Appendix 2—Properties affecting transport and fate.

Table A. Properties affecting the transport and fate of selected pesticide compounds.

[Pesticide compounds selected are those detected most frequently in NAWQA samples (see figs. 4–2 and 4–4), as well as several that were detected infrequently, despite extensive use. All values measured at (or estimated for) 25°C, except for those shown in italics. Unless noted otherwise, (1) values for octanol-water partition coefficient (K_{ow}, dimensionless), soil organic carbon-water partition coefficient (K_{oc}), water solubility (S_w) and Henry's law constant (K_H) are from Mackay and others (1997); (2) transformation half-lives in soil and water were measured in the laboratory (rather than in the field) at neutral pH in the dark, and obtained from the U.S. Department of Agriculture (2005); and (3) all are recommended values selected by the compilation authors when more than one value was available from the literature. Compounds are listed in the same order as in figures 4–2 and 4–4. Numbers of significant figures are identical to those given in original sources. mg/L, milligrams per liter; mL/g, milliliters per gram; NA, data not available from any of the references consulted; Pa•m^3/mol, pascal-cubic meters per mole; >, greater than.]

Pesticide compound (synonym)	log K_{ow}	log K_{oc} (K_{oc} in mL/g)	S_w (mg/L)	log K_H (K_H in Pa•m^3/mol)	Half-life for transformation (days)	
					In aerobic soil	In water
Agricultural herbicides and degradates detected most frequently in water						
Atrazine	2.75	2.00	30	-3.54	146	[1]742
Deethylatrazine	[1,2]1.3	[1,2]1.90	[1]2,700	[1,2]-4.12	[1,2]170	NA
Metolachlor	3.13	2.26	430	-2.63	26	[1,2]410
Cyanazine	2.22	2.3	171	-6.52	[2]17	[2]>200
Alachlor	2.8	2.23	240	-2.7	[1,2]20.4	[1,2]640
Acetochlor	[1]3.0	[1,2]2.38	[1,3]*223*	[1,3]*-2.15*	[1,2,3]*14*	[1]2,300
Metribuzin	[1,3]*1.60*	1.72	[1,3]*1,000*	[1,2]-5.31	172	[2]>200
Bentazon	[1,2]2.80	[1,2]1.54	[1,3]*500*	[1,2,3]*-3.7*	[1,2]35	[1,2,3]*>200*
EPTC	3.2	2.3	370	0.00988	[1,3]*7*	[2]>200
Trifluralin	5.34	4.14	[2]0.5	1.00	169	[2]>32
Molinate	3.21	1.92	970	-0.839	[1,3]*21*	[2]>200
Norflurazon[1]	2.45	2.55	34	-4.46	130	[2]>200
Urban herbicides detected most frequently in water						
Simazine	2.18	2.11	5	-3.46	[2]91	[1,2]>32
Prometon	2.99	2.54	750	-4.05	932	[2]>200
Tebuthiuron	[1,2]1.79	[1]2.1	[1,2]2,400	[1]-4.88	[1]1,050	[2]>2,700
2,4-D	2.81	[1]1.68	890	-3.61	[1,2]2.3	[1,2]732
Diuron	2.78	2.6	40	-3.17	372	>500
Dacthal (DCPA)	[1]4.28	[1]3.75	[1]0.5	[1]-0.66	[1]16	[2]>200
Bromacil	2.11	1.86	815	-4.89	275	[2]>30
Insecticides detected most frequently in water						
Diazinon	3.3	2.76	60	-1.39	39	140
Chlorpyrifos	4.92	3.78	0.73	0.0374	30.5	29
Carbofuran	2.32	2.02	351	-4.30	11	[2]289
Carbaryl	2.36	2.36	120	-4.35	17	11
Malathion	2.8	3.26	145	-2.64	<1	[2]6.3
Dieldrin	5.20	4.08	0.17	0.0492	NA	3,830
Organochlorine pesticide compounds detected most frequently in bed sediment and fish tissue						
p,p′-DDE	5.7	5.0	0.04	0.900	NA	[1,2,3]*>44,000*
p,p′-DDD	5.5	5.0	0.05	-0.194	NA	[2]10,000
p,p′-DDT	6.19	5.4	0.0055	0.37	NA	[1,2,3]*5,000*

Table A. Properties affecting the transport and fate of selected pesticide compounds.—Continued

[Pesticide compounds selected are those detected most frequently in NAWQA samples (see figs. 4–2 and 4–4), as well as several that were detected infrequently, despite extensive use. All values measured at (or estimated for) 25°C, except for those shown in italics. Unless noted otherwise, (1) values for octanol-water partition coefficient (K_{ow}, dimensionless), soil organic carbon-water partition coefficient (K_{oc}), water solubility (S_w) and Henry's law constant (K_H) are from Mackay and others (1997); (2) transformation half-lives in soil and water were measured in the laboratory (rather than in the field) at neutral pH in the dark, and obtained from the U.S. Department of Agriculture (2005); and (3) all are recommended values selected by the compilation authors when more than one value was available from the literature. Compounds are listed in the same order as in figures 4–2 and 4–4. Numbers of significant figures are identical to those given in original sources. mg/L, milligrams per liter; mL/g, milliliters per gram; NA, data not available from any of the references consulted; Pa•m^3/mol, pascal-cubic meters per mole; >, greater than.]

Pesticide compound (synonym)	log K_{ow}	log K_{oc} (K_{oc} in mL/g)	S_w (mg/L)	log K_H (K_H in Pa•m^3/mol)	Half-life for transformation (days)	
					In aerobic soil	In water
o,p'-DDE	5.8	[1,2]5.58	0.1	0.405	NA	NA
o,p'-DDD	6.0	[1,2]5.36	[2]0.10	[1]-2.7	NA	[2]NA
o,p'-DDT	[2]NA	[2]NA	0.026	-0.460	NA	NA
cis-Chlordane	6.0	5.5	0.056	-0.466	NA	[1]>7.2×10^7
trans-Chlordane	6.0	5.5	0.056	-0.582	NA	[1,2]>10,000
Nonachlor [1]	5.66	4.86	0.06	-1.69	NA	NA
Oxychlordane[1]	2.6	2.48	200	-1.52	NA	NA
Dieldrin	5.20	4.08	0.17	0.0492	NA	3,830
Heptachlor epoxide	5.0	4.0	0.35	[1]0.51	NA	NA
Pentachloroanisole [1]	5.66	4.62	0.2	2.91	NA	NA
Hexachlorobenzene	[1]5.31	[1]4.7	[1]0.0062	[1,2]1.69	NA	[1,2]>26,000
Heavily used pesticides not detected frequently in water						
Chlorothalonil	2.64	3.2	0.6	1.77	NA	[2]>200
Dicamba	2.21	[1]1.11	4500	-3.66	[1,2]28	[2]>200
Parathion-methyl (Methyl parathion)	3.0	3.7	25	-1.68	[1,2]3.3	41
Pendimethalin	[1]5.2	[1]4.13	[1]0.275	[1]0.0899	1300	[2]>200
Terbufos	4.48	2.70	5	0.39	5	1.9

[1]Value(s) obtained from sources other than Mackay and others (1997) for K_{ow}, K_{oc}, S_w, and K_H; or U.S. Department of Agriculture (2005) for transformation half-lives. See *http://ca.water.usgs.gov/pnsp/pubs/circ1291/* for data sources.

[2]See *http://ca.water.usgs.gov/pnsp/pubs/circ1291/* for details related to computation or selection of parameter value.

[3]See *http://ca.water.usgs.gov/pnsp/pubs/circ1291/* for temperature of measurement.

References—Appendix 2

Mackay, D., Shiu, W-Y., and Ma, K-C, 1997, Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals, Volume V. Pesticide Chemicals: New York, NY, Lewis Publishers, 812 p.

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