

DATA EVALUATION RECORD
DER 1

SHAUGHNESSY No. 029001
COMMON NAME: 1,3-Dichloropropene, 1,3-D
CHEMICAL NAME: 1,3-Dichloropropene
FORMULATION: Parent (neat)
DATA REQUIREMENT: 162-4

MRID No: 44975502
F.R. Batzer, T.J. Buehrer, D.O. Duebelbeis. November 2, 1999.
The Aerobic Aquatic Metabolism of 1,3-Dichloropropene. Performed
and Submitted by: Global Environmental Chemistry Laboratory-
Indianapolis Lab, Dow AgroSciences LLC, 9330 Zionsville Road,
Indianapolis, Indiana 46268-1054. Study ID 990031.

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Date: *1/24/00*

CONCLUSIONS:

Metabolism - (1,3-D) Aerobic Aquatic

1. Study MRID #44975502 is acceptable and satisfies the aerobic aquatic (162-4) metabolism data requirement for 1,3-Dichloropropene.
2. 1,3-Dichloropropene degraded with a relatively short half-life of 4.9 days (DT_{90} of 16.2 days with a correlation coefficient of 0.9923) in a sandy loam soil flooded with pond water, sealed, and incubated in the dark at 25C for up to 21 days. 1,3-D was at 104.1% of applied at 0 DAT (days after treatment; totaled from the carbon trap 1 and 2, aqueous phase and organic extract) 95.1% at 1 DAT, then decreased to 5.2% at 21 DAT. The degradate CAA (3-chloroallyl alcohol) gave a half-life (non-linear first order regression) of 0.3 days and a DT_{90} of 1.1 day; CAA was at 1.3% of applied at 0 DAT, increased to a maximum of 6.4% of applied at 1 DAT, then decreased slowly to 0.7% of applied by 21 DAT. The degradate cis-CAC (cis 3-chloroacrylic acid) was at 0.1% of applied at 0 DAT, increased to a maximum of 6.5% of applied by 7 DAT, then decreased slowly to 0.4% of applied by 21 DAT. The degradate trans-CAC (trans 3-chloroacrylic acid) was at 0.2% of applied by 0 DAT, increased to a maximum of 3.5% by 7 DAT then decreased to 1.0% by 21 DAT. Mineralization was moderate as up to 42.5% was reported as CO_2 by 21 DAT.

Sieved (2mm) oven dried, sandy loam soil; Bertie County North Carolina (75.6% sand, 16.8% silt, 7.6% clay, 1.13% organic matter, pH 5.9, CEC 2.89 meq/100g) was weighed (10 g) and added to incubation flasks and flooded with filtered (glass wool) pond water (total hardness 88 mg/L as CaCO₃, pH 7.4) to a total depth of 100 ml (ratio of sediment to water 1:10), including the sediment. Sample openings were covered with parafilm and pre-incubated in the dark at 25C for 3 days. Samples were not attached to an oxygen manifold to limit volatilization of parent and degradates (figure 2). A purge and trap was set up to quantify 1,3-D and CO₂ during sample analysis. After pre-incubation the flooded soils were treated with 4 ug/ml of 1,3-dichloropropene-UL¹⁴C (radiochemical purity 99%+) in acetonitrile water 1:1 v/v. Controls were fortified with 120 ul of acetonitrile water 1:1. After dosing all treated samples were sealed and placed in a 5-gallon pail containing a caustic trap to capture CO₂. The pails were sealed and placed in the dark at 25C, and duplicate samples were collected for analysis at 0, 1, 3, 7, 10, 14 and 21 days after treatment. A control sample was also collected during sampling. The analysis procedure for the treated samples emphasized recovery of volatile ¹⁴C activity with a purge and trap system consisting of two carbon traps and a caustic trap in a bubbling tower (figure 2). Once this step was completed the sediment was separated from the aqueous phase and extracted with acidified acetone. The carbon traps were extracted with acetone.

Prior to transferring samples to centrifuge bottles, the aqueous phase was assayed in triplicate by LSC. The aqueous/sediment phases were separated by centrifugation at approximately 2500 rpm for 10 minutes. The aqueous phase was re-assayed in triplicate by LSC after decanting into a bottle for storage. The second LSC assay was conducted to ascertain whether or not there was any loss of volatile ¹⁴C activity during transfers. An aliquot of the aqueous phase was filtered through a 0.44 um PTFE filter prior to HPLC analysis. The sediment was extracted with acetone 0.1 M HCL (90:10 by volume) three times for a least 20 minutes with agitation of a horizontal shaker. Samples were centrifuged at approximately 2500 rpm for 10 minutes and the extract decanted into a storage bottle. The organic extract volumes were measured in a graduated cylinder. Aliquots of the organic extracts were assayed in triplicate by LSC. Sub-samples of the extracts were concentrated prior to HPLC analyses. A harsh extraction of the sediment with 0.2 M NaOH for at least 30 minutes on a horizontal shaker was used as well. The samples were centrifuged at approximately 2500 rpm for 10 minutes. Aliquots of the caustic extracts were assayed in triplicate by LSC. For a subset of samples (with greater than 10% of applied in the caustic extract), a 1-ml aliquot of the caustic extract was treated with 250 ul of 2 M HCL and briefly shaken by hand. The samples were then centrifuged at approximately 10,000 rpm for 15 minutes. the supernatant was removed by pipette and added to a vial containing Ultima Gold XR scintillation cocktail for LSC assay. The precipitate was reconstituted in 1-ml of 0.2 N NaOH and

centrifuged at approximately 10,000 rpm for 15 minutes. The extracted sediment was air dried and then combusted over a 4-minute period. Organic extracts prior to analysis by HPLC and LSC were reduced in volume by heating in an Erlenmeyer flask with a Snyder column.

The aqueous phase of control samples was analyzed for dissolved O₂, redox potential and pH. The redox potential was measured in the sediment phase by inserting the platinum tip of the probe in the sediment phase after the aqueous phase measurement had been obtained.

DATA SUMMARY:

1,3-Dichloropropene-UL-¹⁴C (radiochemical purity 99%+), at 4 mg/L (based on a PRZM/EXAMS model (a 1,3-D concentration of 1390 ppb), degraded with a half-life (non-linear first order regression) of 4.9 days (DT₉₀ of 16.2 days with a correlation coefficient of 0.9923) in a sandy loam soil, pre-incubated for 3 days, and flooded just prior to treatment, then incubated in the dark at 25°C. 1,3-D was at 104.1% of applied at 0 DAT (days after treatment; totaled from the carbon trap 1 and 2, aqueous phase and organic extract) 95.1% at 1 DAT, 64.2% at 3 DAT, 33.7% at 7 DAT, 24.2% at 10 DAT, 16.1% at 14 DAT, 5.2% at 21 DAT.

The degradate CAA (3-chloroallyl alcohol) gave a half-life (non-linear first order regression) of 0.3 days and a DT₉₀ of 1.1 day. CAA was at 1.3% of applied at 0 DAT, increased to a maximum of 6.4% of applied at 1 DAT, then decreased slowly to 0.7% of applied by 21 DAT. The degradate cis-CAC (cis 3-chloroacrylic acid) was at 0.1% of applied at 0 DAT, increased to a maximum of 6.5% of applied by 7 DAT, then decreased slowly to 0.4% of applied by 21 DAT. The degradate trans-CAC (trans 3-chloroacrylic acid) was at 0.2% of applied by 0 DAT, increased to a maximum of 3.5% by 7 DAT then decreased to 1.0% by 21 DAT. A non-linear first order half-life for cis/trans CAC was not determined with Microsoft Excel because of the low levels involved.

The ¹⁴C activity in the aqueous phase of samples from 0, 1 and 3 DAT was subject to fluctuations in recovery during the purge and trap procedure. At 7 DAT the purge and trap was optimized and the observed decline in ¹⁴C activity in the aqueous phase from that point to the end of the study was attributed to mineralization and incorporation into soil sediment organic matter (Table 8).

The ¹⁴C activity trapped by the carbon traps declined from 79.0% of applied at 0 DAT to a low of 1.7% of applied at 21 DAT. Only 1,3-D was observed in the carbon trap extracts. The declining levels of ¹⁴C in the carbon traps was attributed to the degradation of 1,3-D into 3-chloroallyl alcohol, 3-chloroacrylic acid, other minor metabolites, CO₂, and incorporation into sediment organic matter.

The organic extractable ¹⁴C activity ranged from a low of 2.6% of

applied to a high of 9.9% of applied at 7 and 1 DAT, respectively. The caustic extraction of ^{14}C activity increased to 13.3% of applied at 21 DAT. A subset of caustic extracts of the sediment was fractionated at pH 1 into a humic and fulvic acid pool (Table 9). 61% of the caustic extractables were associated with the fulvic acid pool. Unextractable residues increased to a maximum of 16.4% of applied at 21 DAT (Table 8).

Recovery of ^{14}C activity ranged from 77.7 to 98.2% of applied ^{14}C activity. The average recovery for all samples was 91.0% of applied with a standard deviation of 5.3% of applied (Table 8).

DISCUSSION:

1. Aerobic aquatic half-lives (linear and non-linear, first order) were recalculated using Microsofts Excel 2000 with Problem Solver. Estimated half-lives were 4.9 days by linear first order and 4.6 days by non-linear first order; same as those calculated by the study investigators.
2. Linear first order half-life should be used in environmental modeling where the chemical is not directly applied to surface water. Using the non-linear first order half-life which doesn't weigh later sample points more heavily than linear regression, is more appropriate for direct applications to aquatic systems where the earlier degradation applies.
3. Combined (aqueous and sediment phase) total levels of 1,3-D, 3-chloroallyl alcohol, cis/trans 3-chloroacrylic acid were reported and not individual components from the aqueous phase and sediment phase. The study authors state that due to experimental procedures used to collect 1,3-D and CO_2 , perturbed the phase separation of 1,3-D and its metabolites between the aqueous phase and sediment phase, so that partitioning coefficients were not calculated.
4. Acetonitrile represented 0.06% by volume in the study samples.
5. The redox potential was measured in the control samples and not the treated samples because of the volatility of 1,3-D and CO_2 . In order to maintain material balance, 1,3-D treated samples were analyzed with a purge and trap procedure that alters these measurements.
6. Using the method of Currie the limit of detection and quantitation was determined to be 10 dpm and an LOQ of 40 dpm.
7. Regressions, means, standard deviations and correlation coefficients were generated using Microsoft Excel 97. The two compartment model was generated using ModelMaker version 3 Cherwell Scientific Oxford UK. Degradation kinetics calculations are found in appendix C. The DT_{50} values generated from a two compartment model gave values of 4.5, 0.3 and 7.2 days for 1,3-D,

CAA and CAC respectively.

8. The observed aerobic aquatic half-life of 1,3-D (4.9 days) is shorter than a half-life of 5.8 days observed from hydrolysis of 1,3-D in a sterile, pH 7 tris buffer at 25C (from previously reviewed 161-1 studies).

9. Two unknown degradates were observed in HPLC radiochromatograms at 5 minutes (max. of 4.1% at 7 DAT) and at 26 minutes (max. of 3.5% at 21 DAT). No attempt was made to identify these compounds.

10. The dissolved oxygen levels slowly declined from 6.00 to 2.32 mg/L at 1 and 21 DAT, respectively (figure 4). The redox potential in the aqueous phase declined from 230.9 mV at 1 DAT to 105.4 mV at 21 DAT and that of the sediment steadily declined from 239.0 mV at 1 DAT to 83.4 mV at 21 DAT. The pH of the aqueous phase was 6.43 at 0 DAT, then dropped to 6.14 at 1 DAT and then rose to 6.87 at 21 DAT.

DER for MRID 44975302 - (EFE)

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