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Novel calculator for estimation of Freundlich partitioning coefficient

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Abstract

An estimation method for the Freundlich organic carbon normalized partitioning coefficient (K_{foc}) is presented. It is based on regressions developed from batch equilibrium experiments submitted to U.S. EPA for pesticide registration. The regressions represent 18 specific agricultural soils from the U.S. and Europe, and are based on 41 pesticide active ingredients or metabolites. The predictive variable used is the subcooled liquid solubility (S_{sl}), whose calculation requires the compound's solubility, and if a solid (mp > 25 °C), its melting point. S_{sl} represents the compound's solubility as if it were a liquid at room temperature and does not assume that the compound is neutral. The estimation method was tested on 333 pesticides, and estimated means matched published K_{foc} values to within 10× for 83%, 3× for 65%, and 2× for 43%. The estimation method (K_{foc} Estimator v0.1) was further tested against data for 94 herbicides, 55 Superfund Priority Pollutants and 22 polychlorinated biphenyls. The estimated mean and median K_{foc} values were highly correlated ($R^2 > 0.63$ to 0.87) with the measured values. Matching of reported to estimated values was generally good. The herbicides were 51%–54% within 2×, 74%–77% within 3×, and 93%–94% within 10×. The Priority Pollutants were 22%–29% within 2×, 38%–55% within 3×, and 73%–75% within 10×. The estimates for the PCBs were low, but the maximum estimated K_{foc} was consistently within 10 × of the reported K_{oc}. This may be due to the PCB data representing a single soil, rather than the central-tendency estimates produced by K_{foc} Estimator v0.1.

Keywords

Freundlich partition coefficient; Pesticides; Estimation; Agriculture; Soil; K_f; K_{foc}; Subcooled liquid solubility; Exponent

1. Introduction

A coefficient to describe soil-water partitioning is essential to computer modeling of environmental pollutants, including pesticides and industrial chemicals. The organic carbon normalized partitioning coefficient (K_{oc}) and its Freundlich equivalent (K_{foc}) are in common usage for this purpose. In the U.S., these parameters are measured in batch equilibrium studies according to harmonized guideline 835.1230 (U.S. EPA, 2008).

The U.S. EPA Office of Pesticides Programs (OPP) receives dozens of batch equilibrium studies each year, as routine FIFRA (Federal Insecticide, Fungicide and Rodenticide Act) data requirements, for both new pesticides and those under periodic review. Because the soils used in these tests are required to be representative of the area of intended use, particular agricultural soils are used repeatedly in studies submitted to OPP. The pesticide active ingredients that are tested range from neutral organics, to compounds that are ionic, either positively or negatively charged at pH7.

A comprehensive review of the literature for K_{oc} and K_{oc} prediction methods is beyond the scope of this article. Estimation methods for K_{oc} or K_{oc} have been reviewed by Brusseau (1993), Sabljic et al. (1995), Doucette (2003), Shao et al. (2014), and most recently by Vitale and DiGuardo (2019). Many QSARs (Quantitative Structure-Activity Relationships) for K_{oc} or K_{oc} use the octanol/water partitioning coefficient (K_{ow}), Molecular Connectivity Index (MCI) or solubility as the independent variable. In practice, OPP uses the KOCWIN v2.00 program in EPISuite (US EPA, 2012), which gives two estimates, one based on K_{ow} and the other on MCI. The estimates provided do not quantitatively account for ionization of the target compound and are not explicitly related to agricultural soils.

In this paper, K_{oc} is regressed against the S_{oc}, which is essentially an estimate of the solubility of a compound as if it were a liquid at room temperature. The use of S_{oc} (Liu et al., 2013) as the independent variable is intended to make the QSAR equally applicable to neutral and ionic compounds, and to compounds that are solids or liquids at 25 °C.

This paper is an attempt to use measurements of K_{oc} on eighteen agricultural soils to develop a general-purpose QSAR for prediction of both K_{oc} and the associated exponent, 1/n. The significance of this work is in the use of K_{oc} measurements from commonly-tested agricultural soils, based on a common EPA testing guideline, to give central-tendency estimates of K_{oc} for an unmeasured compound from a greater number of soils than otherwise would be submitted. The estimation method is intended to be robust and to work equally well for solids and liquids, as well as neutral and anionic compounds.

2. Materials and methods

Batch equilibrium studies in OPP's electronic data holdings were searched to find studies that had used the same soils, for at least three different compounds (active ingredients or metabolites thereof). A total of 18 soils with studies for at least three, and as many as ten compounds, were identified (Table 1). Eleven were U.S. soils, and seven were from Europe. Soils were identified by name, for example, the Don Uglem clay loam from North Dakota. The soil identity in different batch equilibrium studies was confirmed by comparing percent sand, silt, and clay content, and well as fraction organic carbon.

Table 1 also summarizes the number of compounds tested for each of the soils, along with the range of solubility (of the solid), and the range of melting points (Kelvins) (Lewis et al., 2016). At least 3, and as many as 10 compounds were included in the regressions for each soil. For each regression, estimates of K_{oc} were compared to the measured values to ensure

that the estimates were reasonable (data not shown). Overall, 41 different active ingredients or degradates were included in the 18 regressions.

In order to calculate the S_{scl} , only compounds with reported solubility and melting point were retained for the regressions. S_{scl} was calculated by the method presented in Liu et al. (2013) using the assumption of 56.5 kJ/mol/K for the entropy of fusion. The uncertainty introduced by the use of S_{scl} is in its estimation for solid compounds. The further a compound's melting point is from 25 °C, the greater the possible extrapolation in S_{scl} from the solubility from of the solid-state compound. The assumption for the entropy of fusion may over- or under-estimate the actual value, so the error is believed to largely cancel out.

Reported K_f values, not normalized for the fraction of organic carbon in the soil, were regressed versus calculated S_{scl} values and plotted on a log-log scale. A power regression was run for each soil, because of the very wide range of S_{scl} (8 orders of magnitude in Fig. 1) and K_f (over 3 orders of magnitude) values, so that a straight line was obtained on the log-log plot. Power regressions were used for all soils to be consistent. The resulting slopes, exponents and R^2 values were recorded for each soil.

The regression models for the 18 soils, in the form of the K_{foc} Estimator v0.1 Excel spreadsheet, were used to estimate K_{foc} for 333 pesticides from the Footprint database (Lewis et al., 2016), 94 herbicides (Ahrens, 1994), 55 Superfund Priority Pollutants (US EA, 1996) and 22 Polychlorinated biphenyls (Hansen et al., 1999).

3. Results

Fig. 1 presents the plot for the Speyer 2.2 loamy sand soil from Germany, which had the most data. Note that the relationship between K_f and S_{scl} spans 8 orders of magnitude of S_{scl} . Table 2 presents the slope and exponent of the power function describing the log-log plot of K_f versus sub-cooled liquid solubility for each soil. These are the regression parameters used in the K_{foc} Estimator v0.1 model to produce the 18 individual K_{foc} estimates.

Equations for the Freundlich exponent $1/n$ were estimated by regressing, within the data set for each of the 18 soils, the reported $1/n$ value versus the melting point of each compound. These results are also reported in Table 2.

In general, the regression of $1/n$ versus melting point gave an intercept less than one with a shallow positive slope, or an intercept greater than one with a shallow negative slope, so that a value of $1/n = 1$ was reached at some melting point. With a few exceptions, the intercepts were close to one (0.5–2). Larger intercepts (Ephrata loamy sand) had correspondingly steeper slopes. Only two soils (Horse Camp Bridge and Bosket sandy loam) had intercepts less than one and a negative slope, but in both cases the slope was very close to one and the R^2 value was low (0.002–0.0561), indicating that $1/n$ was close to one in all cases. Overall, these results indicate that $1/n$ is not a strong function of melting point, and that use of a value of $1/n = 1$ would not be unreasonable.

A calculator (Kfoc Estimator v. 0.1) was constructed from the results in Tables 1 and 2 to estimate Kfoc and $1/n$ from the melting point and solubility of 333 pesticide active ingredients found in the Footprint database (Lewis et al., 2016). Each of the 333 pesticides had reported Kfoc, melting point, and solubility data, and were generally organic chemicals. No attempt was made to segregate the 333 pesticides by structural class. Values of pKa were recorded to test whether Kfoc predictions were affected by chemicals being ionized rather than neutral. The calculator estimates Kfoc for each of the 18 soils, then reports the median, average, standard deviation, minimum and maximum values of Kfoc, and calculates $1/n$ for each soil based on the melting point regression.

Fig. 2 shows a plot of the predicted versus reported average Kfoc values for the 333 pesticides. The 1:1 line is indicated, showing general good agreement, with some scatter as expected since many different structural classes, not all expected to partition to organic carbon, are included. Predictions were within a factor of 10 for 83%, within a factor of 3 for 65%, and within a factor of 2 for 43% of the 333 pesticides. The worst predictions were obtained for quaternary ammonium compounds (e.g., paraquat) since these cationic compounds are not expected to partition to organic carbon.

To test whether the Kfoc of ionic compounds was predicted well, the ratio of the predicted and reported Kfoc values was plotted versus the reported pKa for each compound (data not shown). The ratio of predicted Kfoc to reported Kfoc was 1 or less for 99 compounds, and >1 for 74 compounds; 65 were within $2\times$. The lack of an apparent trend in the data suggests that pKa had little influence on the quality of the prediction.

The Kfoc Estimator v. 0.1 program was further tested against published data for Koc for 95 diverse herbicides (WSSA, 1994), 56 Superfund Priority Pollutants (U.S. EPA, 1996), and 22 PCBs (Hansen et al., 1999) measured in one soil. For the herbicides (Fig. 3), the estimated Kfoc values were well-correlated ($R^2 = 0.7685$ vs. median estimates, $R^2 = 0.6347$ vs. mean estimates).

Quaternary ammonium compounds and arsenic-containing compounds were not well-predicted, presumably because their sorption behavior is not correlated to organic carbon content. For the Priority Pollutants (Fig. 4), measured values were predicted with R^2 values of 0.8737 vs. median predicted and 0.8664 vs. mean predicted. Finally, the Koc values for the PCBs (Fig. 5) were estimated with R^2 values of 0.8316 vs. median estimated and 0.8303 vs. mean estimated.

As can be seen in Figs. 3 to 5, the accuracy of the mean and median estimates differs for the three data sets. In Fig. 3, the mean estimates have a slope near 1, while the median estimates have a slope near 0.5. In Fig. 4 for Superfund Priority Pollutants, the regression lines are reasonably near the 1:1 values, with estimates underpredicting to some degree as the values approach 100,000. In Fig. 5, for PCBs, while the estimates are highly correlated with the measured values, there is considerable underestimation. This is probably because the measured values are from a single soil, and so do not represent an 'average' soil in the way that the Kfoc Estimator v0.1 attempts to do. Literature and estimated values for Figs. 3–5 are in the Appendix.

4. Discussion

The calculated S_{sc1} was well-correlated with the reported K_f values, even over 8 orders of magnitude of S_{sc1} for the Speyer 2.2 soil (see Fig. 1). R^2 values for the 18 soils ranged from 0.70 to 0.99, with one exception, indicating that S_{sc1} is a useful independent variable for prediction of K_f .

The correlation between mean and median predicted K_{foc} values from the K_{foc} Estimator v0.1 is shown in Figs. 2 to 5 for different data sets. The data in Fig. 2 (333 pesticide active ingredients) show a fair correlation between the mean predicted K_{foc} and the reported values ($R^2 = 0.39$). This data set includes compounds such as quaternary ammonium cations, whose very strong partitioning behavior does not reflect their very high solubility. These compounds' K_{foc} values are predicted poorly by K_{foc} Estimator v0.1, which contributes to the relatively low R^2 . Even so, predictions were within a factor of 10 for 83%, within a factor of 3 for 65%, and within a factor of 2 for 43% of the 333 pesticides.

Fig. 3 shows the results for a set of 94 herbicides. The correlations between reported K_{oc} estimated mean K_{foc} ($R^2 = 0.63$) and estimated median K_{foc} ($R^2 = 0.77$) are good. The estimated means are within a factor of 2 for 51% of the 94 herbicides, within a factor of 3 for 77% and within a factor of 10 for 94%. The estimated median K_{foc} values are within 2× for 54%, 3× for 74% and 10× for 93% of the 94 herbicides. This indicates generally good agreement between reported and estimated values.

Fig. 4 shows the correlation between reported geometric mean K_{oc} for 55 Superfund Priority Pollutants, and the mean and median estimated K_{foc} values from K_{foc} Estimator v0.1. Correlations are good (mean, $R^2 = 0.86$; median, $R^2 = 0.87$). The estimated mean K_{foc} values are within 2× of reported K_{oc} values for 22%, within 3× for 38% and within 10× for 75% of the 55 compounds. The estimated median K_{foc} values are within 2× for 29%, within 3× for 55% and within 10× for 73% of the 55 compounds. Agreement is not as good as for the 94 herbicides. This may be due to the structural diversity of the 55 Priority Pollutants, and due to the structural differences from pesticides in general.

Fig. 5 shows the correlation between reported $\log K_{oc}$ values for 22 PCB congeners tested on a single soil, and the mean and median estimated K_{foc} values. Correlations are good ($R^2 = 0.83$ for both mean and median). However, the values estimated by K_{foc} Estimator v0.1 are significantly lower than the reported values. The mean estimates run from 2 to 14% of reported K_{oc} , and the median values run from 0.65 to 10.4% of reported K_{oc} . Seven estimated means and only one estimated median are within 10× of reported K_{oc} . Estimated maximum K_{foc} values were within a factor of 10 of the reported K_{oc} . The low estimates for this data set are attributed to the fact that the reported values are for a single soil, while K_{foc} Estimator v0.1 gives the central tendency for estimates from 18 soils. These central tendency values are not intended to reflect any one soil.

5. Conclusions

A calculator (K_{foc} Estimator v. 0.1) for the Freundlich Organic Carbon-normalized partition coefficient (K_{foc}) and its associated exponent ($1/n$) has been constructed from studies

submitted to the U.S. EPA pesticides program. The calculator is based on regressions for 41 active ingredients and metabolites in 18 specific agricultural soils. It produces 18 separate estimates, so soil-to-soil variability may be assessed; mean and median results represent central tendencies across the 18 soils. The use of the subcooled liquid solubility (Sscl) as the independent variable makes the calculator applicable to both neutral and anionic organic compounds. Predictions of Kfoc for 333 active ingredients were within 10× for 83%, 3× for 65%, and 2× for 43%. Predictions are well-correlated with published values for diverse sets of compounds, including herbicides, Priority Pollutants and polychlorinated biphenyls. Testing shows that the Kfoc Estimator is not applicable to quaternary ammonium or organometallic compounds. A copy of Kfoc Estimator v. 0.1 is available from the author.

Acknowledgments

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Appendix. Measured and Estimated Koc/Kfoc Values from Hansen (1999), U.S. EPA (1996) and Ahrens (1994). Values estimated by Kfoc Estimator v. 0.1 marked as “this work.”

CAS No	name	Water solubility mg/L	mp, °C	Geomean Koc	This Work	
					Ea Mean Kfoc	Est Median Kfoc
50-32-5	Benzo(a)pyrene	162E-03	179	968,774	37,561	11,909
72-43-5	Methoxychlor	4,50E-02	82.5	80,000	16,551	8039
50-29-3	DDT	2,50E-02	108.5	677,934	16,493	8025
56-55-3	Benz(a)anthracene	9.40E-03	155	357,537	15,591	7798
117-81-7	Bis(2-ethylhexyl)phthalate	3.40E-01	-50	111,123	10,367	6188
57-74-9	Chlordane	5.60E-02	105	51,310	10,233	6137
72-54-8	DDD	9.00E-02	109.5	45,800	7225	4885
76-44-8	Heptachlor	1.80E-01	95.5	9,528	5844	4129
309-00-2	Aldrin	1.80E-01	104.3	48,685	5237	3902
206-44-0	Fluoranthene	2.06E-01	107	49,096	4716	3654
8001-35-2	Toxaphene	7.40E-01	65	95,816	3394	3284
129-00-0	Pyrene	1.35E-01	156	67,992	3316	2896
85-68-7	Butyl benzyl phthalate	2.69E+00	-35	13,746	3308	2892
120-12-7	Anthracene	4.34E-02	218	23,493	2900	2440
60-57-1	Dieldrin	1.95E-01	175.5	25,546	2267	2043
86-73-7	Fluorene	1.98E+00	116	7,707	1494	1225
83-32-9	Acenaphthene	4.24E+00	95	4,898	1329	1045

CAS No	name	Water solubility mg/L	mp, °C	Geomean Koc	This Work	
					Ea Mean Kfoc	Est Median Kfoc
72-20-8	Endrin	2.50E-01	228	10,811	1224	934
115-29-7	Endosulfan	5.10E-01	209	2,040	1093	825
319-84-6	a-HCH (a-BHC)	2.00E+00	158	1,762	1008	779
58-89-9	g -HCH (Lindane)	6.80E+00	112.5	1,352	937	739
91-20-3	Naphthalene	3.10E+01	80.2	1,191	693	596
106-46-7	1,4-Dichlorobenzene	7.38E+01	53.1	616	631	536
95-50-1	1,2-Dichlorobenzene	1.56E+02	-17	379	606	511
108-38-3	m-Xylene	1.61E+02	-47.4	196	599	504
319-85-7	b-HCH (b-BHC)	2.40E-01	312	2,139	591	496
100-41-4	Ethylbenzene	1.69E-02	-95	204	588	494
95-47-6	o-Xylene	1.78E+02	-25	241	577	482
106-42-3	p-Xylene	1.85E+02	13	311	569	474
127-18-4	Tetrachloroethylene	2.00E+02	-22	265	552	458
120-82-1	1,2,4-Trichlorobenzene	3.00E+02	17	1,659	476	384
100-42-5	Styrene	3.10E+02	-30	912	470	378
108-90-7	Chlorobenzene	4.72E+02	-45	224	403	315
108-88-3	Toluene	5.26E+02	-94	140	388	300
118-74-1	Hexachlorobenzene	6.20E+00	228	80,000	362	277
56-23-5	Carbon tetrachloride	7.93E-r02	-23	152	335	251
84-66-2	Diethylphthalate	1.08E+03	-40.5	82	300	220
79-01-6	Trichloroethylene	1.10E+03	-87	94	298	218
71-55-6	1,1,1-Trichloroethane	1.33E+03	-35	135	278	201
71-43-2	Benzene	1.75E+03	5	62	253	179
98-95-3	Nitrobenzene	2.09E+03	6	119	238	168
75-35-4	1,1 -Dichloroethylene	2.25E+03	-122	65	232	164
78-87-5	1,2-Dichloropropane	2.80E+03	-100.3	47	215	151
79-34-5	1,1,2,2-Tetrachloroethane	2.97E+03	-36	79	210	148
75-25-2	Bromoform	3.10E+03	7.5	126	207	146
79-00-5	1,1,2-Trichloroethane	4.42E-i-03	-37	75	183	128
75-34-3	1,1-Dichloroethane	5.06E-f03	-97	53	175	122
156-60-5	trans-1,2-Dichloroethylene	6.30E+03	-50	38	162	113
67-66-3	Chloroform	7.92E-f-03	-63	53	150	104
107-06-2	1,2-Dichloroethane	8.52E-r03	-35	38	147	101
75-09-2	Methylene chloride	1.30E+04	-95.1	10	127	87
74-83-9	Methyl bromide	1.52E+04	-94	9	121	82
111-44-4	Bis(2-chloroethyl)ether	1.72E+04	-50	76	116	79

U.S. EPA (1996)

PCB#	Log Koc	This Work		Sol mg/L	mp °C	This Work	
		Log est mean	Log est median			Est mean Kfoc	Est median Kfoc
183	6.32	5.06	4.29	4.90E-03	83	114,096	19,631
138	6.2	4.84	4.20	7.29E-03	80.5	68,990	15,718
180	6.37	4.81	4.18	3.85E-03	112	64,527	15,248
153	6.19	4.58	4.08	9.14E-03	103	37,945	11,920
151	6.02	4.47	4.03	1.36E-02	100	29,375	10,611
101	5.78	4.43	4.01	2.63E-02	77	26,612	10,133
118	5.99	4.41	4.00	1.34E-02	109	25,474	9927
87	5.82	4.37	3.98	2.84E-02	81	23,449	9543
44	5.1	4.22	3.91	1.00E-01	47	16,677	8070
49	5.09	4.16	3.87	7.84E-02	67	14,398	7484
70	5.26	4.13	3.86	3.62E-02	106	13,372	7200
95	5.62	4.09	3.84	5.41 E-02	94	12,250	6866
28	4.98	4.05	3.82	1.43E-01	57	11,303	6533
31	4.96	3.99	3.78	1.43E-01	67	9770	5959
66	5.38	3.98	3.77	3.68E-02	128	9568	5880
18	4.79	3.93	3.74	2.99E-01	44	8576	5476
52	5.1	3.93	3.74	1.13E-01	87	8537	5460
60	5.38	3.88	3.71	3.89E-02	142	7634	5070
40	5.14	3.82	3.66	8.07E-02	121	6603	4594
8	4.76	3.79	3.64	5.38E-01	43	6187	4392
15	4.79	3.74	3.60	6.00E-02	149	5467	4024
2	4.58	3.73	3.60	9.00E-01	32	5340	3956

Hansen et al. (1999)

compound	water solubility mg/L	mp, °C	Koc	This Work	
				mean est Kfoc	median est Kfoc
fluridone	12	154–155	1000	526	433
oxyfluorfen	0.1	76–80	5483	10,444	6217
lactofen	0.1	419–455	10000	17,170	8190
fluazifop Butyl Ester	1.1	10	5700	5222	3894
fenoxaprop Ethyl Ester	0.5	89–91	9490	3646	3089
benefin	0.1	65–66.5	9000	12,631	6985
trifluralin	0.3	46–47	7000	8327	5371
ethalfluralin	0.3	57–59	4000	7088	4822
isopropalin	0.08	no data	10,000	28,040	10,384
prodiamine	0.013	122.5–124	13,000	20,643	8973
cinmethylin	6.3	no data	300	855	692

compound	water solubility mg/L	mp, °C	Koc	This Work	
				mean est Kfoc	median est Kfoc
pendimethalin	0.275	47–57	17,200	8083	5267
oxadiazon	0.7	87	3200	3196	2804
sethoxydim pH7	4390	no data	100	184	129
acifluorfen	120	142–160	113	253	180
bifenox	0.398	84–86	10,000	4337	3466
tridiphan	1.8	428	5600	3296	2884
napropamide	73	748–755	700	525	432
norflurazon	28	177	700	320	238
bensulide	25	344	1000	1132	846
desmedipham	7	120	1500	865	698
phenmedipham	10	143–144	2400	618	523
imazaquin	60	219–224	20	171	120
butylate	44	no data	400	984	766
clomazone	1100	25	300	297	218
thiobencarb	30	3.3	1700	1146	857
fomesafen Na	600,000	220–221	60	10	5
haloxyfop acid	433	107–108	60	487	394
isoxaben	1	176–179	380	1117	838
dithiopyr	1.38	65	1638	2936	2483
triclopyr BE	23	148–150	780	432	342
triallate	4	29–30	2400	2619	2268
naptalam	200	185	20	152	105
oryzalin	2.6	141–142	600	1058	806
prometryn	33	118–120	400	486	394
diallate	14	25–30	500	1569	1308
DCPA	0.5	156	5000	1818	1648
metolachlor	488	–40	200	398	310
ametryn	200	84–85	300	338	254
triasulfuron pH7	815	186	121	94	63
pronamide	15	155–156	800	480	389
linuron	75	93–94	400	447	357
siduron	18	133–138	420	527	434
chlorsulfuron	31,800	174–178	40	32	20
alachlor	200	39.5–41.5	124	486	394
pebulate	60	<25	430	871	702
vernolate	108	no data	260	695	597
fluometuron	110	163–164.5	100	219	155
flumetsulam acid	5600	253	700	32	20
atrazine	33	175–177	100	307	226
propachlor	580	77	112	245	174

compound	water solubility mg/L	mp, °C	Koc	This Work	
				mean est Kfoc	median est Kfoc
ethofumesate	110	70–72	340	467	376
molinate	970	<25	190	311	230
propanil	500	85–89	149	239	169
EPTC	370	no data	200	440	350
simazine	6.2	225–227	130	368	282
prometon	720	91–92	150	204	143
cyanazine	160	1673–169	190	187	131
hexazinone	33X100	115–117	54	48	30
cycloate	85	no data	650	762	637
diuron	42	158–159	48CJ	323	241
2,4DB acid	46	120–121	440	427	337
MCPB Na salt	200,000	100–101	20	31	19
triflurosulfuron pH7	110	150–154	80	241	171
dazomet	2000	100–106	10	131	90
diethatyl	105	49–50	1400	572	478
mefluidide	180	183–185	200	160	111
bromacil	815	158–159	32	116	79
methazole	42	123–124	3000	1029	791
metribuzin	1100	1255–1263	60	134	92
terbacil	710	175–177	55	106	72
mecoprop acid	620	94–95	20	209	148
tebuthiuron	2500	161.5–164	80	77	51
picloram	430	no data	90	416	327
sodium chlorate	1,000,000	248	10	8	3
2,4-D acid	900	135–138	20	133	91
MCPA acid	825	118–119	110	157	1(19
primisulfuron pH7	243	203	50	124	85
dicamba acid	4500	114–116	2	91	61
asulam	534,000	135–137	40	18	10
sulfometuron pH7	300	203–205	78	114	78
metsulfuron	2790	158	35	78	51
tribenuron pH7	2040	141	46	98	65
clopyralid	1000	151–152	33	115	78
endothall	100	144	120	266	190
thifensulfuron pH7	2240	186	45	68	44
bentazon	500	137–139	34	160	111
chlorimuron	1200	185–187	110	83	55
glufosinate	1,370000	215	100	9	4
nicosulfuron pH7	12,200	172–173	30	44	27
maleic hydrazide acid	4500	300	250	25	15

compound	water solubility mg/L	mp, °C	Koc	This Work	
				mean est Kfoc	median est Kfoc
amitrole	280,000	159	100	19	11
acrolein	237.628	-87	05	49	31
fosamine	1,790000	175	150	10	5

Ahrens (1994)

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HIGHLIGHTS

- Freundlich soil-water partition coefficient (K_{foc}) is predicted from subcooled liquid solubility.
- Predictions are based on measured values from 41 pesticides in 18 agricultural soils, giving robust central-tendency estimates.
- Mean and Median K_{foc} estimates give estimates within a factor of 10 of literature values for a majority of compounds from 3 of 4 data sets.

Fig. 1. K_f as a function of subcooled liquid solubility for Speyer 2.2 loamy sand ($R^2=0.75$).

Fig. 2.
Footprint Avg kfoc vs predict Avg kfoc N=333.

Fig. 3.
kfoc estimated vs WSS Handbook (Ahrens,1994) koc.

Fig. 4.
Superfund priority poputant Geometrie mean koc vs Estimate mean vs median koc.

Fig. 5.
PCB congener logkoc (Hansen, et al. 1999) vs Estimate mean and median lofkoc.

Table 1

Properties of soils and chemicals used in regressions.

Soil	Soil properties				Chemical Properties		
	Avg f-oc	%sand	%silt	%clay	No. Of chemicals	solid sol. (mg/L)	mp range (K)
CA Fresno Atwater loamy sand	0.0036	82	10	8	3	0.492 to 429	373 to 456
FRG Laacher Hof Axxa sandy loam	0.0173	72.4	22.6	5	5	0.029 to 436	378 to 490
FRG Hoefchen am Hohenseh silt	0.021	8.5	81.3	10.2	5	0.029 to 42,000	378 to 503
NC Pikeville loamy sand	0.014	77	20	3	4	10.9 to 71,000	384 to 474
ND Ostlie East sandy clay loam	0.032	52	24	24	4	0.087 to 2100	337 to 453
NJ Penn silt loam	0.014	25	52	23	3	14 to 2100	377 to 463
WA Ephrata loamy sand	0.0042	75.7	20.5	3.8	3	0.03 to 42,000	490 to 503
SWTZ Gartenacker loam/silt loam	0.021	45	43	12	3	0.98 to 119,000	337 to 369
ND Roger Myron sandy loam	0.012	77	10	13	5	0.087 to 37,100	298 to 453
ND Mutchler sandy (clay) loam	0.018	59	20	21	4	1 to 37,100	359 to 453
ND Horse Camp Bridge silt loam	0.043	21	54	25	5	436 to 69,100	365 to 489
FRG Speyer/LUFA2.2 loamy sand	0.022	82	13.6	4.4	10	0.07 to 8.86E+5	369 to 510
FRG LUFA/Speyer2.1 sand	0.0072	89	7	4	6	0.08 to 400	369 to 510
SWTZ Vetroz silt loam	0.039	18.2	58.5	23.3	4	0.02 to 2.5	332 to 442
SWTZ Les Evouettes silt loam	0.014	31.9	61.1	7	3	0.046 to 2.5	332 to 442
MS Bosket sandy loam	0.0038	49	44	7	3	0.07 to 25,700	375 to 447
SWTZ Illarsaz humicsoil	0.197	humic			3	0.02 to 4	332 to 442
ND Don Uglem clay loam	0.039	39	30	31	5	0.087 to 2100	298 to 453

Table 2

Regression Parameters for Kf vs. Sscl and 1/n vs. Melting Point.

Soil	Kf vs. Sscl (power regression)		1/n vs. Melting Point (linear regression)	
	intercept	exponent	R ²	slope
CA Fresno Atwater loamy sand	2.3734	-0.421	0.87	0.0007
FRG Laacher Hof Axxa sandy loam	32.53	-0.336	0.81	0.0009
FRG Hoefchen am Hohenseh silt	21.079	-0.333	0.79	0.0005
NC Pikeville loamy sand	18.507	-0.167	0.75	-0.0005
ND Ostlie East sandy clay loam	111.43	-0.379	0.79	-0.0005
NJ Penn silt loam	89.923	-0.502	0.97	0.0007
WA Ephrata loamy sand	18.318	-0.381	0.78	-0.0081
SWTZ Gartenacker loam/silt loam	80.412	-0.477	0.99	-0.0015
ND Roger Myron sandy loam	51.163	-0.312	0.70	-0.0007
ND Mutchler sandy (clay) loam	91.721	-0.367	0.92	0.0005
ND Horse Camp Bridge silt loam	4.9906	-0.124	0.03	-0.0002
FRG Speyer/LUFA2.2 loamy sand	78.719	-0.356	0.75	-0.0027
FRG LUFA/Speyer2.1 sand	26.7	-0.287	0.72	-0.0018
SWTZ Vetroz silt loam	502.43	-0.877	0.98	0.0006
SWTZ Les Evouettes silt loam Switz	128.02	-1.092	0.98	0.0012
MS Bosket sandy loam	80.248	-0.378	0.93	-0.0001
SWTZ Illarsaz humic soil	19471947.8	-0.757	0.97	0.0004
ND clay loam Don Uglem	250.43	-0.372	0.71	-0.0006
				1.0761