Environmental Risk Assessment and Remediation: Class #2

Physical-Chemical Properties:

Physical-chemical properties determine how a specific chemical will interact in the environment, how the chemicals move in the environment, and how effectively they can be removed.

Solubility:

Solubility is the degree to which a substance (the solute) will dissolve into another (the solvent)

Factors affecting solubility for non-ioniozable compounds:

- -molecular size
- -functional groups
- -specific interactions (H-bonding)
- -temperature
- -salinity
- -cosolvents

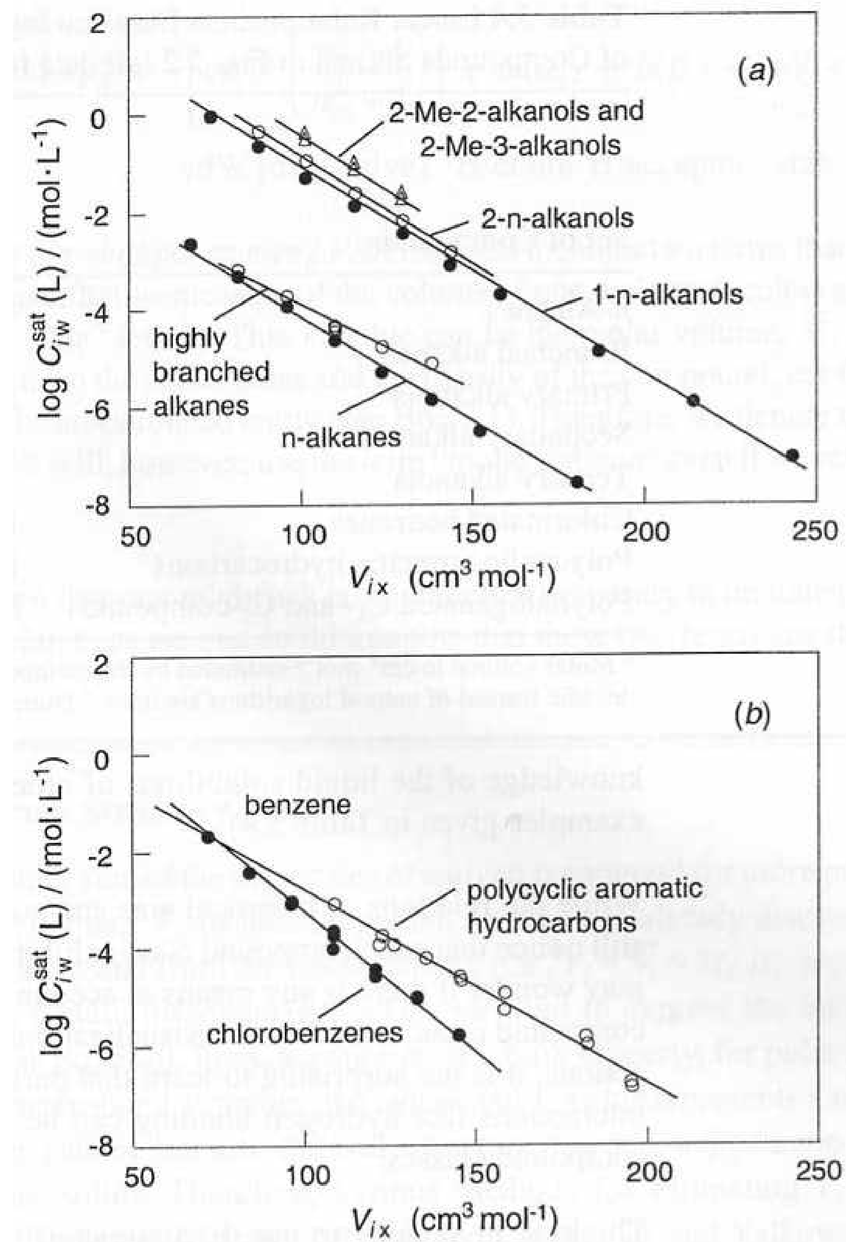

Table 5.4 Linear Relationships Between log C_{iw}^{sat} (L) and V_{ix} [a] for the Various Sets of Compounds Shown in Fig. 5.2 (all data for 25°C)

Set of Compounds	n [c]	log C_{iw}^{sat} (L) /(mol·L^{-1}) $= -a \cdot V_{ix} + b$ [b]		R^2
		a	b	
n-Alkanes	8	0.0442	0.34	0.99
Branched alkanes	7	0.0349	–0.38	0.97
Primary alkanols	10	0.0416	3.01	0.99
Secondary alkanols	5	0.0435	3.52	0.99
Tertiary alkanols	6	0.0438	4.01	0.99
Chlorinated benzenes	13	0.0556	2.27	0.99
Polycyclic aromatic hydrocarbons	13	0.0399	1.90	0.99
Polyhalogenated C_1- and C_2-compounds	27	0.0404	1.85	0.86

[a] Molar volume in cm^3·mol^{-1} estimated by the method discussed in Box. 5.1. [b] Eq. 5-18; note that decadic instead of natural logarithms are used. [c] Number of compounds.

Do example in class to calculate the solubility of an alkane and a PAH

Molar volume (V_{ix}) can be calculated by the method of Abraham and McGowan (1987) where each element is assigned a characteristic atomic volume. The total volume is calculated by summing up all atomic volumes and subtracting 6.56 cm^3/mol for each bond.
Eg. Benzene V_{ix}= (6)(16.35) + (6)(8.71) –(12)(6.56) = 71.6 cm^3/mol

Characteristic atomic volumes

C=16.35	H=8.71	O=12.43	N=14.39
P=24.87	F=10.48	Cl=20.95	Br=26.21
I=34.53	S=22.91	Si=26.83	

Solubility (continued):
Solubility for an ionizable compound is affected by solution pH.
Eg: consider the precipitation of calcium chloride:

$Ca^{+2} + 2OH^{-} \rightarrow Ca(OH)_2$

The solubility product of this reaction is:

$K_{sp} = [Ca^{+2}][OH^{-}] = 7.88 \times 10^{-6}$ square brackets indicate molar concentration

Do example 3-3 in class.

TABLE 3-3
Constants for solubility equilibria[8]

Oxides and hydroxides	log *K* at 25°C
$H_2O(l) = H^+ + OH^-$	−14.00
$Cd^{+2} + H_2O = CdOH^+ + H^+$	−10.1
$Cd^{+2} + 2H_2O + Cd(OH)_2\ (aq) + 2H^+$	−20.4
$Cd^{+2} + 3H_2O = Cd(OH)_3^- + 3H^+$	< −33.3
$Cd^{+2} + 4H_2O = Cd(OH)_4^{-2} + 4H^+$	−47.4
$\beta\text{-}Cd(OH)_2\ (s) + 2H^+ = Cd^{+2} + 2H_2O$	13.65
$Hg^{+2} + H_2O = HgOH^+ + H^+$	−3.4
$Hg^{+2} + 2H_2O = Hg(OH)_2\ (aq) + 2H^+$	−6.2
$Hg^{+2} + 3H_2O = Hg(OH)_3^- + 3H^+$	−21.1
$HgO + 2H^+ = Hg^{+2} + H_2O$	2.56
$PbCO_3\ (s) = Pb^{+2} + CO_3^{-2}$	−13.1

Vapor pressure: