 µg/ml were used to estimate adsorption on the Teflon centrifuge tube. Samples were mechanically shaken for 2, 4, 6, 16, 24, and 48 hours.

Definitive Study

Subsamples (10g) of each soil type were placed into each of 22 Teflon centrifuge tubes, suspended in 19 ml of sterile, 0.01 CaCl2, and then mechanically shaken at 20°C for 40 hours. After pre-equilibration, four samples of each soil type were amended with radiolabeled R402173 (cyanophenyl labeled; SA=2.32 GBq $mmol^{-1}$; radiopurity = >98%) to yield nominal concentrations of 0.03, 0.08, 0.17, 0.97, and 2.0 µg/ml. The co-solvent concentration of acetonitrile was < 0.34%. (Reviewer Note: The water solubility for R402173 was not reported.) The remaining samples of each soil type were not amended with R402173 to serve as treatment controls. The samples were mechanically shaken for 40 hours at 20°C. After equilibration, the samples were centrifuged to separate soil and water phases. Duplicate samples of each soil type were retained for chemical analysis. The remaining samples were used in the desorption study. These samples were treated exactly as described in the adsorption study except the soil pellet of each sample was retained for the desorption study. The soil pellet was suspended in pesticide-free 0.01M $CaCl_2$ and then mechanically shaken for 17 hours at 20°C. Supernatant and soil were taken for chemical analysis.

Analytical

Soil samples were sequentially extracted with acetonitrile. Residues in supernatant samples were extracted using a solid phase extraction.

Soluble radiolabeled residues were separated by 1-D TLC using a hexane:ethyl acetate:glacial acetic acid 30:70:1 (v/v/v) solvent system. Soluble residues were identified by co-chromatography with known standards. The ^{14}C content in supernatant and soil extracts was determined by LSC. The ^{14}C content in extracted soil was determined by combustion-LSC.

VII. Study Author's Conclusions

A. Preliminary studies indicate radiolabeled R402173 reached a pseudo-equilibrium or steady-state condition after 16 to 24 hours of mechanical shaking (Figure 5). The registrant stated R402173 was stable in 0.01M $CaCl_2$ and soil slurries. Radiolabeled R402173 had a low adsorption potential to Teflon centrifuge tubes. (Reviewer Note: The registrant did not provide data to support the adsorption potential of radiolabeled R402173 on Teflon centrifuge tubes.)

B. The material balance of radioactivity ranged from 91 to 100% of applied R402173 in the NRTC soil and 0.17 µg/ml treatment for all other soil types (Tables 10 and 11).

C. The transformation product R402173 was stable (83% to 98% of applied) during the 57 hour batch equilibrium study (Figures 20, 21, and 22). (Reviewer Note: The registrant provided chromatograms with a single peak as evidence of a single compound. However, EFGWB notes the registrant did not provide a standard chromatogram to substantiate identification of R402173.)

D. The Freundlich adsorption coefficients of radiolabeled R402173 was 0.74 ml/g (K_{oc}=25; 1/n=0.96) in a Kenny sandy loam soil, 2.0 ml/g (K_{oc}=86; 1/n=0..93) in a Wisborough Green silty clay soil, 0.27 ml/g (K_{oc}=93;1/n=0.0.95) in a ERTC loamy sand soil, 4.2 ml/g (K_{oc}=200;1/n=0.92) in a NRTC silty clay loam soil, 0.65 ml/g (K_{oc}=37;1/n=0.0.96) in a Hyde Farm sandy clay loam soil, and 2.9 ml/g (K_{oc}=110;1/n=0.96) in the Pickett Piece clay loam soil (Table 6).

E. The registrant classified the mobility of R402173 from medium to very high according to McCall's mobility classification scale. There was an inverse relationship between soil pH and Freundlich adsorption coefficients for R402173. The registrant believes the inverse relationship can be explained by the deprotonation (hydrogen dissociation) of the carboxylic acid (pKa=3.5) functional group on R402173 in acid soils (Figure 3). The registrant stated there is a positive correlation between Freundlich adsorption coefficient of R402173 and soil clay content (Figure 4).

F. The desorption coefficient (K_{oc}) of radiolabeled R402173 was 39 ml/µg (Kd=1.3) in a Kenny sandy loam soil, 170 ml/µg (Kd=5.0) in the Wisborough Green silty clay soil, 180 ml/µg (Kd=0.57) in the ERTC loamy sand soil, 260 ml/µg (Kd=6.8) in the NRTC silty clay loam soil, 57 ml/µg (Kd=1.1) in the Hyde Farm sandy clay loam soil, and 160 ml/µg (Kd=4.4) in a Pickett Piece clay loam soil (Table 8).

VII. Reviewer's Comments

A. The USDA soil taxonomy classification of test soils was taken from MRID 4378182. EFGWB appreciates the registrant's effort to cross-reference the United Kingdom soils into USDA soil taxonomy.

B. The registrant did not provide the water solubility of R402173. EFGWB notes the water solubility of R402173 is needed to evaluate the theoretical upper bound concentration for adsorption. EFGWB believes the absence of water solubility data should not influence acceptance of the study because R402173 is expected to be mobile in terrestrial and aquatic environments.

C. The registrant provided chromatograms with a single peak as evidence of stability of R402173 during equilibration. EFGWB notes the registrant did not provide a reference chromatogram for R402173. In future studies, the registrant should provide a standard chromatogram as reference for retention time.

D. The transformation product R402173 is cross referenced as Compound 30 in registrant data submissions.

A2OXYSTROBIN

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