

Supplemental Information for:

Characterization of clomazone sorption process in four agricultural soils using different kinetic models

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Table S1 Kinetic parameters predicted from the nonlinear analysis of hyperbolic model, and the linear analysis of pseudo-first- and pseudo-second-order kinetic models (the all set of soil/solution contact times is taken)

Soil	RG (Regosol)		PL (Planosol)		CH (Chernozem)		VR (Vertisol)	
Parameters / Initial conc.(mg L ⁻¹)	0.5	15	0.5	15	0.5	15	0.5	15
$q_{\max \text{ exp}}$ (mg kg ⁻¹)	0.97±0.01	27.90±0.19	1.11±0.02	31.44±0.22	1.18±0.04	32.62±0.06	1.31±0.02	35.32±0.08
Hyperbolic								
q_{\max} (mg kg ⁻¹)	1.05±0.03	26.58±0.32	1.14±0.01	30.38±0.52	1.23±0.01	30.90±0.51	1.37±0.02	34.41±0.28
R ²	0.974	0.985	0.992	0.965	0.993	0.966	0.979	0.991
Reduced chi-square	26.4×10 ⁻⁴	0.727	7.7×10 ⁻⁴	2.142	7.6×10 ⁻⁴	2.113	28.9×10 ⁻⁴	0.684
AIC*	-83.025	1.251	-101.475	17.461	-101.627	17.260	-81.654	0.337
Pseudo-first order								
q_{\max} (mg kg ⁻¹)	0.50±0.06	6.41±0.26	0.17±0.03	7.72±0.46	0.22±0.08	6.54±0.20	0.09±0.04	3.27±0.29
k_1 (h ⁻¹)	0.33±0.02	0.15±0.01	0.29±0.02	0.32±0.01	0.47±0.07	0.19±0.01	0.53±0.09	0.14±0.01
R ²	0.811	0.891	0.597	0.947	0.528	0.955	0.472	0.586
Residual sum of squares	1.035	0.106	2.220	0.227	7.834	0.070	12.663	0.545
AIC	-0.749	103.035	7.159	107.891	8.399	108.737	12.425	112.384
Pseudo-second order								
q_{\max} (mg kg ⁻¹)	1.01±0.01	27.85±0.25	1.11±0.01	32.57±0.29	1.20±0.01	32.89±0.19	1.32±0.01	35.46±0.17
k_2 (kg mg ⁻¹ h ⁻¹)	1.16±0.12	0.11±0.00	5.21±0.02	0.09±0.00	3.05±0.02	0.11±0.00	4.93±0.02	0.18±0.00
h (mg kg ⁻¹ h ⁻¹)	1.19±0.12	85.47±0.25	6.45±0.03	91.74±0.28	4.41±0.03	113.64±1.91	8.62±0.03	227.27±1.70
R ²	0.998	0.999	0.999	0.999	0.999	0.999	0.999	0.999
Residual sum of squares	1.249	5.4×10 ⁻⁴	0.078	7.3×10 ⁻⁴	0.107	3.1×10 ⁻⁴	0.110	2.6×10 ⁻⁴
AIC	-83.025	1.251	-101.475	17.461	-101.627	17.260	-81.654	0.337

* AIC - Akaike's Information Criterion Test.

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Table S2 Pearson correlation between clomazone sorption parameters obtained by hyperbolic and pseudo-first-order kinetic models and selected soil properties^a

	Hyperbolic model				Pseudo-first order model			
	$q_{\max \text{ exp}}$		q_{\max}		q_{\max}		k_1	
					Initial concentration (mg L ⁻¹)			
	0.5	15	0.5	15	0.5	15	0.5	15
OC	0.873 (0.127)	0.853 (0.147)	0.886 (0.114)	0.788 (0.201)	0.670 (0.330)	0.599 (0.401)	0.935 (0.065)	0.370 (0.630)
Clay	0.869 (0.131)	0.879 (0.121)	0.845 (0.155)	0.924 (0.076)	0.882 (0.118)	0.656 (0.344)	0.529 (0.471)	0.038 (0.962)
pH	0.413 (0.587)	0.465 (0.535)	0.318 (0.682)	0.531 (0.469)	0.708 (0.292)	0.029 (0.971)	0.150 (0.850)	0.652 (0.348)
Silt	0.579 (0.421)	0.636 (0.364)	0.455 (0.545)	0.627 (0.373)	0.855 (0.145)	0.156 (0.844)	0.105 (0.895)	0.692 (0.308)
Sand	0.839 (0.161)	0.874 (0.126)	0.764 (0.236)	0.898 (0.102)	0.981* (0.019)	0.349 (0.651)	0.392 (0.608)	0.358 (0.642)

^a OC-organic carbon content. Values in parentheses are *p* values of the correlations.

* Significance at the 0.05 level.

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Table S3 Pearson correlation between clomazone sorption parameters obtained by pseudo-second-order kinetic model and selected soil properties^a

	Pseudo-second order model					
	q_{\max}		k_2		h	
	Initial concentration (mg L ⁻¹)					
	0.5	15	0.5	15	0.5	15
OC	0.901 (0.099)	0.788 (0.212)	0.350 (0.650)	0.611 (0.389)	0.565 (0.435)	0.698 (0.302)
Clay	0.836 (0.164)	0.893 (0.107)	0.868 (0.132)	0.713 (0.287)	0.974* (0.026)	0.851 (0.149)
pH	0.326 (0.673)	0.580 (0.420)	0.917 (0.083)	0.102 (0.898)	0.783 (0.217)	0.290 (0.710)
Silt	0.500 (0.500)	0.748 (0.252)	0.871 (0.129)	0.086 (0.914)	0.734 (0.266)	0.166 (0.834)
Sand	0.781 (0.219)	0.936 (0.064)	0.980* (0.020)	0.419 (0.581)	0.982* (0.018)	0.629 (0.371)

^a OC-organic carbon content. Values in parentheses are *p* values of the correlations.

* Significance at the 0.05 level.

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Table S4 Kinetic parameters predicted from the linear analysis of Elovich and intraparticle diffusion (IPD) models, and nonlinear analysis of intraparticle diffusion dimensionless (IPDD) and two-site nonequilibrium model (TSNE) (the all set of soil/solution contact times is taken)

Soil	RG (Regosol)		PL (Planosol)		CH (Chernozem)		VR (Vertisol)	
Parameters / Initial conc.(mg L ⁻¹)	0.5	15	0.5	15	0.5	15	0.5	15
Elovich								
K _d (exp) (mL g ⁻¹)	3.19±0,11	3.00±0,14	4.01±0,09	3.65±0,11	4.54±0,13	3.89±0,15	5.58±0,09	4.51±0,13
(1/Y)ln(XY) (mg kg ⁻¹)	0.52±0.03	22.03±0.23	0.86±0.03	26.54±0.19	0.86±0.03	27.66±0.21	1.02±0.04	32.08±0.21
1/Y (mg kg ⁻¹)	0.18±0.02	1.97±0.13	0.11±0.02	1.81±0.11	0.14±0.02	1.58±0.12	0.13±0.02	1.10±0.12
X (mg kg ⁻¹ h ⁻¹)	3.2±0.0	(14.4±0.3)×10 ⁴	329.5±5.0	(42.4±0.1)×10 ⁵	66.3±1.0	(63.7±0.2)×10 ⁶	252.3±4.5	(54.3±0.2)×10 ¹¹
%*	53.48±3.10	78.96±0.82	77.93±2.71	84.41±0.60	72.72±2.53	84.79±0.64	77.48±3.05	90.83±0.59
R ²	0.907	0.952	0.779	0.959	0.857	0.936	0.738	0.880
Residual sum of squares	0.086	5.049	0.085	3.644	0.085	4.42	0.168	4.265
IPD								
k _{int,1} (mg kg ⁻¹ min ^{-0.5})	0.06±0.00	1.27±0.09	0.07±0.00	0.23±0.02	0.06±0.00	0.20±0.02	0.09±0.00	0.13±0.02
C (mg kg ⁻¹)	0.03±0.00	13.14±0.57	0.34±0.04	24.68±0.39	0.38±0.06	26.00±0.35	0.31±0.03	31.05±0.42
R ²	0.993	0.989	0.976	0.921	0.943	0.917	0.992	0.872
Residual sum of squares	0.00267	0.14666	0.00381	7.03462	0.01323	5.75264	0.00236	8.10803
k _{int,2} (mg kg ⁻¹ min ^{-0.5})	0.001±0.000	0.15±0.01	0.0005±0.0002		0.002±0.001		0.0002±0.0001	
C (mg kg ⁻¹)	0.92±0.01	22.30±0.28	1.09±0.01		1.13±0.01		1.31±0.01	
R ²	0.741	0.947	0.430		0.559		0.698	
Residual sum of squares	1.6×10 ⁻⁴	1.384	3.5×10 ⁻⁶		0.004		6.9×10 ⁻⁵	
IPDD								
R _i	1.00±0.02	0.44±0.02	0.65±0.03	0.24±0.01	0.60±0.04	0.19±0.01	0.76±0.02	0.12±0.01
R ²	0.989	0.987	0.968	0.907	0.917	0.870	0.991	0.751
Reduced chi-square	6.6×10 ⁻⁴	1.1×10 ⁻⁴	9.1×10 ⁻⁴	5.9×10 ⁻⁴	0.003	6.5×10 ⁻⁴	2.9×10 ⁻⁴	5.4×10 ⁻⁴
TSNE								
K (ml g ⁻¹)	3.23±0.03	2.81±0.01	3.98±0.01	3.86±0.02	4.55±0.01	3.93±0.02	5.67±0.02	4.46±0.02
F	0.016±0.003	0.579±0.062	0.227±0.010	0.656±0.051	0.216±0.011	0.695±0.051	0.167±0.012	0.790±0.082
k ₂ (h ⁻¹)	0.310±0.036	0.461±0.091	0.819±0.029	0.149±0.036	0.557±0.029	0.155±0.034	0.692±0.051	0.301±0.090
R ²	0.974	0.896	0.996	0.935	0.993	0.943	0.982	0.842
Reduced chi-square	4.5×10 ⁻⁴	1.4×10 ⁻⁴	1.8×10 ⁻⁵	8.2×10 ⁻⁵	5.3×10 ⁻⁵	5.5×10 ⁻⁵	1.4×10 ⁻⁴	7.4×10 ⁻⁵

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Table S5 Pearson correlation between clomazone sorption parameters obtained by Elovich model and selected soil properties^a

	Elovich model					
	(1/Y) ln(XY)		1/Y		X	
			Initial concentration (mg L ⁻¹)			
	0.5	15	0.5	15	0.5	15
OC	0.758 (0.242)	0.823 (0.177)	0.317 (0.683)	0.843 (0.157)	0.076 (0.924)	0.556 (0.444)
Clay	0.888 (0.112)	0.911 (0.089)	0.701 (0.299)	0.850 (0.150)	0.796 (0.204)	0.849 (0.150)
pH	0.618 (0.382)	0.489 (0.511)	0.864 (0.136)	0.291 (0.709)	0.993** (0.007)	0.337 (0.663)
Silt	0.789 (0.211)	0.599 (0.401)	0.970* (0.030)	0.345 (0.655)	0.605 (0.222)	0.081 (0.919)
Sand	0.953* (0.047)	0.876 (0.124)	0.920 (0.080)	0.715 (0.285)	0.889 (0.111)	0.587 (0.413)

^a OC-organic carbon content. Values in parentheses are *p* values of the correlations.

* Significance at the 0.05 level.

* Significance at the 0.01 level.

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Table S6 Pearson correlation between clomazone sorption parameters obtained by intraparticle diffusion (Weber-Morris model) and intraparticle diffusion dimensionless models and selected soil properties^a

	Intraparticle diffusion model						Intraparticle diffusion dimensionless model	
	$k_{int,1}$		C_1		$k_{int,2}$	C_2	R_i	
			Initial concentration (mg L ⁻¹)					
	0.5	15	0.5	15	0.5	0.5	0.5	15
OC	0.458 (0.542)	0.716 (0.284)	0.681 (0.319)	0.802 (0.198)	0.239 (0.761)	0.816 (0.184)	0.577 (0.423)	0.843 (0.157)
Clay	0.943 (0.057)	0.740 (0.260)	0.563 (0.437)	0.965 (0.135)	0.677 (0.323)	0.917 (0.083)	0.382 (0.617)	0.824 (0.176)
pH	0.573 (0.427)	0.598 (0.402)	0.496 (0.504)	0.561 (0.439)	0.734 (0.266)	0.491 (0.509)	0.422 (0.578)	0.497 (0.503)
Silt	0.261 (0.739)	0.913 (0.087)	0.936 (0.064)	0.771 (0.229)	0.091 (0.909)	0.583 (0.416)	0.931 (0.069)	0.761 (0.239)
Sand	0.735 (0.265)	0.917 (0.083)	0.814 (0.186)	0.929 (0.071)	0.481 (0.519)	0.873 (0.127)	0.695 (0.305)	0.898 (0.102)

^a OC-organic carbon content. Values in parentheses are *p* values of the correlations.

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Table S7 Pearson correlation between clomazone sorption parameters obtained by two-site nonequilibrium (TSNE) model and selected soil properties^a

	Two-site nonequilibrium model							
	K_d (exp)		K		F		k_2	
					Initial concentration (mg L ⁻¹)			
	0.5	15	0.5	15	0.5	15	0.5	15
OC	0.869 (0.131)	0.849 (0.151)	0.867 (0.133)	0.787 (0.213)	0.531 (0.469)	0.853 (0.147)	0.276 (0.724)	0.419 (0.581)
Clay	0.871 (0.129)	0.890 (0.110)	0.868 (0.132)	0.886 (0.114)	0.515 (0.485)	0.887 (0.113)	0.757 (0.243)	0.309 (0.691)
pH	0.379 (0.621)	0.451 (0.549)	0.359 (0.641)	0.582 (0.418)	0.583 (0.417)	0.411 (0.588)	0.914 (0.086)	0.479 (0.521)
Silt	0.510 (0.490)	0.590 (0.410)	0.474 (0.526)	0.761 (0.239)	0.981* (0.019)	0.526 (0.474)	0.933 (0.067)	0.947 (0.053)
Sand	0.808 (0.192)	0.859 (0.141)	0.788 (0.212)	0.938 (0.062)	0.805 (0.195)	0.826 (0.174)	0.938 (0.062)	0.655 (0.345)

^a OC-organic carbon content. Values in parentheses are *p* values of the correlations.

* Significance at the 0.05 level.