

Quantitative Prediction Of Atrazine Sorption In A Manitoba Soil Using Conventional Chemical Kinetics Instead Of Empirical Parameters.

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SUPPORTING INFORMATION

Table S1
Spreadsheet formulas For Kinetics

Z₁: Column O
$+I\$22*((@EXP(\$N10*\$L10))-1)$
$+I\$22*((@EXP(\$N11*\$L11))-1)$
$+I\$22*((@EXP(\$N12*\$L12))-1)$
$+I\$22*((@EXP(\$N13*\$L13))-1)$
$+I\$22*((@EXP(\$N14*(\$L14-\$L13)))-1)+\$O13$
$+I\$22*((@EXP(\$N15*(\$L15-\$L10)))-1)+\$O\11

Z₂: Column P
$(\$I\$20*(@EXP(\$N10*\$L10))-\$I\$21)$
$(\$I\$20*(@EXP(\$N11*\$L11))-\$I\$21)$
$(\$I\$20*(@EXP(\$N12*\$L12))-\$I\$21)$
$(\$I\$20*(@EXP(\$N13*\$L13))-\$I\$21)$
$(\$I\$20*(@EXP(\$N14*(\$L14-\$L13)))-\$I\$24)+\$P13$
$(\$I\$20*(@EXP(\$N15*(\$L15-\$L10)))-\$I\$24)+\$P\$11$

Columns Q & R	
(Z₁/Z₂) + Y	M₁
(Mol/L)	(Mol/L)
$+\$O10/\$P10+\$Y10$	$+\$I\$21-\$Q10$
$+\$O11/\$P11+\$Y11$	$+\$I\$21-\$Q11$
$+\$O12/\$P12+\$Y12$	$+\$I\$21-\$Q12$
$+\$O13/\$P13+\$Y13$	$+\$I\$21-\$Q13$
$+\$O14/\$P14+\$Y14$	$+\$I\$21-\$Q14$
$+\$O15/\$P15+\$Y15$	$+\$I\$21-\$Q15$

Column Y
$Y = \theta_{d1}(W/V)$
(Mol/L)
$+\$V10*(1-@EXP(-\$Z10*(\$L10-\$L\$10)))$
$+\$V11*(1-@EXP(-\$Z11*(\$L11-\$L\$10)))$
$+\$V12*(1-@EXP(-\$Z12*(\$L12-\$L\$10)))$
$+\$V13*(1-@EXP(-\$Z13*(\$L13-\$L\$10)))$
$+\$V14*(1-@EXP(-\$Z14*(\$L14-\$L\$10)))$
$+\$V15*(1-@EXP(-\$Z15*(\$L15-\$L\$10)))$

Table S2
Spreadsheet Entries For Iterative Calculations

ITERATIONS			
Copy Formulas AD & AE		To Values AB & AC	
Labile Sorption	Bound Res.	Labile Sorption	Bound Res.
*****	*****	*****	*****
Values	Values	For Iteration	For Iteration
$\theta_{a1}(W/V)$	$\theta_{d1}(W/V)$	$\theta_{a1}(W/V)$	$\theta_{d1}(W/V)$
(Mol/L)	(Mol/L)	(Mol/L)	(Mol/L)
*****	*****	*****	*****
0.0000E+00	0.0000E+00	+\$V10	+\$Y10
1.8219E-07	1.2384E-09	+\$V11	+\$Y11

TABLE S3: Model 4a Calibration

Experimental Rate Coefficients			
No.	t	k _{r1}	k _d
	DAYS	g/(Mol x days)	DAYS ⁻¹
1	0.000		
2	0.130	1.2667E+07	5.2465E-02
3	0.180	9.8906E+06	4.9055E-02
4	0.250	8.3890E+06	4.2640E-02
5	0.500	9.9334E+06	4.3179E-02
6	1.000	2.8535E+06	4.4242E-02
7	1.100	2.6274E+06	4.4019E-02
8	1.200	2.4391E+06	4.3798E-02
9	1.250	2.3563E+06	4.3689E-02
10	2.000	1.6118E+06	4.2108E-02
11	2.125	1.5390E+06	4.1855E-02
12	2.200	1.4993E+06	4.1704E-02
13	2.250	1.4733E+06	4.1622E-02
14	3.000	1.2001E+06	4.0169E-02
15	3.050	1.1867E+06	4.0076E-02
16	3.100	1.1737E+06	3.9985E-02
17	3.150	1.1611E+06	3.9893E-02
18	3.200	1.1489E+06	3.9803E-02
19	3.250	1.1371E+06	3.9713E-02
20	3.900	1.0113E+06	3.8581E-02
21	4.000	9.9598E+05	3.8404E-02
22	4.150	9.8750E+05	3.7805E-02
23	4.200	9.6701E+05	3.8070E-02
24	4.250	9.6020E+05	3.7987E-02
25	7.000	7.3940E+05	3.3948E-02
26	7.125	7.3360E+05	3.3785E-02
27	7.200	7.3022E+05	3.3688E-02
28	7.250	7.2800E+05	3.3624E-02
29	8.000	6.9844E+05	3.2688E-02
30	8.050	6.9668E+05	3.2628E-02
31	8.150	6.9324E+05	3.2507E-02
32	8.200	6.9155E+05	3.2448E-02
33	8.250	6.8989E+05	3.2388E-02
34	9.000	6.6742E+05	3.1520E-02
35	9.250	6.6084E+05	3.1242E-02
36	10.000	6.4338E+05	3.0435E-02
37	10.100	6.4128E+05	3.0330E-02
38	10.200	6.3923E+05	3.0227E-02
39	10.250	6.3822E+05	3.0175E-02
40	11.000	6.2444E+05	2.9423E-02
41	11.050	6.2361E+05	2.9374E-02
42	11.150	6.2196E+05	2.9277E-02
43	14.000	5.8754E+05	2.6760E-02
44	14.050	5.8711E+05	2.6720E-02
45	14.125	5.8647E+05	2.6659E-02
46	14.200	5.8584E+05	2.6600E-02
47	15.000	5.7974E+05	2.5977E-02
48	15.050	5.7939E+05	2.5940E-02
49	15.125	5.7888E+05	2.5883E-02
50	15.200	5.7836E+05	2.5827E-02
51	15.250	5.7805E+05	2.5789E-02
52	16.000	5.7408E+05	2.5162E-02
53	16.050	5.7324E+05	2.5204E-02
54	16.150	5.7270E+05	2.5133E-02
55	16.250	5.7270E+05	2.5044E-02
56	16.800	5.6950E+05	2.4680E-02
57	17.000	5.6862E+05	2.4544E-02
58	17.050	5.6841E+05	2.4510E-02
59	17.100	5.6820E+05	2.4476E-02
60	17.200	5.6779E+05	2.4409E-02
61	18.000	5.6486E+05	2.3885E-02
62	18.050	5.6470E+05	2.3853E-02
63	18.125	5.6446E+05	2.3806E-02
64	18.200	5.6423E+05	2.3758E-02