Partitioning of contaminants

When chemicals are discharged into the environment it is important to understand their fate.

A) Two-phase partition processes in the environment

A number of 2 phase distributions can exist …

Described by the Freundlich equation:

$C_1 = K_f (C_2)^n$

C_1 =
K_f =
C_2 =
n is

If C_1 is soil and C_2 is water, what does a large K_f represent?

n describes the curvature of the plot

Invalid if solubility is exceeded (e.g. NAPL).

Can also be log transformed to give

$\log C_1 = \log K_f + n \log C_2$ look familiar?

By plotting this, $\log K_f$ can be estimated.

I Air/water partitioning: Henry's Law part II

Henry's constant (H) = $\frac{\text{partial pressure of compound in air}}{\text{Conc in water } (C_W)}$

Units?

II Biota/water partitioning: Octanol/water coefficient

$K_{OW} = C_O / C_W$

Biota/water coefficient

$K_B = C_B / C_W$

Partitioning into lipids (C_L)

C_L / C_W = constant

$C_B = f_{lipid} C_L$

f_{lipid} = lipid fraction

$K_B = C_B / C_W$

$= f_{lipid} C_L / C_W$

Since octanol is a good surrogate for biota lipid, then $C_L = C_O$

$K_B = f_{lipid} C_L / C_W$

$= f_{lipid} C_O / C_W$

$= f_{lipid} K_{OW}$

$K_B = f_{lipid} K_{OW}$

The lipid fraction for fish is about 5% or 0.05

So, K_B =

III Solid phases/water partitioning: K_D

K_D =

$K_D = C_S / C_W$

C_{SOC} / C_W = constant

C_{SOC} =
f_{OC} =

Since compounds will distribute into the soil organic carbon

$C_S = f_{OC} C_{SOC}$

$K_D = C_S / C_W$

$= f_{OC} C_{SOC} / C_W$

Assume that octanol is a good surrogate for organic matter and x is a factor related to the organic carbon content of the solid phase

$K_D = x f_{OC} C_O / C_W$

$= x f_{OC} K_{OW}$

$\boxed{K_D = x f_{OC} K_{OW}}$

For most soils, x = 0.41 and f_{OC} ranges from 0.02 - 0.04.

$K_D = (0.41) f_{OC} K_{OW}$

Chemical (mw)	BP °C	water sol mg/L	vapor pres Pa @ 25°C	K_{OW}
Pentane (72)	36	40	68000	$10^{3.5}$
TCE (131)	87	1100	9200	$10^{2.3}$
MTBE (88)	54	50000	33000	10^{1}

What are the Henrys' constants for the above compounds?

Which is likely to partition more into fish? less likely? how about soil?

Which is most soluble in octanol? least soluble?

What are the K_D values for a soil containing 1.5% C? How does doubling the % C influence K_D?