sTest Material:	R613636 (Transformation product of Chlorothalonil)
MRID	49342705
Title:	Blair, L. R613636. R613636 - Adsorption/Desorption Properties in Five Soils. Final Report.
EPA PC Code:	081901 (for Chlorothalonil)
OCSPP Guideline:	835.1230

For CDM Smith

Primary Reviewer: Teresa Nelis **Signature:** Teresa Nelis

Date: 9/25/14

Secondary Reviewer: Kindra Bozicevich **Signature:** Kindra Bgwich

Date: 9/25/14

QC/QA Manager: Joan Gaidos **Signature:** Joan S S

Date: 9/25/14

Adsorption and desorption of R613636, transformation product of chlorothalonil, in five soils.

Report:	MRID 49342705. Blair, L. 2014. R613636. R613636 – Adsorption/Desorption Properties in Five Soils. Final Report. Unpublished study performed by Charles River, Preclinical Services, Tranent, Edinburgh, UK; sponsored and submitted by Syngenta Crop Protection, LLC, Greensboro, NC. Report Number 35043. Study Number 222269. Task Number TK0046550. Experimental initiation September 19, 2013 and completion February 13, 2014 (p. 5). Study completion date March 13, 2014.
Document No.:	MRID 49342705
Guideline:	OCSPP 835.1230
Statements:	The study was conducted in accordance with OECD Principles of GLP (p. 3). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-4). A Certification of Authenticity statement was not provided.
Classification:	This study is Acceptable. Minor deficiencies include determining mass balances and stability tests on select samples rather than across all soils and test concentrations.
PC Code:	081901 (for chlorothalonil)
Reviewer:	Sheng Lin, Ph.D. Physical Scientist

Signature: SHENG LIN
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Date: 2020.12.28 12:37:41 -05'00'
Date: 11/14/19

Executive Summary

In a batch equilibrium study, two U.S. soils and three European soils (pH range 6.2 to 8.2) were used to measure sorption of [^{14}C]-R613636, a transformation product of chlorothalonil, in darkness at 20 ± 2°C. Determined Freundlich Adsorption Coefficient (K_F) values ranged from 2.3 to 8.1 L/kg (mean K_F = 4.5 L/kg); respective K_{FOC} values ranged from 130 to 325 L/kg (mean K_{FOC} = 246 L/kg).[1] Freundlich Desorption Coefficients ($K_{F\text{-}des}$) (ranged 1.7 to 8.3 L/kg, mean K_F = 4.1 L/kg) were similar to the corresponding Freundlich Adsorption Coefficients, indicating that sorption of R613636 was relatively reversible. Percent adsorption ranged from 18.1 to 66.4% across all test soils, and percent desorption, as percent of the adsorbed, ranged from 21.9 to 79.6% across all test soils. Relatively moderate Freundlich Adsorption Coefficients and percent adsorption indicate R613636 was not strongly adsorbed to the soils tested. Freundlich exponents corresponding to adsorption K_F values ranged from 0.81 to 0.91 across all test soils, indicating sorption data was slightly non-linear, i.e. sorption was not independent of the test substance concentration.

[1] Sorption is a generic term that applies to absorption, adsorption, and desorption processes. Adsorption refers to sorption onto a two-dimensional surface; absorption refers to sorption into a three dimensional matrix. Both types of sorption occur in soils and sediments. Desorption refers to a sorbate becoming desorbed from a sorbent. Desorption distribution coefficients are measured by removing solution from a sorption experiment and adding fresh solution, so that all material measured in solution will be the desorbed material. The guideline uses the term adsorption in place of sorption and refers to the initial measurement of sorption.

Table 3 summarizes the adsorption coefficients measured in the study. **Table 4** summarizes the desorption coefficients measured in the study.

Mass balances ranged from 101.7 to 107.2% of the applied radioactivity for select samples. TLC analysis of select samples showed that [^{14}C]-R613636 was stable, accounting for ≥ 99.4% in the adsorption and desorption phases and soil extracts.

Coefficients of variation (CV) were 0.6 and 0.3 across all [^{14}C]-R613636 treated soils for adsorption K_F and K_{Foc}, respectively, and 0.7 and 0.4 across all [^{14}C]-R613636 treated soils for desorption K_F and K_{Foc}, respectively. K_{Foc} would be a better predictor of sorption across soils.

Results Synopsis:

Table 1. Summary of Adsorption/Desorption Results[A]

Soil/ Sediment, % OC pH	Regressed K_d (L/kg-soil)			Range of K_d (L/kg-soil)	Regressed K_{OC} (L/kg-OC)	K_F ((L/kg-soil)$^{-1/n}$)			1/n for adsorption	K_{FOC} (L/kg-OC)$^{-1/n}$)	Ceq Range (mg/L)
	Value ± SE	r^2	p-value		Value ± SE	Value ± SE	r^2	p-value	Value ± SE	Value ± SE	
Adsorption											
North Dakota Sandy loam (2.5% OC, pH 7.7)	8.7 ± 0.3	0.989	3.4E-10	7.8-18.3	349 ± 12	8.1 ± 1.0	0.998	6.8E-12	0.86 ± 0.0	325 ± 41	0.004-0.625
White Swan Loam (1.2% OC, pH 6.4)	3.8 ± 0.1	0.995	1.7E-11	3.4-6.3	314 ± 8	3.7 ± 1.0	0.998	8.1E-11	0.89 ± 0.0	307 ± 86	0.007-0.829
Marsillargues Silty Clay (1.0% OC, pH 8.2)	2.3 ± 0.1	0.988	7.2E-10	2.0-4.0	228 ± 9	2.3 ± 1.1	0.994	3.8E-07	0.88 ± 0.0	232 ± 106	0.008-0.938
18 Acres Sandy clay loam (2.5% OC, pH 6.2)	5.9 ± 0.2	0.992	7.7E-11	5.5-9.0	237 ± 7	5.9 ± 1.0	0.997	1.3E-10	0.91 ± 0.0	237 ± 42	0.006-0.719
Gartenacker Loam (1.9% OC, pH 7.7)	2.6 ± 0.1	0.991	2.1E-10	2.4-6.1	136 ± 4	2.5 ± 1.0	0.997	5.2E-09	0.81 ± 0.0	130 ± 55	0.007-0.908
Desorption											
North Dakota Sandy loam (2.5% OC, pH 7.7)	10.6 ± 0.5	0.980	6.1E-09	9.0-28.5	423 ± 20	8.3 ± 1.1	0.996	3.9E-10	0.80 ± 0.0	330 ± 42	0.002-0.294
White Swan Loam (1.2% OC, pH 6.4)	3.5 ±0.2	0.972	2.6E-08	2.6-7.0	290 ± 16	2.9 ± 1.1	0.991	1.9E-06	0.85 ± 0.0	241 ± 91	0.003-0.285
Marsillargues Silty Clay (1.0% OC, pH 8.2)	2.2 ±0.2	0.920	3.1E-06	1.6-8.5	218 ± 21	1.7 ± 1.2	0.942	4.6E-02	0.78 ± 0.1	169 ± 125	0.003-0.243
18 Acres Sandy clay loam (2.5% OC, pH 6.2)	6.9 ±0.3	0.983	2.9E-09	6.1-19.5	278 ± 12	5.7 ± 1.1	0.988	1.9E-07	0.84 ± 0.0	230 ± 45	0.002-0.291

Soil/ Sediment, % OC pH	Regressed K_d (L/kg-soil)			Range of K_d (L/kg-soil)	Regressed K_{OC} (L/kg-OC)	K_F ((L/kg-soil)$^{-1/n}$)			1/n for adsorption	K_{FOC} (L/kg-OC)$^{-1/n}$)	Ceq Range (mg/L)
	Value ± SE	r^2	p-value		Value ± SE	Value ± SE	r^2	p-value	Value ± SE	Value ± SE	
Gartenacker Loam (1.9% OC, pH 7.7)	2.7 ±0.2	0.950	3.8E-07	2.2-7.0	142 ± 11	1.9 ± 1.1	0.975	1.3 E-03	0.77 ± 0.0	102 ± 60	0.003-0.253

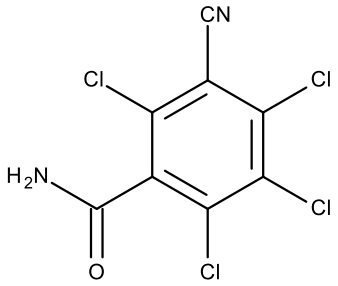
Abbreviations: SE = standard error of regression.

[A] Data were obtained from Tables 2-6, pp. 27-31 of the study report, and reviewer-calculated values. See Attachment 2 for equations used for calculations.

I. Material and Methods

A. Materials

1. Test Material: [^{14}C]-R613636 (p. 12)
Batch/Lot number: ILA-303.7A
Specific radioactivity: 51.7 µCi/mg
Radiochemical purity: ≥93.7% (by HPLC and TLC, pp. 12, 18; Figures 1-2, pp. 33-34)
Chemical Purity: Not reported
Solubility in water: Not reported



* = Location of the radiolabel

2. Reference Compounds: non-radiolabelled R613636, standard and purity not provided

3. Soils/Sediment: The study was conducted using two U.S. test soils and three European test soils (p. 13; Table 1, p. 26). Pesticide use history at the collection sites included: North Dakota sandy loam (Roundup in 2007 and 2009, Glyphosate and Mustang max in 2008), White Swan loam (no pesticides since 2005), Gartenacker loam (no pesticides applied in at least last 5 years), 18 Acres sandy clay loam (no pesticides used since 2000), and Marsillargues silty clay (no pesticides used in at least the last year). Sampling depth was specified for three of the five soils; Gartenacker and 18 Acres samples were collected from the upper 5-20 cm of soil, and Marsillargues samples were collected from the upper 2-10 cm of soil. The soils were air dried, sieved (2 mm), and then stored at ambient temperature prior to use. A summary of the physical and chemical properties of the soils using USDA Soil Taxonomy is provided in **Table 2**. The U.S. test soils were representative of use sites.

Table 2. Description of Soil/Sediment

Soil Name	Gartenacker	18 Acres	Marsillargues	North Dakota	White Swan
Origin	Vouvry, Les Barges, Switzerland	Jealott's Hill Farm, Bracknell, UK	La Paluzette, Marsillargues, France	Gardener, Cass County, North Dakota	Yakima County, Washington
USDA Textural Class	Loam	Sandy clay loam	Silty clay	Sandy loam	Loam
% Sand	45	51	6	63	35
% Silt	43	24	56	20	46
% Clay	12	25	39	17	19
%OC	1.9	2.5	1.0	2.5	1.2
CEC (meq/100 g)	10.8	18.9	12.2	17.4	16.6
pH in water	7.7	6.2	8.2	7.7	6.4
pH in $CaCl_2$	7.2	5.5	7.7	7.3	6.1
% moisture (1/3 bar)	28.8	23.6	29.3	21.5	23.4
Water holding capacity (g/100 g)	Not reported	Not reported	Not reported	Not reported	Not reported
Soil Taxonomy	Entisols, Fluvents	Alfisols, Aqualf	Entisols, Aquents	Mollisols, Albolls	Aridisols, Cambids
$CaCO_3$ (%)	Not reported	Not reported	Not reported	Not reported	Not reported

Data were obtained from Table 1, p. 26 of the study report.

B. Study design

1. **Experimental conditions:** Preliminary tests were conducted to examine R613636 solubility, adsorption to test containers, stability of the test material in 0.01 M $CaCl_2$ solution, optimal soil:solution ratio, study equilibrium times, and effect of test substance concentration on pH (pp. 19-20; Appendix 2, pp. 52-64). Solubility testing determined that 0.1% acetonitrile as a co-solvent would be used to make stock and test solutions. Polyethylene tubes were used in the definitive study because there was no significant adsorption of the test substance to the polyethylene tubes when tested overnight in the absence of soil. Soil:solution ratios of 1:1, 1:10, and 1:50 (w/w) were tested on all soils over a period of 16 hours. TLC results showed adsorption was within the optimum range (20-80%) for the test substance at the 1:10 soil:solution ratio for all soils, except one replicate Marsillargues soil (19.8%), and a soil:solution ratio of 1:10 (w/w) was selected for the definitive study (Appendix 2, Table A, p. 55). Plots of % adsorbed over 24 hours for all five soils were used to select 4 hours as the adsorption equilibrium time in the definitive study (Appendix 2, Figure A, p. 59). Separate desorption equilibrium time tests were conducted on all five soils and a desorption equilibrium time of 4 hours was selected for the definitive study (Appendix 2, Figure B, p. 62). The test substance had a small effect of slightly decreasing the soil pH of most of the soils after the test substance was added to the soils and placed on a shaker for 4 hours (Appendix 2, Table G, p. 64).

For the definitive study, ten replicates of each test soil (*ca* 1 g oven dry weight) were pre-equilibrated overnight at 20 ± 2°C with 10 mL of 0.01 M $CaCl_2$ solution (pp. 14-16). The samples were treated with 10 µL aliquots of [^{14}C]-R613636, dissolved in acetonitrile, to give nominal concentrations of 0.01, 0.25, 0.50, 0.75 and 1.00 µg/mL at soil:solution ratios of 1:10 for all soils studied. For the adsorption study, the samples were shaken in the dark at 20 ± 2°C for 4 hours. Following centrifugation, the supernatants were decanted, weighed and duplicate aliquots analyzed by Liquid Scintillation Counting (LSC). For the desorption study, immediately after removing the adsorption supernatant, an amount of fresh 0.01 M $CaCl_2$ solution equivalent to the amount removed was added to each of the soil samples, and the samples were shaken in the dark at 20 ± 2°C for 4 hours. Following centrifugation, the supernatants were decanted, weighed and duplicate aliquots analyzed by LSC. Representative soils were subjected to soil extraction prior to analysis.

2. **Analytical procedures:** Radioactivity in the aqueous supernatants, soil extracts, and in combusted non-extractable soil debris was determined by Liquid Scintillation Counting (Appendix 3, p. 65). The soils were extracted by shaking with acetonitrile:0.3M HCl (4:1, v:v; 2 x 10mL) and the extracts were pooled and brought to 25 mL with acetonitrile prior to analysis (p. 17). To verify test substance stability, normal phase TLC (Merck KGA, silica UV_{254} plates developed in ethylacetate:ethanol:acetic acid:water) using a Fuji FLA-5000 Bioimaging analyzer was performed (p. 17; Appendix 3, p. 66). TLC analysis was performed on all adsorption and desorption supernatants and combined soil extracts from North Dakota soils (highest Kd soil type), and only on the adsorption and desorption supernatants and combined soil extracts from the 0.50 µg/mL concentration tests on the remaining soil types (p. 22). The Limit of Quantification (LOQ) was set as < 0.01ppm for the samples analyzed by LSC (Appendix 5, p. 76). Limits of Quantification (LOQ) for TLC and HPLC analyses were not reported.

II. Results and Discussion

A. Mass Balance: Recovery ranged from 101.7 to 107.2% of the applied radioactivity, which meets the acceptable limit of 90% or greater, over all test concentrations for the North Dakota sandy loam, and for the remaining soils at the 0.50 µg/mL concentration only (Table 10, p. 35; See Reviewer's Comments).

B. Transformation of Parent Compound: TLC analysis of adsorption and desorption supernatants and soil extracts was conducted for all test concentrations for the North Dakota soil, and for the 0.50 µg/mL test substance trials on the other soils studied. TLC analysis showed that [^{14}C]-R613636 was stable in the adsorption phase (≥ 99.4% of the radioactivity), desorption phase (100%), and combined soil extracts (100%) for all the soils tested, which is within acceptable limits (Table 9, p. 34; See Reviewer's Comments).

C. Findings: Reported values were calculated using linear regression (Excel) and the equations and methods are discussed in the calculations section.

Equilibration concentrations in water were appropriate for all treated soils and ranged from 0.004 to 0.938 µg/mL following the adsorption phase and 0.002 to 0.294 µg/mL following the desorption phase (Tables 2-6, pp. 27-31).

Percent adsorption ranged from 45.5 to 66.4% for the North Dakota sandy loam, 26.6 to 40.0% for the White Swan loam, 18.1 to 30.0% for the Marsillargues silty clay, 36.4 to 49.1% for the 18 Acres sandy clay loam, and 21.2 to 40.9% for the Gartenacker loam (Tables 2-6, pp. 27-31). Percent desorption, as percent of the adsorbed, ranged from 21.9 to 46.0% for the North Dakota sandy loam, 52.3 to 73.6% for the White Swan loam, 45.2 to 79.6% for the Marsillargues silty clay, 26.4 to 56.0% for the 18 Acres sandy clay loam, and 51.1 to 74.6% for the Gartenacker loam (Tables 2-6, pp. 27-31). Coefficients of variation (CV) were 0.6 and 0.3 across all soils for adsorption K_F and K_{Foc}, respectively, and 0.7 and 0.4 across all soils for desorption K_F and K_{Foc}, respectively.

Table 3. Description of Adsorption Coefficients[A]

Soil	K_d (L/kg)	K_{oc}	K_F (L/kg)	K_{Foc}
North Dakota Sandy loam	8.7	349	8.1	325
White Swan Silt loam	3.8	314	3.7	307
Marsillargues Silty clay	2.3	228	2.3	232
18 Acres Sandy clay loam	5.9	237	5.9	237
Gartenacker Loam	2.6	136	2.5	130

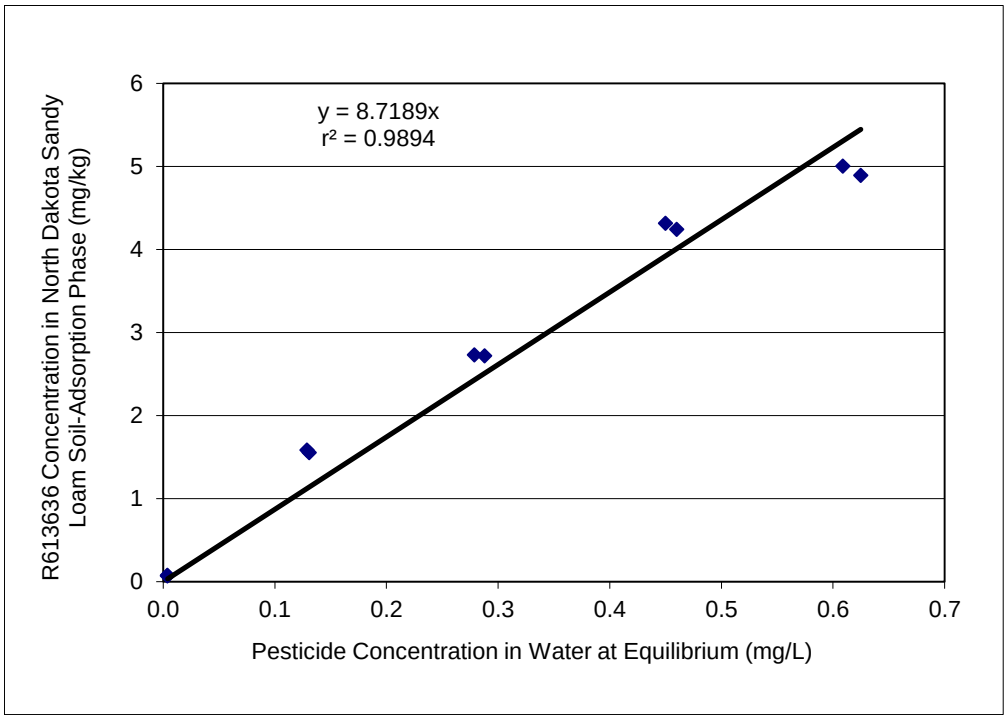
[A] Reviewer-calculated values using data obtained from Tables 2-6, pp. 27-31 of the study report.

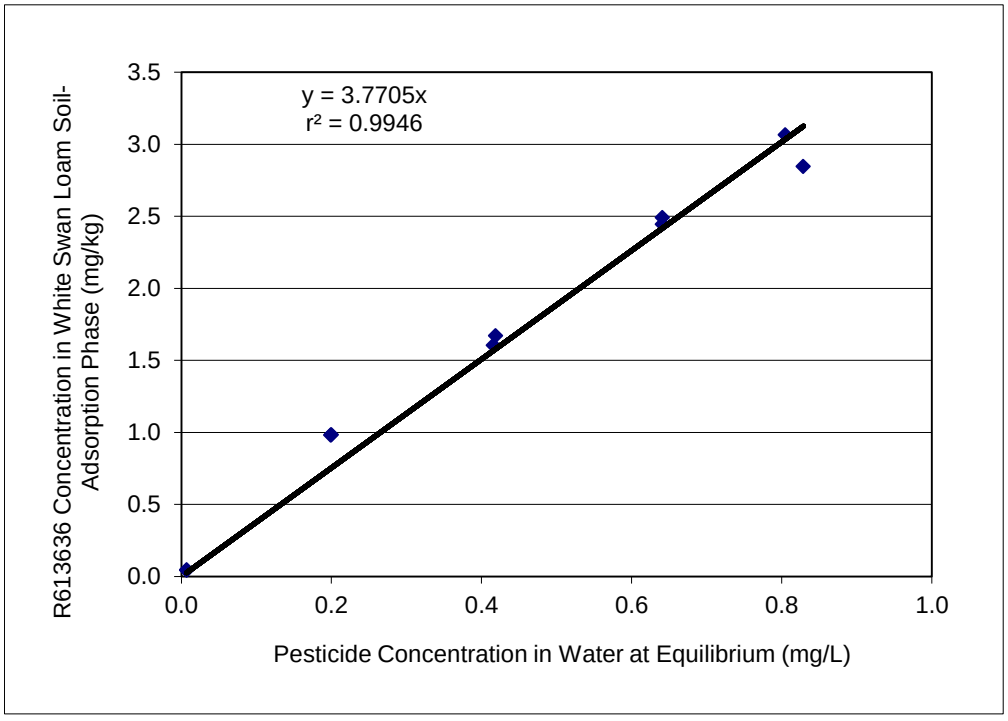
Table 4. Description of Desorption Coefficients[A]

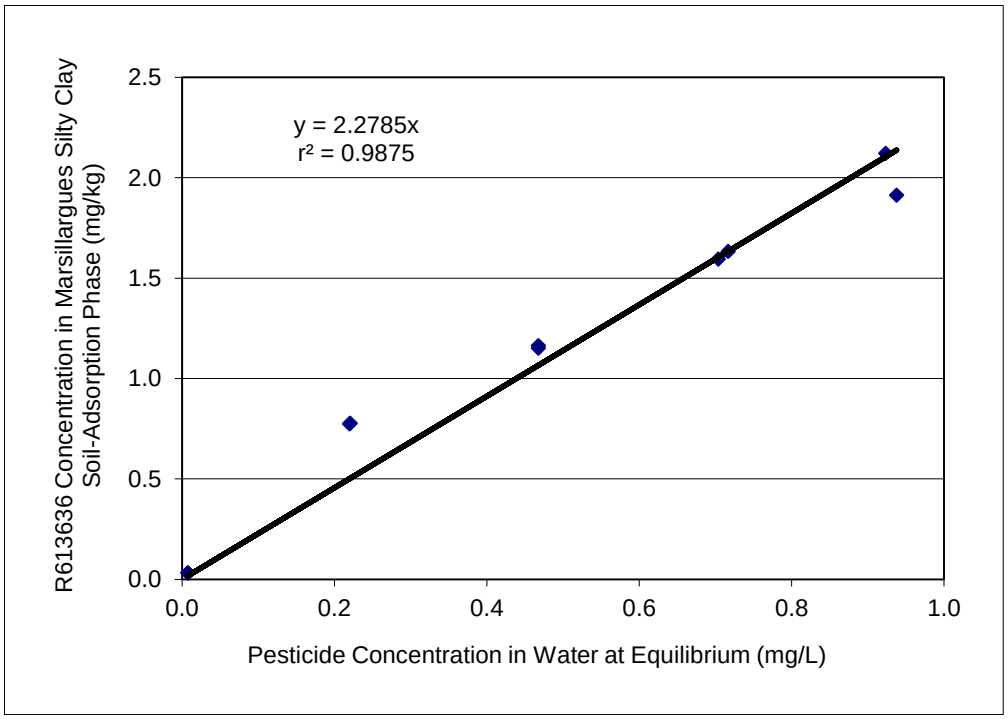
Soil	K_{des} (L/kg)	$K_{oc\text{-}des}$	K_{Fdes} (L/kg)	$K_{Foc\text{-}des}$
North Dakota Sandy loam	10.6	423	8.3	330
White Swan Silt loam	3.5	290	2.9	241
Marsillargues Silty clay	2.2	218	1.7	169
18 Acres Sandy clay loam	6.9	278	5.8	230
Gartenacker Loam	2.7	142	2.0	102

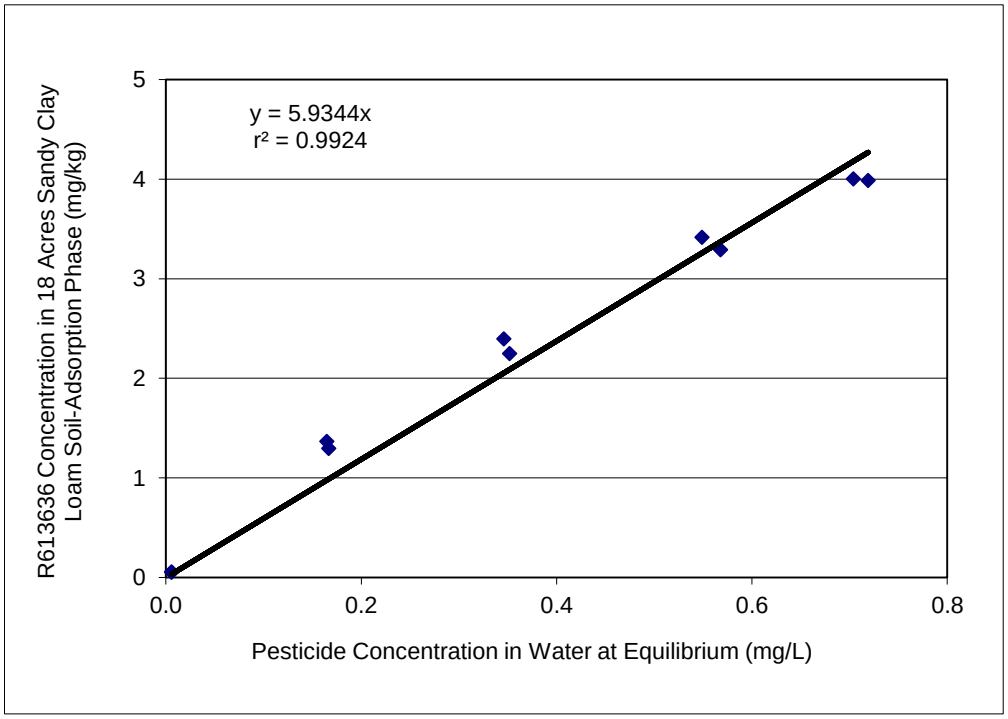
[A] Reviewer-calculated values using data obtained from Tables 2-6, pp. 27-31 of the study report.

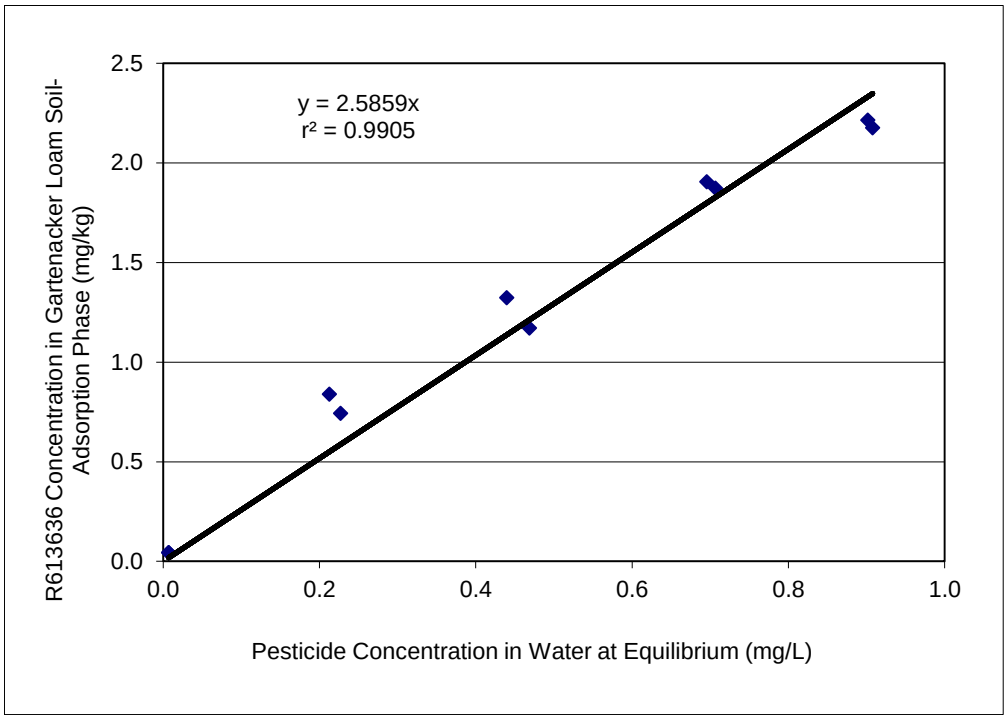
Reviewer-calculated Freundlich sorption coefficients were in agreement with the study-reported values (p. 21; Tables 7-8, pp. 32-33; Figures 3-4, pp. 39-44).

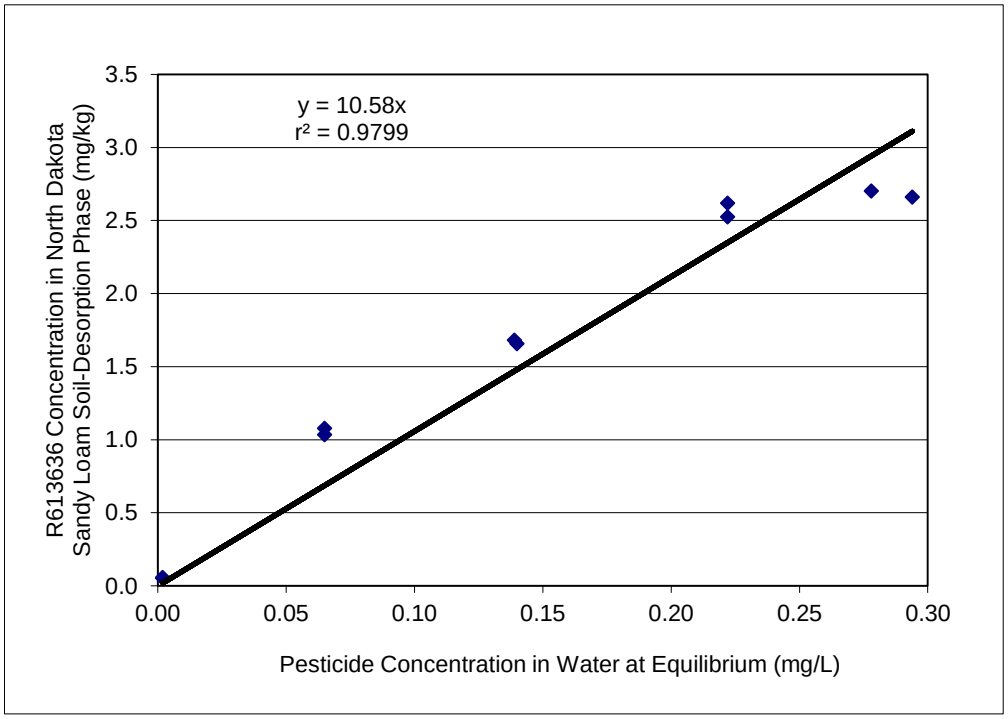

y = 8.7189x
r² = 0.9894
R613636 Concentration in North Dakota Sandy Loam Soil-Adsorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0
1
2
3
4
5
6
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

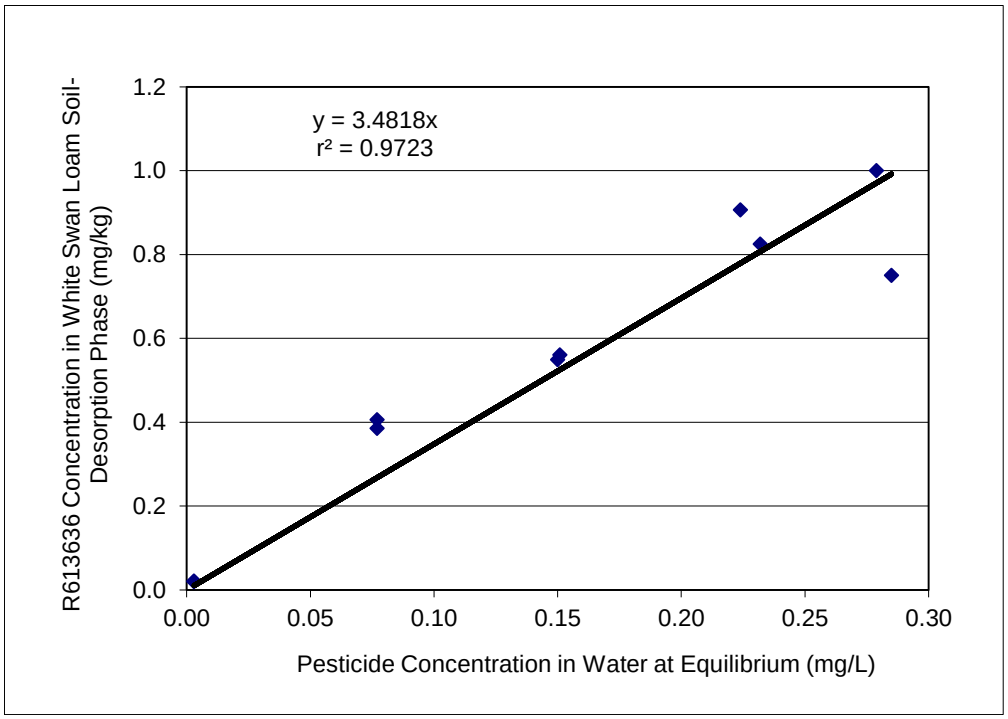

y = 3.7705x
r² = 0.9946
R613636 Concentration in White Swan Loam Soil-Adsorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0.0
0.2
0.4
0.6
0.8
1.0

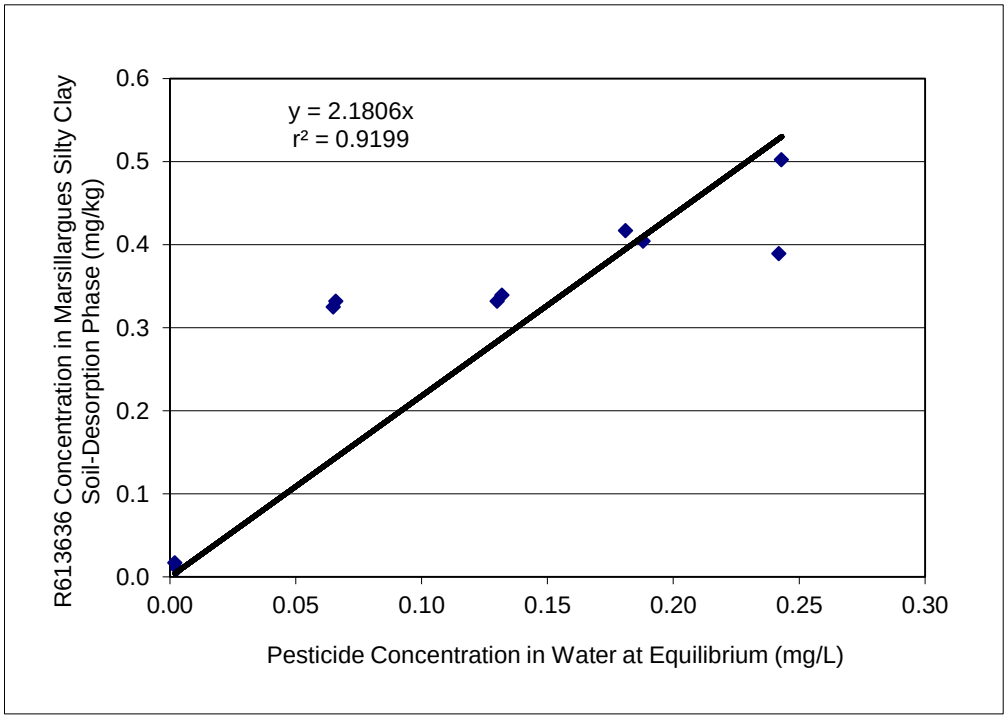

y = 2.2785x
r² = 0.9875
R613636 Concentration in Marsillargues Silty Clay Soil-Adsorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0.0
0.5
1.0
1.5
2.0
2.5
0.0
0.2
0.4
0.6
0.8
1.0

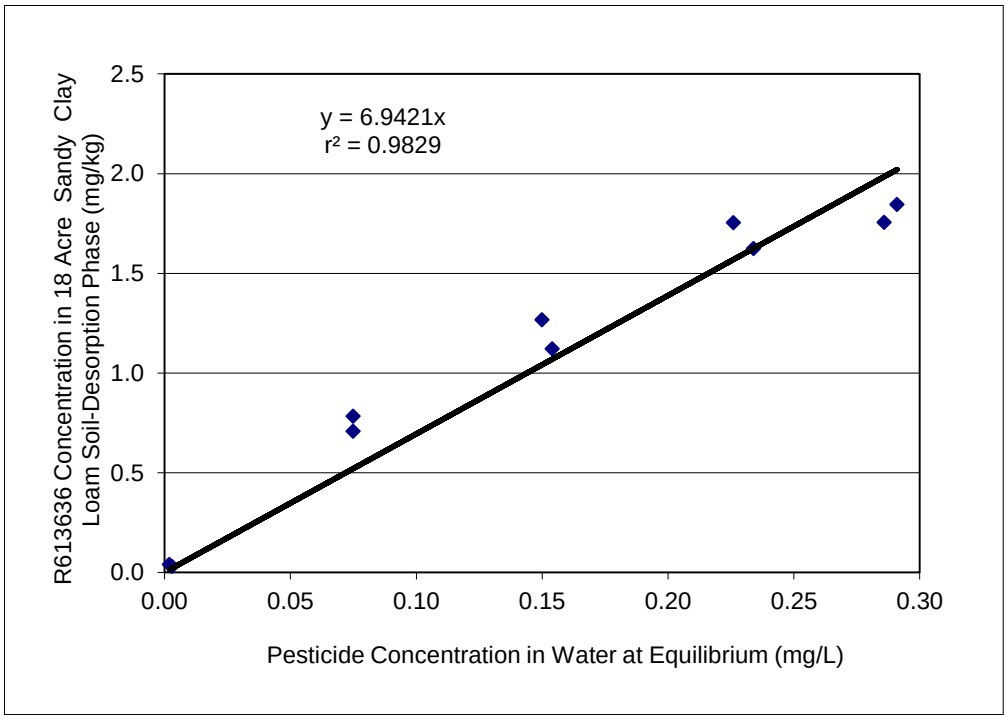

y = 5.9344x
r² = 0.9924
R613636 Concentration in 18 Acres Sandy Clay Loam Soil-Adsorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0
1
2
3
4
5
0.0
0.2
0.4
0.6
0.8

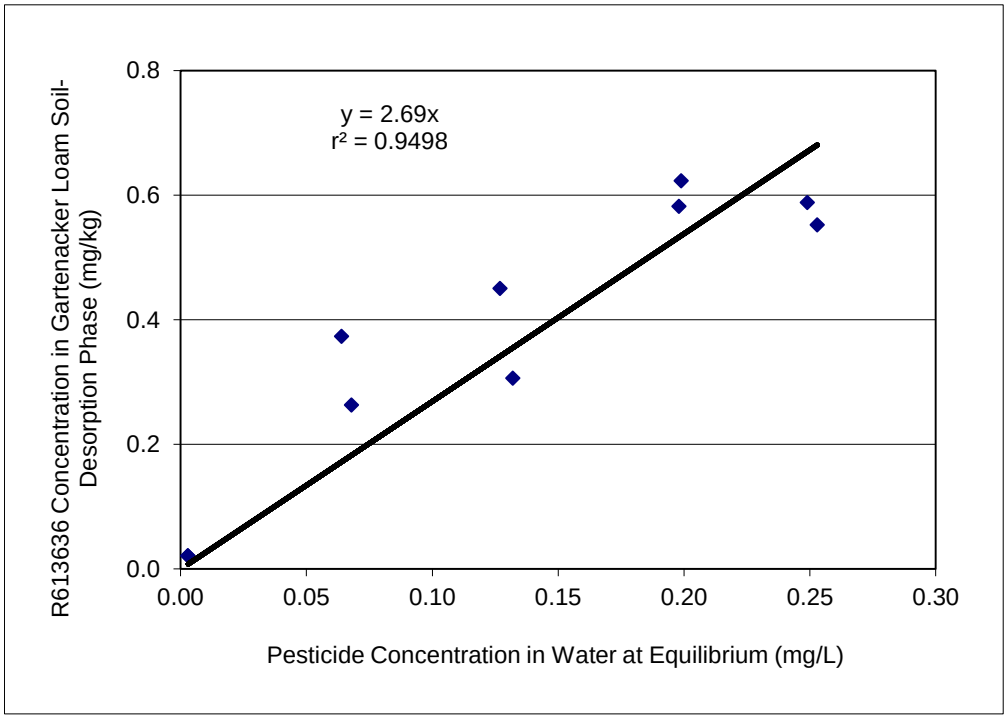

y = 2.5859x
r² = 0.9905
R613636 Concentration in Gartenacker Loam Soil-Adsorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0.0
0.5
1.0
1.5
2.0
2.5
0.0
0.2
0.4
0.6
0.8
1.0


y = 10.58x
r² = 0.9799
R613636 Concentration in North Dakota Sandy Loam Soil-Desorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0.00
0.05
0.10
0.15
0.20
0.25
0.30


y = 3.4818x
r² = 0.9723
R613636 Concentration in White Swan Loam Soil-Desorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.00
0.05
0.10
0.15
0.20
0.25
0.30


y = 2.1806x
r² = 0.9199
R613636 Concentration in Marsillargues Silty Clay Soil-Desorption Phase (mg/kg)
Pesticide Concentration in Water at Equilibrium (mg/L)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.00
0.05
0.10
0.15
0.20
0.25
0.30



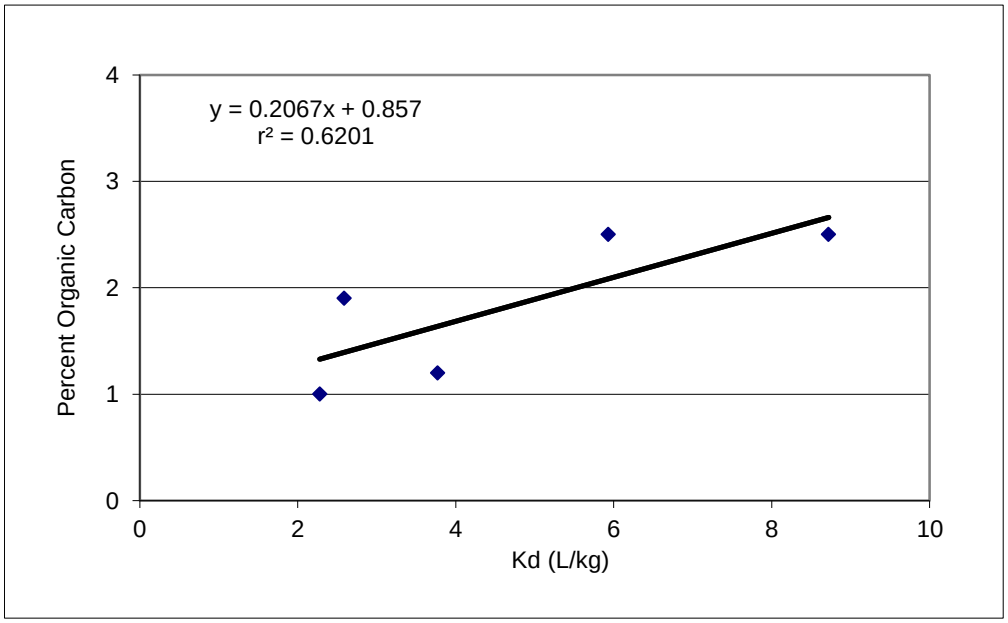


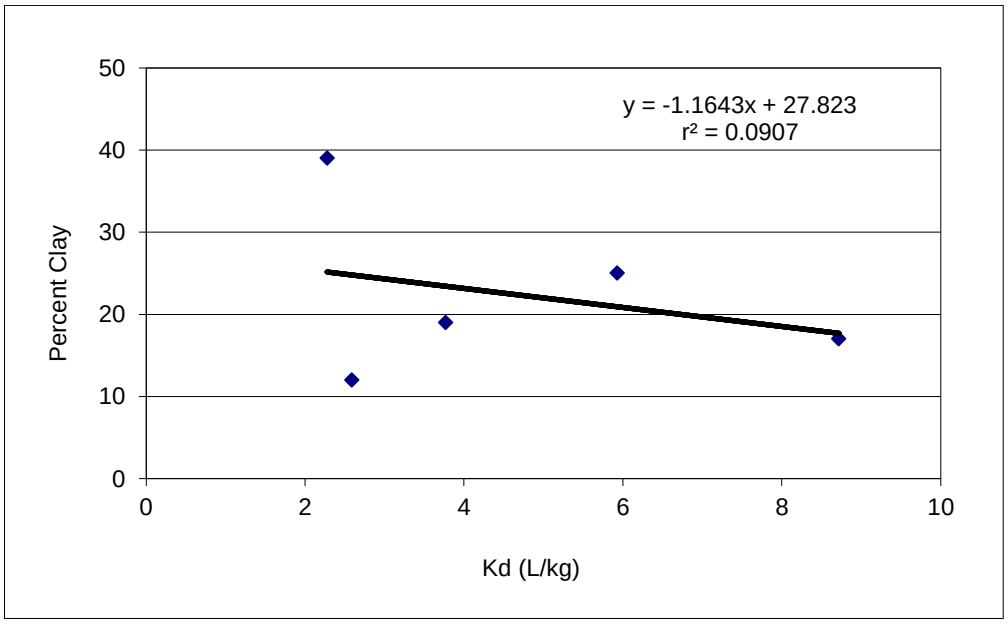
The results of the regression of K_d by percent organic carbon, percent clay, and CEC are tabulated below:

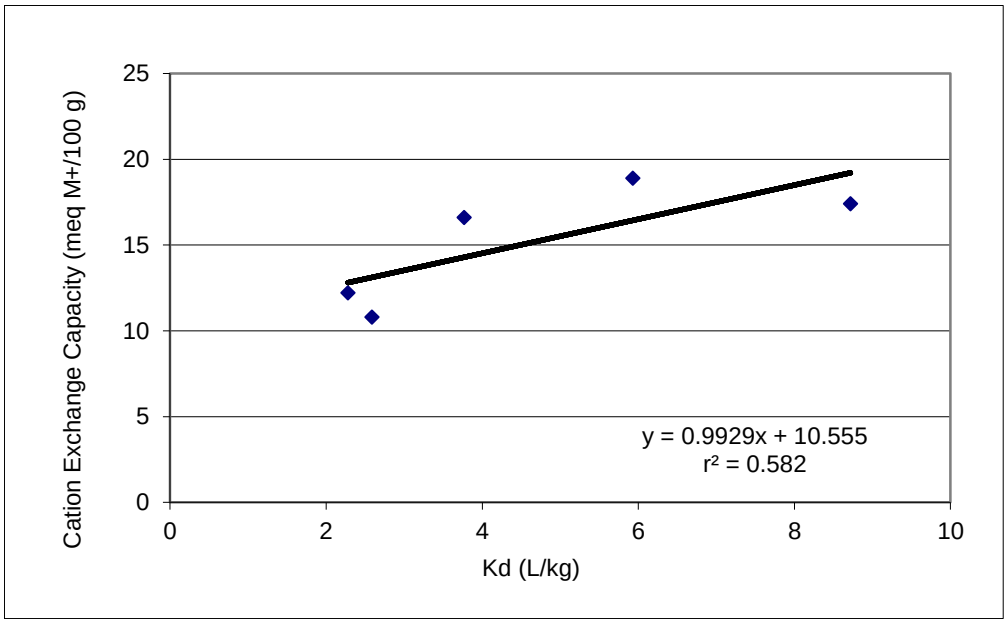
Table 5. Summary of Regressed Kd vs %OC, %Clay, and CEC[A]

Parameter	r^2	p-value
Kd vs. % organic carbon	0.620	0.114
Kd vs. % clay	0.091	0.623
Kd vs. CEC	0.582	0.134

[A] Reviewer-calculated values using data obtained from Tables 2-6, pp. 27-31 of the study report.







The data indicate slight correlations between the adsorption of R613636 to soil and percent organic carbon and CEC. No correlation was observed between the adsorption of R613636 and percent clay.

III. Study Deficiencies and Reviewer's Comments

1. Three of the five soils studied were collected from France, United Kingdom, and Switzerland, and it was not established that these foreign soils were comparable to soils that would be found at the intended use sites in the United States.

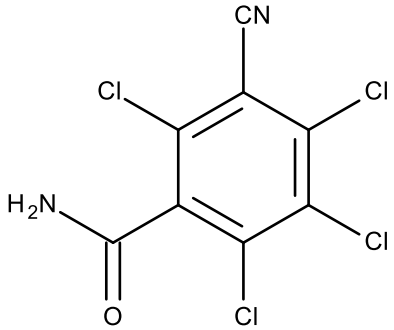
2. Mass balances and stability tests were determined using select samples (all test concentrations for the North Dakota sandy loam soil; 0.5 µg/mL test concentration for the White Swan silt loam, Marsillargues silty clay, 18 Acres sandy clay loam and Gartenacker loam), rather than across all soils and test concentrations.

3. Limits of Quantification (LOQ) for LSC was stated to be <0.01 ppm, and Limits of Detection (LOD) and Quantification (LOQ) for TLC analyses were not reported.

IV. References

1. U.S. Environmental Protection Agency. 2008. Fate, Transport and Transformation Test Guidelines, OPPTS 835.1230, Adsorption/Desorption (Batch Equilibrium). Office of Prevention, Pesticides and Toxic Substances, Washington, DC. EPA 712-C-08-019.

DER ATTACHMENT 1. R613636 and Its Environmental Transformation Products. [A]

Code Name/ Synonym	Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)	Final %AR (study length)
PARENT						
R613636	**IUPAC:** 2,3,4,6-Tetrachloro-5-cyano-benzamide **CAS No.:** 61073-19-6 **Formula:** $C_8H_2Cl_4N_2O$ **MW:** 283.9 g/mol **SMILES:** C(#N)c1c(c(c(c(c1Cl)Cl)Cl)C(=O)N)Cl		835.1230 Batch equilibrium	49342705	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: Calculations

Calculations were performed by the reviewer using Excel and the following equations.

Ceq range is the range of test concentrations in water at equilibrium.
Cs is the test concentrations sorbed to soil or sediment at equilibrium.

K_d –Distribution Coefficient for Adsorption = C_s/C_{eq} (eq 1)

- Regressed K_d is calculated using linear regression of Cs versus Ceq with a forced zero intercept over the range of measured Ceq for each soil/sediment.
- Range of K_d reflects the range of each K_d measured at a specific concentration in a soil/sediment

K_{OC} -Organic Carbon Normalized Adsorption Coefficient = regressed K_d *100/% OC (eq 2)

Standard Error (SE) of K_{OC}= K_d SE *100/%OC (eq 3)

K_F -Freundlich Adsorption Coefficient and the Freundlich exponent (1/n) were calculated using nonlinear regression of $C_s = K_F$ x Ceq $^{1/n}$. Cs should be expressed in mg/kg and Ceq should be expressed in mg/L in the regression. (eq 4)

K_{FOC} –Organic Carbon Normalized Adsorption Coefficient = K_F*100/%OC (eq 5)

Standard Error (SE) of K_{FOC}= K_F SE *100/%OC (eq 6)

K_{DES} –Apparent Desorption Coefficient = C_s/C_{eq} where C_s and C_{eq} are measured after an initial sorption measurement and the soil/sediment is placed in a new solution and allowed to equilibrate, so that any material in solution desorbed from the soil/sediment. (eq 7)

- Regressed K_{DES} is calculated using linear regression of Cs versus Ceq over the range of Ceq measured with a forced zero intercept for each soil/sediment.
- Range of K_{DES} reflects the range of each K_{DES} measured at a specific concentration in a soil/sediment

$K_{OC\text{-}DES}$ -Organic Carbon Normalized Apparent Desorption Coefficient = regressed K_{DES} *100/% OC (eq 8)

Standard Error of Koc-$_{DES}$ = K_{DES} SE* 100/%OC (eq 9)

$K_{F\text{-}DES}$ -Freundlich Desorption Coefficient and the Freundlich Desorption exponent (1/n)

were calculated using nonlinear regression of $C_s = K_{F\text{-}DES} \times Ceq^{1/n}$ (eq 10)

$K_{FOC\text{-}DES}$ -Organic Carbon Normalized Freundlich Desorption Coefficient= $K_{F\text{-}DES}$*100/%OC (eq 11)

Standard Error of $K_{FOC\text{-}DES} = K_F$ SE *100/%OC (eq 12)