

Article

Sorption/Desorption and Kinetics of Atrazine, Chlorfenvinphos, Endosulfan Sulfate and Trifluralin on Agro-Industrial and Composted Organic Wastes

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Table S1. physicochemical properties of the studied pesticides.

Pesticide	Type	2D structure diagram	Chem. Family	Chem. Formula	Molecular Weight (mol ⁻¹)	S _w (20 °C mg L ⁻¹)	DT50 typical (days)	GUS	K _{oc} (mL g ⁻¹)	Log K _{ow}
Atrazine	Herbicide		Triazine	C ₈ H ₁₄ ClN ₅	215.68	35	75	3.20	100	2.75
Endosulfan sulfate	Metabolite		Organochlorine	C ₉ H ₆ Cl ₆ O ₄ S	422.93	0.48	-	-	5194	3.66
Chlorfenvinphos	Insecticide, Acaricide		Organophosphate	C ₁₂ H ₁₄ Cl ₃ O ₄	359.57	145	40	1.87	680	3.85
Trifluralin	Herbicide		Dinitroaniline	C ₁₃ H ₁₆ F ₃ N ₃ O ₄	335.28	0.221	181	0.13	15800	5.27

Footnotes: S_w (20 °C mg L⁻¹): Water solubility. DT50: typical half life. GUS: GUS indexes coefficient. K_{oc}: normalized organic carbon coefficient. K_{ow}: octanol/water coefficient. Data from PPDB (2020).

Table S2. Correlation coefficients between sorption-desorption and kinetic parameters and pesticides physicochemical properties ($n = 4$, $p < 0.05$).

	Molecular Weight (mol ⁻¹)	S _w (20 °C mg/L)	DT50 typical(days)	GUS	K _{oc} (mL/g)	Log K _{ow}	Molecular Weight (mol ⁻¹)	S _w (20 °C mg/L)	DT50 typical(days)	GUS	K _{oc} (mL/g)	Log K _{ow}
Sorption capacity (%) (600 mg - Effect of adsorbent dose)							K ₂					
OR1	0.89	0.44	-0.22	-0.64	0.31	0.57	0.05	-0.45	0.97	-0.48	0.42	0.68
OR2	0.85	-0.11	0.37	-0.93	0.70	0.95	0.46	-0.66	0.77	-0.84	0.84	0.93
OR3	0.88	-0.08	0.31	-0.93	0.70	0.94	0.48	-0.83	0.58	-0.84	0.96	0.85
OR4	0.82	-0.36	0.44	-0.99	0.86	0.99	0.06	-0.42	0.97	-0.49	0.41	0.68
K _i							X _i					
OR1	0.14	0.85	-0.90	0.38	-0.55	-0.52	0.89	-0.01	0.27	-0.91	0.65	0.91
OR2	-0.53	0.79	-0.58	0.87	-0.96	-0.89	0.83	-0.27	0.42	-0.97	0.81	0.99
OR3	0.06	1.00	-0.61	0.40	-0.69	-0.44	0.80	-0.37	0.46	-0.98	0.86	1.00
OR4	0.28	0.81	-0.91	0.24	-0.42	-0.40	0.67	-0.50	0.62	-0.95	0.87	0.99
N _{fa}							K _{fa}					
OR1	0.04	-0.93	0.80	-0.53	0.73	0.62	0.76	-0.62	0.27	-0.94	0.99	0.88
OR2	0.60	0.61	0.04	-0.41	0.00	0.45	0.36	-0.83	0.74	-0.78	0.88	0.84
OR3	0.72	-0.59	0.48	-0.97	0.96	0.97	0.42	-0.63	0.81	-0.81	0.79	0.91
OR4	0.92	-0.07	0.23	-0.94	0.72	0.92	0.32	-0.70	0.85	-0.75	0.77	0.86
K _d							K _{oc}					
OR1	0.50	-0.75	0.67	-0.87	0.92	0.91	0.50	-0.75	0.67	-0.87	0.92	0.91
OR2	0.32	-0.64	0.87	-0.74	0.73	0.87	0.32	-0.64	0.87	-0.74	0.73	0.87
OR3	0.24	-0.57	0.92	-0.67	0.63	0.82	0.24	-0.57	0.92	-0.67	0.63	0.82
OR4	0.25	-0.57	0.92	-0.67	0.63	0.82	0.25	-0.57	0.92	-0.67	0.63	0.82
N _{fd}							K _{fd}					
OR1	0.27	0.97	-0.50	0.16	-0.52	-0.19		-0.88	0.75	-0.71	0.85	0.77
OR2	0.56	-0.21	-0.85	-0.26	0.43	0.02	0.46	-0.76	0.87	-0.72	0.59	0.87
OR3	0.68	-0.36	-0.76	-0.41	0.56	0.17	0.63	-0.88	0.75	-0.85	0.74	0.95
OR4	-0.62	0.87	-0.76	0.84	-0.73	-0.95	0.75	-0.94	0.63	-0.92	0.84	0.99
H							%D					
OR1	-0.33	-0.91	0.76	-0.17	0.45	0.28	0.05	1.00	-0.60	0.40	-0.70	-0.43
OR2	-0.06	-0.31	1.00	-0.26	0.08	0.49	-0.37	0.86	-0.68	0.78	-0.91	-0.82
OR3	-0.17	-0.21	0.99	-0.16	-0.02	0.39	0.31	0.95	-0.64	0.16	-0.49	-0.23
OR4	0.28	-0.62	0.95	-0.58	0.42	0.76	-0.20	0.95	-0.67	0.64	-0.85	-0.68

Table S3. Determination coefficients between sorption-desorption and kinetic parameters and physicochemical properties of organic wastes ($p < 0.05$).

	%TOC	BET	pH	C	N	O	Na	Mg	Al	Si	P	S	Cl	K	Ca	Ti	Fe	Cu	
<i>n</i>	4	4	4	4	2	4	2	3	2	3	1	2	3	3	3	1	2	1	<i>n</i>
Sorption capacity (%) (600 mg - Effect of adsorbent dose)																			
AT	0.52	-0.47	-0.92	0.95	n/a	-0.20	n/a	-0.39	n/a	-0.01	n/a	n/a	-0.52	0.49	-0.52	n/a	n/a	n/a	4
TF	-0.46	0.40	0.89	-0.93	n/a	0.27	n/a	0.04	n/a	-0.34	n/a	n/a	0.18	-0.15	0.19	n/a	n/a	n/a	4
CF	0.78	-0.87	-0.97	0.95	n/a	0.36	n/a	-0.99	n/a	-0.87	n/a	1.00	-1.00	1.00	-1.00	n/a	n/a	n/a	4
ES	0.03	0.33	0.75	-0.62	n/a	0.20	n/a	0.05	n/a	-0.33	n/a	n/a	0.20	-0.17	0.20	n/a	n/a	n/a	4
Q _e exp																			
AT	0.42	-0.51	-0.94	0.92	n/a	-0.14	n/a	-0.35	n/a	0.03	n/a	n/a	-0.48	0.46	-0.49	n/a	n/a	n/a	4
TF	-0.24	0.38	0.87	-0.83	n/a	0.26	n/a	0.03	n/a	-0.35	n/a	n/a	0.18	-0.15	0.18	n/a	n/a	n/a	4
CF	0.86	-0.83	-0.94	0.96	n/a	0.32	n/a	-0.99	n/a	-0.97	n/a	n/a	-0.96	0.96	-0.95	n/a	n/a	n/a	4
ES	0.19	0.30	0.63	-0.46	n/a	0.12	n/a	0.09	n/a	-0.30	n/a	n/a	0.23	-0.20	0.24	n/a	n/a	n/a	4
K ₂																			
AT	0.86	-0.84	-0.42	0.43	n/a	0.84	n/a	-0.88	n/a	-1.00	n/a	n/a	-0.81	0.83	**	n/a	n/a	n/a	4
TF	0.66	-0.96	-0.89	0.79	n/a	0.60	n/a	-0.96	n/a	-0.78	n/a	n/a	-0.99	0.98	-0.99	n/a	n/a	n/a	4
CF	0.52	-0.71	-0.10	0.02	n/a	0.98	n/a	-0.95	n/a	-1.00	n/a	n/a	-0.90	0.91	-0.90	n/a	n/a	n/a	4
ES	0.67	-0.49	-0.90	0.98	n/a	-0.15	n/a	-0.95	n/a	-1.00	n/a	n/a	-0.90	0.91	-0.90	n/a	n/a	n/a	4
K _i																			
AT	-0.98	0.83	0.62	-0.68	n/a	-0.62	n/a	0.83	n/a	0.98	n/a	n/a	0.74	-0.76	0.74	n/a	n/a	n/a	4
TF	-0.10	-0.56	-0.56	0.31	n/a	0.36	n/a	-0.50	n/a	-0.13	n/a	n/a	-0.62	0.60	-0.62	n/a	n/a	n/a	4
CF	-0.50	0.91	0.87	-0.72	n/a	-0.55	n/a	0.87	n/a	0.62	n/a	n/a	0.93	-0.92	0.93	n/a	n/a	n/a	4
ES	-0.33	0.88	0.61	-0.40	n/a	-0.77	n/a	0.88	n/a	0.64	n/a	n/a	0.94	-0.93	0.94	n/a	n/a	n/a	4
X _i																			
AT	0.91	-0.90	-0.88	0.89	n/a	0.49	n/a	-0.97	n/a	-0.99	n/a	n/a	-0.93	0.94	-0.93	n/a	n/a	n/a	4
TF	-0.02	-0.21	0.46	-0.56	n/a	0.78	n/a	-0.95	n/a	-1.00	n/a	n/a	-0.90	0.91	-0.89	n/a	n/a	n/a	4
CF	0.62	-0.89	-0.96	0.86	n/a	0.43	n/a	-0.90	n/a	-0.67	n/a	n/a	-0.96	0.95	-0.96	n/a	n/a	n/a	4
ES	0.44	-0.87	-0.38	0.21	n/a	0.96	n/a	-0.99	n/a	-0.87	n/a	n/a	-1.00	1.00	-1.00	n/a	n/a	n/a	4
n _{fa}																			
AT	0.03	-0.51	-0.77	0.60	n/a	0.06	n/a	-0.33	n/a	0.05	n/a	n/a	-0.47	0.44	-0.47	n/a	n/a	n/a	4
TF	-0.27	-0.21	-0.56	0.39	n/a	-0.19	n/a	0.00	n/a	0.38	n/a	n/a	-0.14	0.11	-0.15	n/a	n/a	n/a	4
CF	-0.77	0.17	0.09	-0.31	n/a	-0.12	n/a	0.13	n/a	0.50	n/a	n/a	-0.02	-0.01	-0.02	n/a	n/a	n/a	4
ES	-0.35	-0.18	-0.49	0.30	n/a	-0.16	n/a	-0.01	n/a	0.37	n/a	n/a	-0.15	0.13	-0.16	n/a	n/a	n/a	4
K _{fa}																			
AT	-0.28	0.73	0.88	-0.71	n/a	-0.28	n/a	0.62	n/a	0.27	n/a	n/a	0.72	-0.70	0.73	n/a	n/a	n/a	4
TF	0.09	0.29	0.71	-0.58	n/a	0.22	n/a	0.01	n/a	-0.37	n/a	n/a	0.15	-0.12	0.16	n/a	n/a	n/a	4
CF	0.34	0.14	0.50	-0.33	n/a	0.24	n/a	-0.07	n/a	-0.44	n/a	n/a	0.07	-0.05	0.08	n/a	n/a	n/a	4
ES	0.22	0.24	0.61	-0.45	n/a	0.20	n/a	0.00	n/a	-0.38	n/a	n/a	0.14	-0.12	0.15	n/a	n/a	n/a	4
K _d																			
AT	0.43	-0.50	-0.94	0.92	n/a	-0.16	n/a	-0.34	n/a	0.05	n/a	n/a	-0.47	0.44	-0.47	n/a	n/a	n/a	4
TF	-0.04	0.37	0.79	-0.68	n/a	0.19	n/a	0.08	n/a	-0.30	n/a	n/a	0.22	-0.20	0.23	n/a	n/a	n/a	4
CF	-0.17	0.65	0.84	-0.66	n/a	-0.20	n/a	0.51	n/a	0.14	n/a	n/a	0.63	-0.61	0.63	n/a	n/a	n/a	4
ES	0.12	0.35	0.68	-0.51	n/a	0.09	n/a	0.14	n/a	-0.25	n/a	n/a	0.28	-0.25	0.29	n/a	n/a	n/a	4
K _{oc}																			
AT	-0.74	0.09	0.24	-0.49	n/a	0.15	n/a	-0.10	n/a	0.29	n/a	n/a	-0.24	0.21	-0.25	n/a	n/a	n/a	4
TF	-0.25	0.42	0.88	-0.83	n/a	0.22	n/a	0.11	n/a	-0.28	n/a	n/a	0.25	-0.22	0.26	n/a	n/a	n/a	4
CF	-0.49	0.70	0.98	-0.92	n/a	-0.10	n/a	0.69	n/a	0.36	n/a	n/a	0.78	-0.77	0.79	n/a	n/a	n/a	4
ES	-0.45	0.47	0.93	-0.93	n/a	0.19	n/a	0.29	n/a	-0.09	n/a	n/a	0.43	-0.40	0.43	n/a	n/a	n/a	4
n _{fd}																			
AT	-0.49	0.60	-0.04	0.09	n/a	-0.94	n/a	0.90	n/a	1.00	n/a	n/a	0.83	-0.85	0.83	n/a	n/a	n/a	4
TF	0.20	-0.36	-0.85	0.81	n/a	-0.27	n/a	0.00	n/a	0.38	n/a	n/a	-0.14	0.11	-0.15	n/a	n/a	n/a	4
CF	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	2

ES	-0.27	-0.21	-0.57	0.39	n/a	-0.19	n/a	0.00	n/a	0.38	n/a	n/a	-0.14	0.11	-0.15	n/a	n/a	n/a	4
K _{id}																			
AT	0.75	-0.96	-0.57	0.49	n/a	0.90	n/a	-0.99	n/a	-0.96	n/a	n/a	-0.96	0.97	-0.96	n/a	n/a	n/a	4
TF	-0.19	0.37	0.85	-0.80	n/a	0.26	n/a	0.01	n/a	-0.37	n/a	n/a	0.15	-0.12	0.16	n/a	n/a	n/a	4
CF	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	2
ES	0.16	0.38	0.64	-0.45	n/a	0.01	n/a	0.20	n/a	-0.19	n/a	n/a	0.34	-0.31	0.34	n/a	n/a	n/a	4
H																			
AT	0.55	-0.71	-0.10	0.03	n/a	0.98	n/a	-0.95	n/a	-1.00	n/a	n/a	-0.89	0.90	-0.89	n/a	n/a	n/a	4
TF	0.01	0.30	0.76	-0.65	n/a	0.25	n/a	-0.01	n/a	-0.39	n/a	n/a	0.13	-0.10	0.14	n/a	n/a	n/a	4
CF	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	2
ES	-0.06	0.55	0.79	-0.61	n/a	-0.10	n/a	0.38	n/a	0.00	n/a	n/a	0.51	-0.48	0.51	n/a	n/a	n/a	4
%D																			
AT	-0.91	0.65	0.31	-0.41	n/a	-0.65	n/a	0.68	n/a	0.91	n/a	n/a	0.57	-0.59	0.56	n/a	n/a	n/a	4
TF	0.22	-0.37	-0.86	0.82	n/a	-0.27	n/a	0.00	n/a	0.38	n/a	n/a	-0.14	0.12	-0.15	n/a	n/a	n/a	4
CF	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	2
ES	0.03	-0.69	-0.55	0.30	n/a	0.56	n/a	-0.67	n/a	-0.34	n/a	n/a	-0.77	0.75	-0.78	n/a	n/a	n/a	4

Footnotes: AT: Atrazine, TF: Trifluralin, CF: chlorfenvinphos, ES: endosulfan sulfate. Kinetic parameters: Q_e exp (quantity of pesticide adsorbed at equilibrium), K_2 (Ho and McKay rate constants), K_i (intraparticle diffusion rate constant), X_i (Morris-Weber constant, proportional to the boundary layer thickness). Sorption constants: n_{fa} (Freundlich coefficient correlated to adsorption intensity), K_{fa} (Freundlich constant correlated to the maximum multilayer adsorption capacity). K_d (lineal sorption constant, calculated for one sorption concentration ($200 \mu\text{g L}^{-1}$)), K_{oc} (normalized organic carbon coefficient, calculated as $(K_d/\%COT) \cdot 100$, where $K_d = Q_e/C_e$), n_{fd} (Freundlich coefficient correlated to desorption intensity) Desorption constants: K_{fd} (Freundlich constant correlated to the maximum multilayer desorption capacity), H (hysteresis coefficient), %D (desorption percentages). In bold: significant correlations.

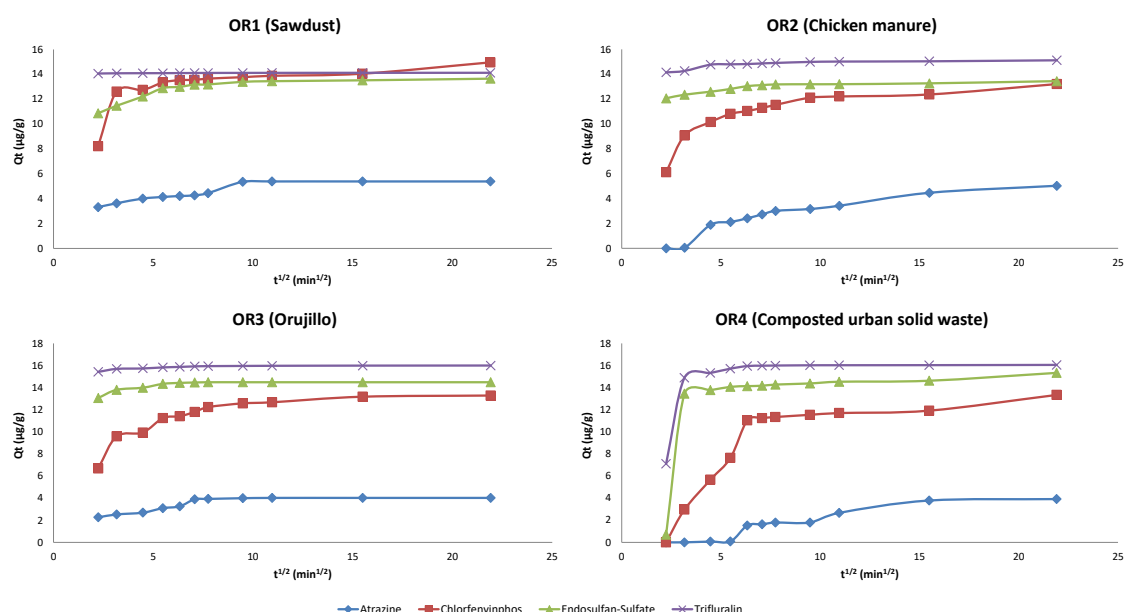


Figure S1. Weber-Morris intraparticle diffusion model of each studied adsorbent for the different pesticides.

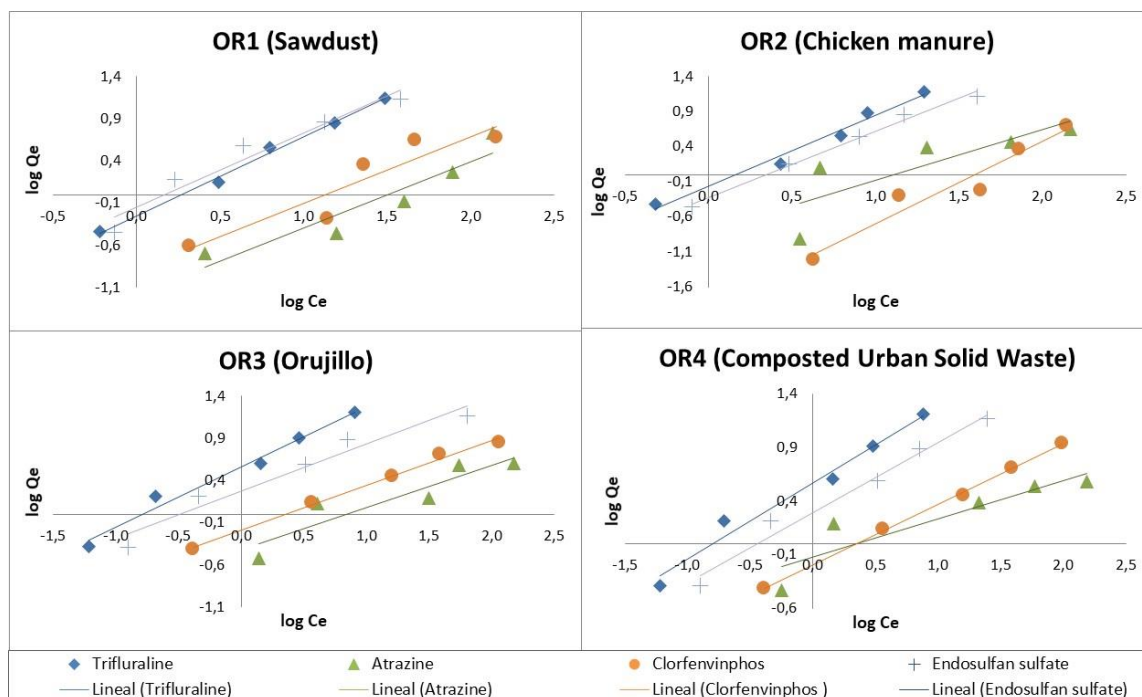


Figure S2. Freundlich sorption isotherms of all pesticides on each organic residue.

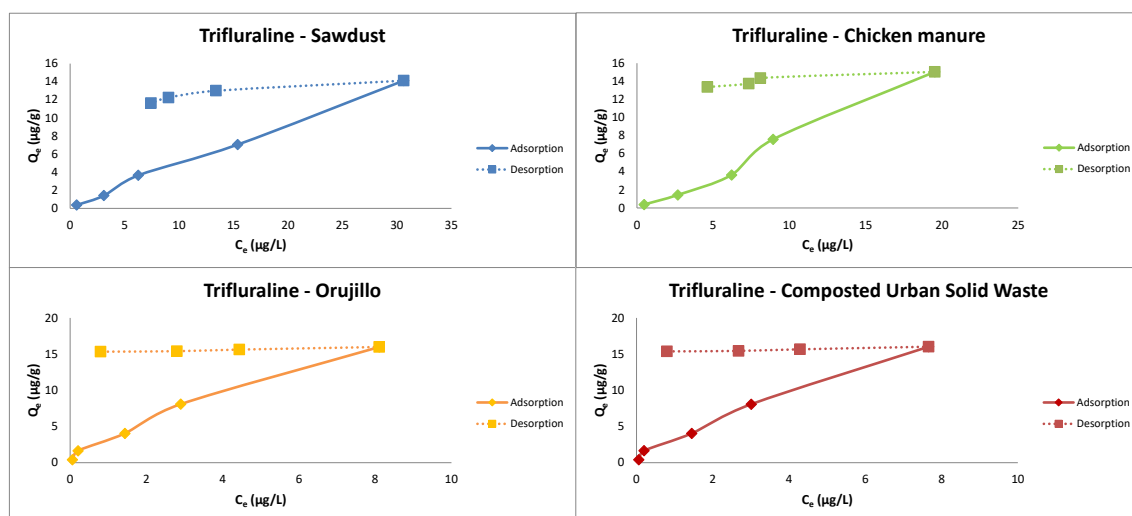


Figure S3. Sorption - desorption isotherms trifluralin on each organic residue.

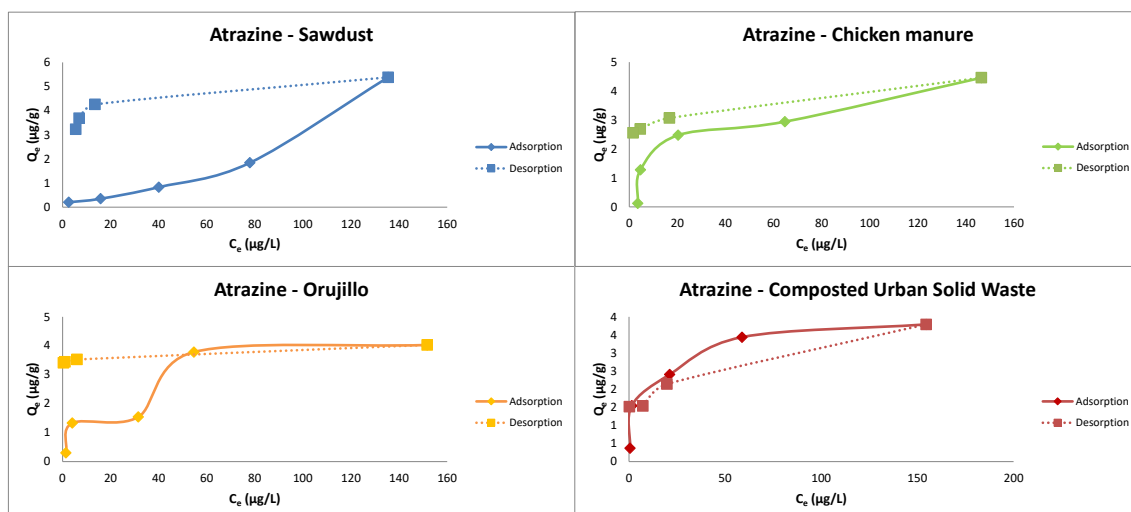


Figure S4. Sorption - desorption isotherms atrazine on each organic residue.

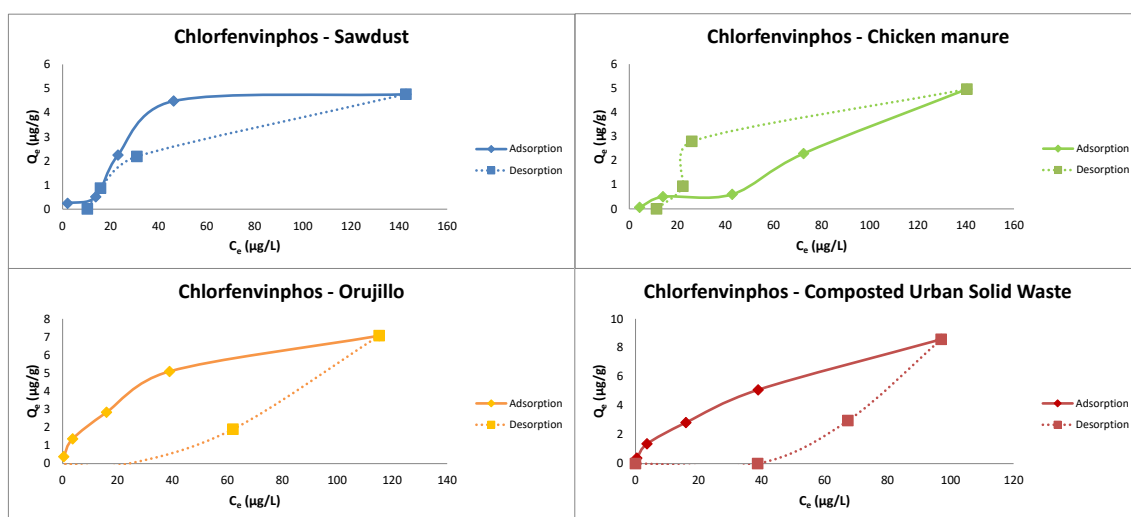


Figure S5. Sorption - desorption isotherms chlorfenvinphos on each organic residue.

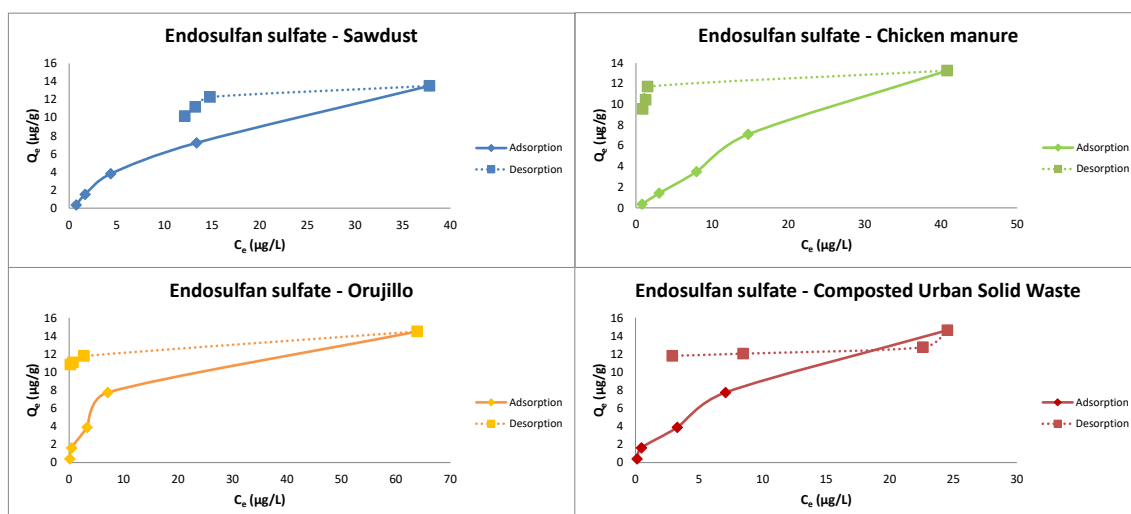


Figure S6. Sorption - desorption isotherms endosulfan sulfate on each organic residue.