Vapor Pressure Estimation

- The following pp-LFER has been developed to estimate the vapor pressure at 298 K using data from 200 chemicals including apolar, monopolar, and bipolar compounds and covering more than 12 orders of magnitude in vapor pressure:

$$\log p_{iL}^{*}(298K)(\text{Pa}) = -0.89L_i - 0.44S_i^2 - 5.43A_iB_i + 6.51 \quad (8\text{-}19)$$

Example: Estimate the vapor pressure of tetrachloroethene (also known as PCE or perchloroethylene) at 298 K.

Solution: PCE is frequently used for dry cleaning of fabrics. The acute toxicity of tetrachloroethene "is moderate to low". Reports of human injury are uncommon despite its wide usage in dry cleaning and degreasing. However, it is probably carcinogenic to humans. The Abraham parameters for it are from Appendix C: V_i = 0.84, L_i = 3.58, S_i = 0.44, and $A_i = B_i = 0$. Substituting in (8-19), we obtain

$$\log p_{iL}^{*} = 3.2386 \rightarrow p_{iL}^{*} = 1732 \text{ Pa} = 0.0173 \text{ bar at 298 K.}$$

Table 7.3 Solute Descriptors (Abraham parameters) for our Companion Compounds (see structures in Table 3.1)

Compound (i)	McGowan molar volume ($cm^3\ mol^{-1}$)/100 V_i	log $K_{i\text{hexadecane-air}}$ at 25°C L_i	Excess molar Refraction E_i	Dipolarity/ polarizability constant S_i	H-donating parameter A_i	H-accepting parameter B_i
Methyl bromide	0.42	1.63	0.37	0.43	0.00	0.10
PCE	0.84	3.58	0.64	0.44	0.00	0.00
MTBE	0.87	2.38	0.02	0.21	0.00	0.59
Benzene	0.72	2.79	0.61	0.52	0.00	0.14
Phenol	0.78	3.77	0.81	0.89	0.60	0.30
Lindane	1.58	7.57	1.45	1.28	0.00	0.50
Aniline	0.82	3.93	0.96	0.96	0.26	0.41
n-Hexane	0.95	2.67	0.00	0.00	0.00	0.00
TNT	1.38	7.27	1.57	1.78	0.11	0.48
Atrazine	1.62	7.78	1.22	1.29	0.17	1.01
D5	2.93	5.24	−0.70	−0.10	0.00	0.50
PCB 153	2.06	9.59	2.17	1.74	0.00	0.11
PBDE 99	2.26	11.71		1.51	0.00	0.44
Triclosan	1.87	8.96	1.85	1.81	0.92	0.30
DDT	2.22	10.02	1.81	1.76	0.00	0.16
Phenanthrene	1.45	7.58	1.94	1.25	0.00	0.24
Benzo(a)pyrene	1.95	11.47	3.63	1.82	0.00	0.31

pp-LFERs Modeling to Estimate K_{iocw}

Table 13.3 pp-LFERs for Some NOM–Water Systems ($\log K_{iocw}(\mathrm{L\,kg_{oc}^{-1}}) = v_{ocw}V_i + e_{ocw}E_i + s_{ocw}S_i + a_{ocw}A_i + b_{ocw}B_i + c$ and $\log K_{iocw}(\mathrm{L\,kg_{oc}^{-1}}) = v_{ocw}V_i + l_{ocw}L_i + s_{ocw}S_i + a_{ocw}A_i + b_{ocw}B_i + c$) at 25°C or 15°C[a]

NOM Type	Eq.	v_{ocw}	l_{ocw}	e_{ocw}	s_{ocw}	a_{ocw}	b_{ocw}	c	r^2	n[b]	S.D.
SOM[c]	13-8	+2.28		+1.10	−0.72	+0.15	−1.98	+0.14	0.98	75	
Pahokee peat[d]	13-9	+2.99		+0.81	−0.61	−0.21	−3.44	−0.29	0.92	79	0.25
Pahokee peat(low conc)[e]	13-10	+3.71		+0.31	+1.27	−0.10	−3.94	−1.04	0.91	51	0.34
Pahokee peat (high conc)[e]	13-11	+3.51		+0.43	+0.19	+0.02	−3.83	−0.82	0.90	51	0.34
Aldrich humic acid[f]	13-12	+3.94		+0.29	−0.52	+0.36	−3.40	−0.85	0.97	52	0.29
Suwannee River fulvic acid[f]	13-13	+2.86		+0.63	−0.63	+0.05	−2.48	−1.21	0.85	34	0.24
Pahokee peat[d]	13-14	+1.20	+0.54		−0.98	−0.42	−3.34	+0.02	0.93	79	0.24
Aldrich humic acid[f]	13-15	+2.65	+0.40		−0.72	+0.49	−3.42	−0.92	0.97	51	0.32
Aldrich humic acid(dry)[g]	13-16	+1.81	+0.45		−1.25	−0.40	−2.31	−0.16		74	
Suwannee River fulvic acid[f]	13-17	+1.54	+0.34		−0.69	+0.02	−2.43	−0.82	0.82	34	0.26
Suwannee River fulvic acid(dry)[g]	13-18	+3.68	+0.05		−0.96	−0.11	−3.51	−0.79		87	

[a]Contain solute descriptors for the size of the compound (V_i), the excess molar refraction (E_i) or the log $K_{i\text{hexadecane-air}}$ (L_i), the H-donor property (A_i), the H-acceptor property (B_i), and a "dipolarity/polarizability" parameter (S_i), plus the complementary fitted system descriptors characterizing the NOM phases involved (lower case letters).
[b]Number of compounds used for LFER.
[c]Data from Nguyen et al. (2005); log K_{iocw} range: 1 to 7.
[d]Data from Bronner and Goss (2011b); log K_{iocw} range: 1 to 4.5.
[e]Data from Endo et al. (2009); log K_{iocw} range: 1 to 6. low conc = 4.3 mg kg^{-1}oc, high conc = 430 mg kg^{-1}oc.
[f]Data from Neale et al. (2012); Aldrich: log K_{iocw} range: 2 to 7; Suwannee River: log K_{iocw} range: 1 to 4.
[g]K_{iocw} calculated at 15°C using Eq. 13-19 with pp-LFER for OC–air partitioning from Niederer et al. (2007) and pp-LFER for air–water partitioning from Goss (2006). dry = partially hydrated state (RH = 98%).

Table 16.2 pp-LFERs for Some Biological Phase–Water $\log K_{ibpw}(\mathrm{L_w\,kg_{bp}^{-1}}) = v_{bpw}V_i + l_{bpw}L_i + s_{bpw}S_i + a_{bpw}A_i + b_{bpw}B_i + c$), and Biological Phase–Air ($\log K_{ibpa}(\mathrm{L_a\,kg_{bp}^{-1}}) = v_{bpa}V_i + l_{bpa}L_i + s_{bpa}S_i + a_{bpa}A_i + b_{bpa}B_i + c$) systems at 37°C[a,b]

Phases		Fitted System Descriptors									
Biological phase–water	Equation	v_{bpw}	l_{bpw}	e_{bpw}	s_{bpw}	a_{bpw}	b_{bpw}	c_{bpw}	r^2	n[c]	S.D.
Storage lipids[d]	16-7	+4.11		+0.70	−1.08	−1.72	−4.14	−0.07	0.98	247	0.29
Membrane lipids[e]	16-8	+3.30		+0.74	−0.72	+0.11	−3.63	+0.29	0.98	131	0.27
Muscle protein[f]	16-9	+3.01		+0.51	−0.51	+0.26	−2.98	−0.80	0.95	46	0.22
BSA[g]	16-10	+2.82		+0.36	−0.26	+0.37	−3.23	+0.14	0.78	82	0.42
Octanol (bp = o)[h]	16-11	+3.74		+0.46	−1.03	−0.13	−3.22	+0.15			
Storage lipids[d]	16-12	+1.99	+0.58		−1.62	−1.93	−4.15	+0.55	0.99	247	0.20
Membrane lipids[e]	16-13	+1.73	+0.49		−0.93	−0.18	−3.75	+0.49	0.98	131	0.28
Muscle protein[f]	16-14	+2.13	+0.33		−0.59	+0.21	−3.17	−1.09	0.95	46	0.23
BSA[g]	16-15	+1.84	+0.28		−0.46	+0.20	−3.18	+0.20	0.79	82	0.41
Octanol (bp = o)[i]	16-16	+2.54	+0.37		−1.37	−0.32	−3.22	+0.35			
Air–water[j]		v_{aw}	l_{aw}		s_{aw}	a_{aw}	b_{aw}	c_{aw}			
	16-17	+2.21	−0.31		−2.26	−3.60	−4.37	+0.63	0.99	374	0.18
Biological phase–air[k]		v_{bpa}	l_{bpa}		s_{bpa}	a_{bpa}	b_{bpa}	c_{bpa}			
Storage lipids	16-18	−0.22	+0.89		+0.64	+1.67	+0.22	−0.08		247	
Membrane lipids	16-19	−0.48	+0.80		+1.33	+3.42	+0.62	−0.14		131	
Muscle protein	16-20	−0.08	+0.64		+1.67	+3.81	+1.20	−1.72		46	
BSA	16-21	−0.37	+0.59		+1.80	+3.80	+1.19	−0.43		82	
Octanol(bp = o)	16-22	−0.33	+0.68		+0.89	+3.28	+1.15	−0.28			

[a]Contains solute descriptors for the size of the compound (V_i), the excess molar refraction (E_i) or the log $K_{i\text{hexadecane-air}}$ (L_i), the H-donor property (A_i), the H-acceptor property (B_i), and a "dipolarity/polarizability" parameter (S_i), plus the complementary fitted system descriptors characterizing the phase involved (lower case letters).
[b]K_{ibpw} and K_{ibpa} are given in $\mathrm{L_w\,kg^{-1}}$ bp and $\mathrm{L_a\,kg^{-1}}$ bp respectively.
[c]Number of compounds used for LFER.
[d]Data from Geissler et al. (2012); log K_{istlpw} range: −1 to 10.
[e]Data from Endo et al. (2011); log K_{imlpw} range: −1 to 8.
[f]Data from Endo et al. (2012); log $K_{improtw}$ range: 1 to 5.
[g]BSA = Bovin Serum Albumin; Data from Endo and Goss (2011); log K_{ibsaw} range: 1 to 6.
[h]Data from Endo et al. (2013).
[i]Data from Endo (2014).
[j]Data from Endo et al. (2013).
[k]For the biological phase–air systems, only the equation containing L_i is given because it has been derived by the thermodynamic cycle using the corresponding pp-LFER for air–water partitioning, which uses L_i to take care of entropic contributions when partitioning from or to the gas phase (see Chapter 7): $K_{ibpa} = K_{ibpw}/K_{iaw}$ or $\log K_{ibpa} = \log K_{ibpw} - \log K_{iaw}$.

DDT is a persistent organic pollutant (one of Our Companion Compound) that is readily adsorbed to soils and sediments, which can act both as sinks and as long-term sources of exposure affecting organisms. It's partitioning in the environment is very important.

10% 2) Estimate the octanol-water partition constant for DDT at 298 K using the corresponding pp-LFER.

10% 3) Estimate the air-water partition constant for DDT at 298 K using the corresponding pp-LFER.

10% 4) Estimate the octanol-air partition constant for DDT at 298 K using the results of Problems 1) and 2).

10% 5) Estimate the NOM-water partition coefficient for DDT at 298 K (in L/kg) using the corresponding pp-LFER. Assume that the NOM is Pahokee peat.