
Test Material:	3,4-Dichloroaniline (transformation product of propanil)
MRID	47165602
Title:	Penketh, S. 2004. Propanil metabolite adsorption/desorption in three soils.
EPA PC Code:	028201
OCSPP Guideline:	835.1230

For Cambridge Environmental

Primary Reviewer: Kindra Bozicevich **Signature:** 

Date: 1/19/12

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Date: 1/19/12

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Date: 1/19/12

IIA 7.5 Determination of Adsorption and Desorption of 3,4-Dichloroaniline, a Transformation Product of Propanil, Using the Batch Equilibrium Method.

The adsorption/desorption of 3,4-dichloroaniline, a transformation product of propanil, was studied in three European soils at measured test concentrations of 0.49-54.8 mg a.i./kg soil or 0.098-10.2 mg a.i./kg soil in the dark at *ca*. 20°C for up to 24 hours.

Report:	Penketh, S. 2004. Propanil metabolite adsorption/desorption in three soils. Unpublished study performed by Huntingdon Life Sciences, Ltd., Cambridgeshire, England; submitted by Propanil Consortium, Washington, DC. Project Identity JSV/012. Experimental initiation June 16, 2003 and completion September 18, 2003 (p. 11). Final report issued May 12, 2004.
Document No.:	MRID 47165602
Guideline:	Conducted under: OECD Guideline 106 Reviewed under: OCSPP 835.1230
Statements:	The study was conducted in accordance with UK GLP Regulations 1999, EC Commission Directive 1999/11/EC, and OECD Principles of Good Laboratory Practice ENV/MC/CHEM(98)17 (pp. 3, 6). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided. A Certification of Authenticity was not provided.
Classification:	This study is classified as supplemental. Deviations from the objectives of USEPA guidelines included: the study was conducted using 3,4-Dichloroaniline, a transformation product of the parent compound propanil. Mass balances were incomplete. It was not established that the foreign soils used in this study were comparable to soils that would be found at the intended use sites in the United States, and only two types of soil were represented. There are calculation errors in the last column of Table 2-4, % applied adsorbed.
PC Code:	028201 (Propanil) and 600166 (3,4-Dichloroaniline)
EPA Reviewer:	He Zhong, Ph.D. Biologist Signature: Date: 2/27/2012

Executive Summary

The adsorption/desorption characteristics of [phenyl-U-^{14}C]3,4-dichloroaniline (3,4-DCA) were studied using a sandy clay loam soil [Elmton; pH 7.4; organic carbon 5.9%] from the United Kingdom, a sandy clay loam soil [Marques de Tamarit; pH 7.5; organic carbon 0.5%] from Spain, and a loamy sand soil [Pavia; pH 6.7, organic carbon 0.6%] from Italy in a batch equilibrium experiment. The adsorption phase of the study was carried out by equilibrating soil with 3,4-DCA at measured test concentrations of 0.49, 1.02, 2.63, 10.5, 54.8 mg a.i./kg soil for the Elmton sandy clay loam soil in the dark at *ca*. 20°C for 24 hours and 0.098, 0.204, 0.532, 2.0, 10.2 mg a.i/kg soil for the Marques de Tamarit sandy clay loam and Pavia loamy sand soils in the dark at *ca*. 20°C for 8 hours. The equilibrating solution used was 0.01M $CaCl_2$ solution, with soil solution ratios of 1:10 (w:v) for the Elmton sandy clay loam soil and 1:2 (w:v) for the Marques de Tamarit sandy clay loam and Pavia loamy sand soils. The desorption phase of the study was carried out by replacing the

adsorption solution with an equivalent volume of 0.01M $CaCl_2$ solution and equilibrating for 8 or 24 hours. Two desorption steps (24 hours per step for the Elmton sandy clay loam soil and 8 hours per step for the Marques de Tamarit sandy clay loam and Pavia loamy sand soils) were conducted for all test soils. Adsorption and desorption supernatants were analyzed using LSC. High-dose adsorption supernatants and concentrated soil extracts were quantified using HPLC.

Based on HPLC analysis of the high-dose adsorption supernatants and soil extracts, 3,4-DCA comprised >94% of the recovered radioactivity in the samples. Following the second desorption step, 3,4-DCA was stable in the high-dose Elmton sandy clay loam soil aqueous solutions and extracts, accounting for >96% of the recovered radioactivity, but showed degradation in the remaining high-dose soil aqueous solutions and extracts, accounting for 4.9-21.8% and 30.2-61.5% of the recovered radioactivity, respectively.

At the end of the adsorption phase, mass balances for 3,4-DCA residues in high-dose soils were 92.4% of the applied radioactivity for the Elmton sandy clay loam soil, 95.0% of the applied for the Marques de Tamarit sandy clay loam soil, and 98.0% of the applied for the Pavia loamy sand soil. At the end of the adsorption and two desorption phases, mass balances for 3,4-DCA residues in high-dose soils ranged from 96.2-96.9% of the applied radioactivity for the Elmton sandy clay loam soil, 93.0-95.6% of the applied for the Marques de Tamarit sandy clay loam soil, and 94.9-96.2% of the applied for the Pavia loamy sand soil.

Following 24 hours of equilibration, a maximum of 90.5% of the applied was adsorbed to the Elmton sandy clay loam soil. Following 8 hours of equilibration, maximums of 62.3% and 78.9% of the applied were adsorbed to the Marques de Tamarit sandy clay loam and Pavia loamy sand soils, respectively. Percent desorbed as % of the adsorbed could not be determined from the available data.

Table 1. Results Synopsis.

Soil type:		**Elmton Sandy clay loam**	**Marques de Tamarit Sandy clay loam**	**Pavia Loamy sand**
Adsorption				
Average K_d		69.8 ± 26.7	2.4 ± 0.9	5.3 ± 1.9
Average K_{oc}		1182	488	883
Regression	K_d	35.2	1.4	3.0
	Freundlich K_F	36.7	1.67	3.3
Freundlich K_{Foc}		622	334	548
Desorption 1				
Average K_d		112.9	6.8	12.9
Average K_{oc}		Not reported.	Not reported.	Not reported.
Freundlich K_F		44.0	3.93	5.57
Freundlich K_{Foc}		746	786	928
Desorption 2				
Average K_d		197.6	123.5	58.7
Average K_{oc}		Not reported.	Not reported.	Not reported.
Freundlich K_F		64.2	68.2	32.3
Freundlich K_{Foc}		1090	13600	5380

I. Materials and Methods

A. Materials

1. Test Material: [Phenyl-U-^{14}C]3,4-dichloroaniline (p. 12).
Radiopurity: >97%.
Specific activity: 20.8 mCi/mmol; 4.75 MBq/mg.
Batch number: NPE/HLS247/3.

2. Reference

Compounds: 3,4-Dichloroaniline (p. 13).
Purity: 98.8%.
Batch number: HB011667. 3.

3. Soil Characteristics

Table 2. Description of Soil Collection and Storage.

Description	Elmton Sandy clay loam	Marques de Tamarit Sandy clay loam	Pavia Loamy sand
Geographic location	Worcestershire, UK	Catalunya, Spain	Cascina Vallaza, Italy
Pesticide use history at the collection site	Not reported.		
Collection procedures	Not reported.		
Sampling depth (cm)	Not reported.		
Storage conditions	Not reported.		
Storage length	Not reported.		
Soil preparation	Sieved (2 mm).		

Data were obtained from pp. 13-14 and Table 1, p. 26 of the study report.

Table 3. Properties of the Soils.

Property		Elmton	Marques de Tamarit	Pavia
Soil texture (USDA)[1]		Sandy clay loam	Sandy clay loam	Loamy sand
% Sand		50.32	54.78	81.70
% Silt		25.50	24.61	13.30
% Clay		24.19	20.61	5.00
pH	Water	8.2	8.0	6.8
	0.01M $CaCl_2$	7.4	7.5	6.7
Organic carbon (%)		5.9	0.5	0.6
Organic matter (%)		10.1	0.9	1.0
CEC (meq/100 g)		32.2	6.2	4.0
Moisture at 0.33 bar (%)		Not reported.		
Bulk density (g/cm^3)		Not reported.		
Microbial Activity (CFU/g)		Not reported.		
Soil taxonomic classification		Not reported.		
Soil mapping unit (for EPA)		Not reported.		

Data were obtained from Table 1, p. 26 of the study report.
1 Textural classifications were confirmed by the reviewer using the NRCS soil texture calculator which calculates texture based on the percent sand and clay.

1. Preliminary study: Preliminary tests were conducted using the Elmton sandy clay loam soil at a nominal test concentration of 50 mg a.i./kg to determine the soil:solution ratios and equilibration times to be used in the definitive study and adsorption of the test substance to the surface of the test containers (p. 15). The results indicated that the definitive study should be conducted using a soil

solution ratio of 1:10 (w:v) and an equilibration time of 24 hours for the Elmton sandy clay loam soil, and a soil:solution ratio of 1:2 (w:v) and an equilibration time of 8 hours for the Marques de Tamarit sandy clay loam and Pavia loamy sand soils (p. 22). There was no significant adsorption (<2%) of the test substance to the glass test containers.

2. Definitive study experimental conditions:

Table 4. Study Design for the Adsorption Phase.

Parameters		**Elmton Sandy clay loam**	**Marques de Tamarit Sandy clay loam**	**Pavia Loamy sand**
Condition of soil (air dried/fresh)[1]		Air-dried.	Air-dried.	Air-dried.
Have these soils been used for other laboratory studies? (specify which)		No.		
Soil (g/replicate)		2	10	10
Equilibrium solution used (eg: 0.01N $CaCl_2$)		0.01M $CaCl_2$		
Control used (with salt solution only) (Yes/No)		Yes.		
Test material concentrations[2]	Nominal application rates (mg a.i./kg soil)	0.5, 1.0, 2.5, 10.0, 50.0	0.1, 0.2, 0.5, 2.0, 10.0	0.1, 0.2, 0.5, 2.0, 10.0
	Analytically measured concentrations (mg a.i./kg soil)	0.49, 1.02, 2.63, 10.5, 54.8	0.098, 0.204, 0.532, 2.0, 10.2	0.098, 0.204, 0.532, 2.0, 10.2
Identity and concentration of co-solvent, if any		Ethyl acetate, final concentration of 0.1% (v:v) for two highest test concentrations. Ethyl acetate:ethanol (95:5, v:v), final concentration of 0.1% (v:v) for remaining test concentrations.		
Soil:solution ratio (w:v)		1:10	1:2	1:2
Initial pH of the equilibration solution, if provided		Not reported.		
No. of replications	Controls	Duplicate.		
	Treatments	Duplicate. Triplicate at highest test concentration.		
Equilibration	Time	24	8	8
	Temperature (°C)	*ca.* 20		
	Darkness (Yes/No)	Yes		
	Shaking method	Orbital shaker		
	Shaking time	24	8	8
Method of separation of supernatant (eg., centrifugation)		Centrifugation		
Centrifugation	Speed (rpm)	2600		
	Duration (min)	45-49		
	Method of separation of soil and solution	Decanted.		

Data were obtained from pp. 13-15 and Appendix 2, p. 45 of the study report.
1 Soils were pre-equilibrated by shaking with *ca.* 19 mL 0.01M $CaCl_2$ solution in the dark at 20-25°C for *ca.* 18 hours.
2 Test material concentrations were calculated by the reviewer by converting µg/mL to mg a.i./kg using the following

equation: [test concentration (µg/mL) × total volume of test material (mL)] ÷ amount of soil (g); e.g. lowest test concentration Elmton sandy clay loam soil [0.05 µg/mL × 20 mL] ÷ 2 g = 0.5 mg a.i./kg soil.

Table 5. Study Design for the Desorption Phase.

Parameters		**Elmton Sandy clay loam**	**Marques de Tamarit Sandy clay loam**	**Pavia Loamy sand**
Were the soil residues from the adsorption phase used? If not, describe the method for adsorption using a separate adsorption		Yes		
Amount of test material present in the adsorbed state/adsorbed amount (mg a.i./kg soil)	0.5/0.1	0.4211	0.06079	0.07704
	1.0/0.2	0.8680	0.1213	0.1561
	2.5/0.5	2.200	0.3018	0.3913
	10.0/2.0	8.275	0.8920	1.295
	50.0/10.0	40.02	4.12	6.008
No. of desorption steps		2		
Equilibration solution and quantity used per treatment for desorption (eg., 0.01M $CaCl_2$)		0.01M $CaCl_2$; 20 mL		
Soil:solution ratio (w:v)		1:10	1:2	1:2
Replications	Controls	Duplicate.		
	Treatments	Duplicate.		
Desorption equilibration	Time	24	8	8
	Temperature (°C)	*ca*. 20		
	Darkness	Yes.		
	Shaking method	Orbital shaker		
	Shaking time	24	8	8
Centrifugation	Speed (rpm)	2600		
	Duration (min)	45-49		
	Method of separation of soil and solution	Decanted.		

Data were obtained from pp. 14, 16 and Tables 2-4, pp. 27-29 of the study report.

3. Description of analytical procedures:

Extraction/clean up/concentration methods: For each soil type treated at the highest test concentration, one soil sample collected after adsorption and two samples collected after the desorption phases were extracted three times with acetonitrile by sonicating for 15 minutes and then shaking for 20 minutes (p. 17). The extracts were separated by centrifugation, pooled (10% by volume), reduced under nitrogen, and dissolved in acetonitrile prior to analysis using HPLC.

Total ^{14}C measurement: Duplicate aliquots of the adsorption and desorption supernatants were analyzed for total radioactivity using LSC (p. 16).

Non-extractable residues, if any: Extracted soils were air-dried, homogenized, and combusted prior to analysis using LSC (p. 17).

Derivatization method, if used: A derivatization method was not employed in this study.

Identification and quantification of parent compound: High-dose adsorption and desorption supernatants and concentrated soil extracts were analyzed for 3,4-DCA using reversed phase HPLC (Solvent A: acetonitrile containing 0.1% H_3PO_4; Solvent B: water containing 0.1% H_3PO_4) with UV (254 nm) and radio detection (pp. 16-19). The samples were co-chromatographed with an unlabeled reference substance of 3,4-DCA.

Detection limits (LOD, LOQ) for the parent compound: Limits of detection (LOD) and quantitation (LOD) were not reported.

II. Results and Discussion

A. Test Conditions: The experimental temperature employed during the study was reported to be maintained at *ca*. 20°C; supporting details were not provided. Based on HPLC analysis of the high-dose adsorption supernatants and soil extracts, 3,4-DCA comprised >94% of the recovered radioactivity in the samples (p. 23; Table 12, p. 37). Following the second desorption, 3,4-DCA was stable in the high-dose Elmton sandy clay loam soil aqueous solutions and extracts, accounting for >96% of the recovered radioactivity, but showed degradation in the remaining high-dose soil aqueous solutions and extracts, accounting for 4.9-21.8% and 30.2-61.5% of the recovered radioactivity, respectively (Table 13, p. 38).

B. Mass Balance: At the end of the adsorption phase, mass balances for 3,4-DCA residues in high-dose soils were 92.4%, 95.0%, and 98.0% of the applied radioactivity for the Elmton sandy clay loam, the Marques de Tamarit sandy clay loam soil, and the Pavia loamy sand soils, respectively (Table 10, p. 35).

At the end of the adsorption and two desorption phases, mass balances for 3,4-DCA residues in high-dose soils ranged from 96.2-96.9% of the applied radioactivity for the Elmton sandy clay loam soil, 93.0-95.6% of the applied for the Marques de Tamarit sandy clay loam soil, and 94.9-96.2% of the applied for the Pavia loamy sand soil (Table 11, p. 36).

Table 6a. Recovery of 3,4-DCA Residues, Expressed as Percentage of Applied Radioactivity, in High-Dose Soils after Adsorption (n = 1).

Matrices	Elmton Sandy clay loam	Marques de Tamarit Sandy clay loam	Pavia Loamy sand
At the end of the adsorption phase			
Supernatant solution	19.2	44.8	33.8
Solid phase (extracted)	48.0	47.3	54.2
Non-extractable residues in soil, if measured	25.2	2.9	10.0
Total recovery	92.4	95.0	98.0
At the end of the desorption phase			
Supernatant solution	Not determined.		
Solid phase (extracted)	Not determined.		
Non-extractable residues in soil, if measured	Not determined.		
Total recovery	Not determined.		

Data were obtained from Table 10, p. 35 of the study report.

Table 6b. Recovery of 3,4-DCA Residues, Expressed as Percentage of Applied Radioactivity, in High-Dose soils after Adsorption/Desorption (n = 2).

Matrices	Elmton Sandy clay loam	Marques de Tamarit Sandy clay loam	Pavia Loamy sand
At the end of the adsorption phase			
Supernatant solution	20.0, 19.6	45.3, 44.3	32.2, 32.4
Solid phase (extracted)	Not determined.		
Non-extractable residues in soil, if measured	Not determined.		
Total recovery	Not determined.		
At the end of the desorption phase			
Supernatant solution Desorption 1	12.0, 11.6	14.9, 14.6	16.5, 15.5
Supernatant solution Desorption 2	6.6, 6.7	3.4, 3.7	5.0, 3.5
Solid phase (extracted)	24.4, 24.5	14.7, 16.8	21.7, 18.4
Non-extractable residues in soil, if measured	33.0, 34.5	17.3, 13.6	20.8, 25.1
Total recovery	96.2, 96.9	95.6, 93.0	96.2, 94.9

Data were obtained from Table 11 p. 36 of the study report.

Table 7. Concentration of 3,4-DCA Residues in the Solid and Liquid Phases at the End of Adsorption (n = 2).

Concentration (mg a.i./kg soil)	**Elmton Sandy clay loam**		
	on soil (mg a.i./kg)	**in solution (µg a.i./mL)**	**% adsorbed**
0.49	0.4211	0.00441	85.9
1.02	0.8680	0.01051	85.1
2.63	2.200	0.03118	83.7
10.5	8.275	0.1708	78.8
54.8	40.02	1.223	73.0
Concentration (mg a.i./kg soil)	**Marques de Tamarit Sandy clay loam**		
	on soil (mg a.i./kg)	**in solution (µg a.i./mL)**	**% adsorbed**
0.098	0.06079	0.01808	62.0
0.204	0.1213	0.04108	59.5
0.532	0.3018	0.1130	56.7
2.0	0.8920	0.5436	44.6
10.2	4.12	2.982	40.4
Concentration (mg a.i./kg soil)	**Pavia Loamy sand**		
	on soil (mg a.i./kg)	**in solution (µg a.i./mL)**	**% adsorbed**
0.098	0.07704	0.01015	78.6
0.204	0.1561	0.02405	76,5
0.532	0.3913	0.0694	73.6
2.0	1.295	0.3472	64.8
10.2	6.008	2.063	58.9

Data were obtained from Tables 2-4, pp. 27-29 of the study report.

Table 8. Concentration of 3,4-DCA Residues in the Solid and Liquid Phases at the End of the Second Desorption Phase (n = 2).

Concentration (mg a.i./kg soil)	Elmton Sandy clay loam		
	on soil (mg a.i./kg)	in solution (μg a.i./mL)	% desorbed as % of the adsorbed
0.49	0.4078	0.001352	ND
1.02	0.7868	0.003145	ND
2.63	2.075	0.009301	ND
10.5	7.408	0.05326	ND
54.8	32.24	0.4405	ND
Concentration (mg a.i./kg soil)	**Marques de Tamarit Sandy clay loam**		
	on soil (mg a.i./kg)	**in solution (μg a.i./mL)**	**% desorbed as % of the adsorbed**
0.098	0.01591	0.0001444	ND
0.204	0.03229	0.0002321	ND
0.532	0.08316	0.0004916	ND
2.0	0.2378	0.002309	ND
10.2	1.1101	0.01180	ND
Concentration (mg a.i./kg soil)	**Pavia Loamy sand**		
	on soil (mg a.i./kg)	**in solution (μg a.i./mL)**	**% desorbed as % of the adsorbed**
0.098	0.04192	0.0006223	ND
0.204	0.08416	0.001158	ND
0.532	0.2055	0.003379	ND
2.0	0.6217	0.01476	ND
10.2	2.902	0.06044	ND

Data were obtained from Tables 6-8, pp. 31-33 of the study report.
ND = Not determined.

Table 9. Reviewer-Calculated Adsorption Constants of 3,4-DCA in the Soils.

Soil	Adsorption										
	K_d (average and SD)	Regression Analysis			K_{oc}	Regression Analysis					K_{Foc}
		K_d	r^2	p-value		K_F	p-value	r^2	1/n	p-value	
Elmton Sandy clay loam	69.8 ± 26.7	35.2	0.9948	1.01E-05	1182	36.7	6.44E-07	0.9998	0.81	1.20E-06	622
Marques de Tamarit Sandy clay loam	2.4 ± 0.9	1.4	0.9976	2.16E-06	488	1.67	0.002	0.9982	0.82	3.24E-05	334
Pavia Loamy sand	5.3 ± 1.9	3.0	0.9968	3.75E-06	883	3.3	4.97E-05	0.9994	0.82	5.99E-06	548

Data were obtained from DER Attachment 2.

K_d values were reviewer-calculated using Equation 2 as follows: $K_d = [(C_0V_0-C_{aq}V_0)/m]/C_{aq}$, where

K_d = adsorption coefficient (mL/g);
C_0= Initial mass concentration of the test solution in contact with the soil (µg/mL);
V_0 = Initial volume of the aqueous phase in contact with the soil during the adsorption test (mL);
C_{aq} = mass concentration of the test substance in the aqueous phase at adsorption equilibrium (µg/mL); and
m = quantity of the soil phase, expressed in dry mass of soil (g).

K_{oc} values were reviewer-calculated using Equation 3 as follows: $K_{oc} = (K_d/OC\%) \times 100$, where

Koc = organic carbon normalized adsorption coefficient (mL/g);
K_d = adsorption coefficient (mL/g); and
OC% = percent organic carbon in the soil.

K_F values were reviewer-calculated using Equation 5 as follows: $(C_0V_0-C_{aq}V_0)/m = K_F \times (C_{aq})^{1/n}$; where

C_0= Initial mass concentration of the test solution in contact with the soil (µg/mL);
V_0 = Initial volume of the aqueous phase in contact with the soil during the adsorption test (mL);
C_{aq} = mass concentration of the test substance in the aqueous phase at adsorption equilibrium (µg/mL);
m = quantity of the soil phase, expressed in dry mass of soil (g);
K_F = Freundlich adsorption coefficient $(\mu g/g)/(\mu g/mL)^{1/n}$; and
1/n = Freundlich exponent.

K_{Foc} values were reviewer-calculated using Equation 6 as follows: $K_{Foc} = (K_F/OC\%) \times 100$, where

K_{Foc} = organic carbon normalized Freundlich adsorption coefficient $(\mu g/g \text{ organic carbon})(\mu g/mL)^{1/n}$;
K_F = Freundlich adsorption coefficient $(\mu g/g)(\mu g/mL)^{1/n}$; and
OC% = percent organic carbon in the soil.

Table 10. Study Author-Calculated Constants of 3,4-DCA in the Soils Following Desorption.

Soil	Desorption 1					
	K_d	K_F	1/n	r^2	K_{oc}	K_{Foc}
Elmton Sandy clay loam	112.9	44.0	0.78	NR	NR	746
Marques de Tamarit Sandy clay loam	6.8	3.93	0.85	NR	NR	786
Pavia Loamy sand	12.9	5.57	0.78	NR	NR	928
Soil	**Desorption 2**					
	K_d	K_F	1/n	r^2	K_{oc}	K_{Foc}
Elmton Sandy clay loam	197.6	64.2	0.76	NR	NR	1090
Marques de Tamarit Sandy clay loam	123.5	68.2	0.92	NR	NR	13600
Pavia Loamy sand	58.7	32.3	0.89	NR	NR	5380

Data were obtained from Table 9, p. 34 of the study report and DER Attachment 2.
NR = Not reported.
K_d - Adsorption and desorption coefficients; K_F - Freundlich adsorption and desorption coefficients; 1/n - Slope of Freundlich adsorption/desorption isotherms; K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon); r^2 - Regression coefficient of Freundlich equation.

C. ADSORPTION: Following 24 hours of equilibration, a maximum of 90.5% of the applied was adsorbed to the Elmton sandy clay loam soil (Table 2, p. 27). Following 8 hours of equilibration, maximums of 62.3% and 78.9% of the applied was adsorbed to the Marques de Tamarit sandy clay loam and Pavia loamy sand soils, respectively (Tables 3-4, pp. 28-29).

D. DESORPTION: Percent desorbed as % of the adsorbed could not be determined from the available data.

III. Study Deficiencies and Reviewer's Comments

1. This preliminary study (Tier 1) was conducted using a transformation product of the parent compound propanil.

2. Mass balances were incomplete. Mass balance data were provided for the soils dosed at the highest test concentration only. Material balances should be provided for all test soil/test concentration combinations.

3. It was not established that the foreign soils used in this study were comparable to soils that would be found at the intended use sites in the United States.

4. Only two types of soil and three soil locations were represented, sandy clay loam and loamy sand and United Kingdom, Spain and Italy respectively. Five soils at one concentration are needed for a Tier 2 study for the adsorption kinetics test. Five test substance concentrations

are needed for a Tier 3 study for the adsorption isotherms and desorption kinetics/desorption isotherms. The characteristics of the soils should be sufficiently different so as to represent full spectrum of the types of soil representative of the proposed use areas.

5. Single samples of the high-dose aqueous solutions and soil extracts for each test soil were analyzed for 3,4-DCA following the adsorption phase (study report Table 12, p, 37). It is preferred that duplicate samples be analyzed to obtain a more accurate determination of the data.

6. Using the Standardized Soil Mobility Classification Guidance according to the Food and Agriculture Organization (FAO) of the United Nations adopted by USEPA and using reviewer calculated adsorption K_{oc} values presented in Table 9, 3,4-DCA is characterized as being moderately to slightly mobile in the test soils. Based on the McCall scale, the study author determined that 3,4-DCA would be of low to medium mobility (p. 24).

7. The following K_F values were calculated by the study author:

Table 11. Study Author-Calculated Constants of 3,4-DCA in the Soils.

Soil	Adsorption					
	K_d	**K_F[1]**	**1/n**	**r^2**	**K_{oc}**	**K_{Foc}**
Elmton Sandy clay loam	69.8	34.5	0.81	NR	NR	585
Marques de Tamarit Sandy clay loam	2.4	1.63	0.81	NR	NR	326
Pavia Loamy sand	5.3	3.26	0.81	NR	NR	543

Data were obtained from Table 5, p. 30 of the study report and DER Attachment 2.
K_d - Adsorption and desorption coefficients; K_F - Freundlich adsorption and desorption coefficients; 1/n - Slope of Freundlich adsorption/desorption isotherms; K_{oc} - Coefficient adsorption per organic carbon (K_d or K x 100/% organic carbon); r^2 - Regression coefficient of Freundlich equation.
1 Freundlich adsorption K_F values were calculated by the study author using the following equation (p. 20 of the study report):

$\log (C^{ads}_s) = \log K^{ads}_F + 1/n \log C^{ads}_{aq}$, where
C^{ads}_s = soil concentration after adsorption (μg/g);
C^{ads}_{aq} = concentration of supernatant after adsorption (μg/mL);
1/n = exponential constant or slope; and
K^{ads}_F = Freundlich adsorption constant.

8. The following values for adsorption K_d vs. % organic carbon, pH, % clay, and CEC were calculated by the reviewer:

Table 12. Reviewer-Calculated Adsorption Regression for 3,4-DCA.

Parameter	Adsorption- Regression Analysis				
	Slope	**p-value**	**Intercept**	**p-value**	**r^2**
Kd vs. % organic carbon	0.081	0.014	0.237	0.183	0.9995
Kd vs. pH	0.004	0.764	7.093	0.039	0.1315
Kd vs. % clay	0.165	0.578	12.342	0.385	0.3782
Kd vs. CEC	0.410	0.069	3.551	0.297	0.9884

Data were obtained from DER Attachment 2.

IV. References

1. U.S. Environmental Protection Agency. 2003. Guidance for Calculating Sorption Coefficients in Batch Equilibrium Studies.

2. U.S. Environmental Protection Agency. 2006. Standardized Soil Mobility Classification Guidance.

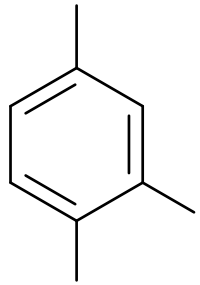
3. U.S. Environmental Protection Agency. 2008. Fate, Transport and Transformation Test Guidelines, OCSPP 835.1230, adsorption/desorption (batch equilibrium). Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-08-019.

4. U.S. Environmental Protection Agency. 2009. Technical Advisory: Calculation and reporting of Partition Coefficient Data from Batch Equilibrium Experiments.

5. U.S. Environmental Protection Agency. 2009. Technical Direction on the Preparation of Data Evaluation Records (DER).

6. NRCS. Soil texture calculator. Available at: http://soils.usda.gov/technical/aids/investigations/texture/.

DER ATTACHMENT 1. 3,4-DCA (Transformation Product of Propanil). [A]

Code Name/ Synonym	Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)	Final %AR (study length)
PARENT						
3,4-DCA	3,4-Dichloroaniline **Formula:** $C_6H_5C1_2N$ **MW:** 162.02 g/mol **SMILES:** c1cc(c(cc1N)Cl)Cl		835.1230 Batch equilibrium	47165602	NA	NA
MAJOR (>10%) TRANSFORMATION PRODUCTS						
No major transformation products were identified.						
MINOR (<10%) TRANSFORMATION PRODUCTS						
No minor transformation products were identified.						
REFERENCE COMPOUNDS NOT IDENTIFIED						
All compounds used as reference compounds were identified.						

[A] AR means “applied radioactivity”. MW means “molecular weight”. NA means "not applicable".

Attachment 2: Statistics Spreadsheets and Graphs