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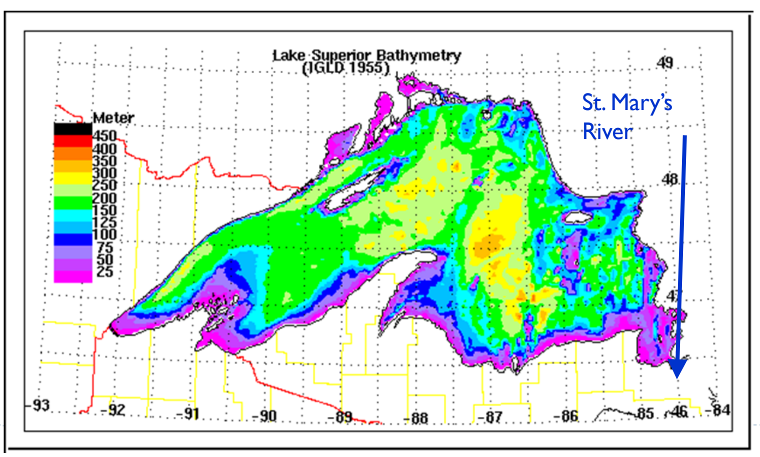
CEE 697z
Organic Compounds in Water and Wastewater

PCBs:
Introduction and Properties

Lecture #34

PCBs in the Lake Superior

- Reference: Jeremiason, Hornbuckle and Eisenreich, Environmental Science and Technology, 28:903 (1994)



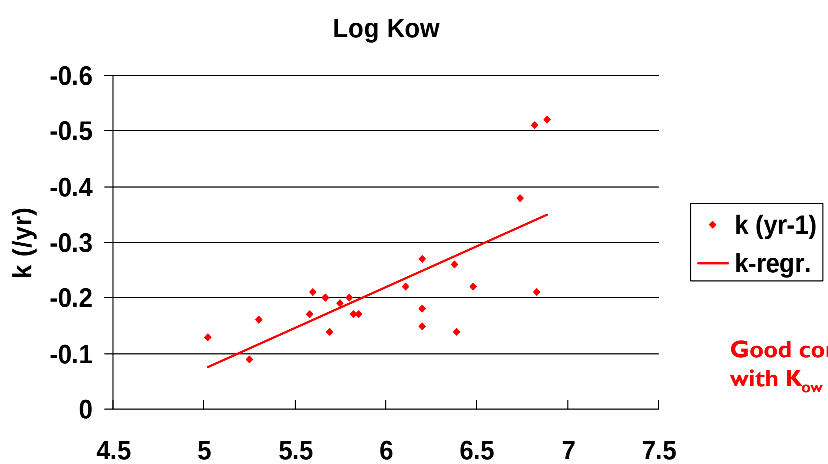
Empirical Models

$$\sum\nolimits_{25} PCB = \left(\sum\nolimits_{25} PCB_o\right) e^{-0.20t}$$

$$\sum\nolimits_{82} PCB = \left(\sum\nolimits_{82} PCB_o\right) e^{-0.22t}$$

- Data tell us that about 26,500 kg has been lost from the water column between 1980 and 1992

Loss rates depend on specific congener



Good correlation with K_{ow}

Sorption

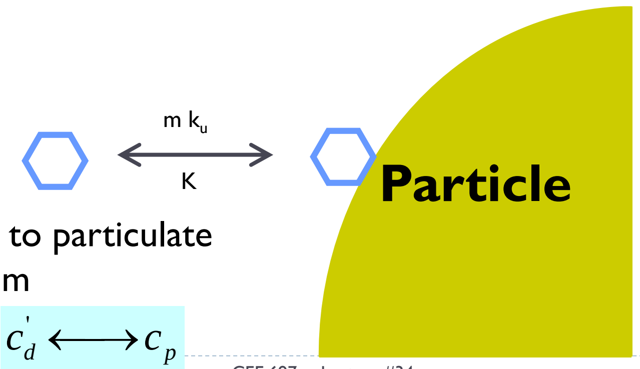
- Definitions

$c_d^{'} \equiv$ dissolved toxicant

$c_p \equiv$ particulate toxicant

and: $c_d = \phi c_d^{'}$

so: $c_T = c_p + c_d$



- dissolved to particulate equilibrium

$$c_d^{'} \longleftrightarrow c_p$$

Langmuir Isotherm

- At Equilibrium
  - Rate of adsorption = rate of desorption

$$R_{ad} = R_{de}$$

$$k_{ad} M c_d (\nu_m - \nu) = k_{de} M \nu$$

- So, solving for the sorbed concentration (ν)

$$\nu = \frac{\nu_m c_d}{\frac{k_{de}}{k_{ad}} + c_d}$$

Limiting Cases

- When C_d is small, and there are lots of surface sites
  - Common situation for trace "toxics" like PCBs

$$\nu = \frac{\nu_m c_d}{\frac{k_{de}}{k_{ad}} + c_d} \approx \frac{\nu_m c_d}{\frac{k_{de}}{k_{ad}}} = \boxed{\frac{\nu_m k_{ad}}{k_{de}}} c_d$$

$$\nu = K_d c_d$$

  - So the bulk particulate concentration is:

$$c_p = m\nu = mK_d c_d$$

  - And the total toxicant is:

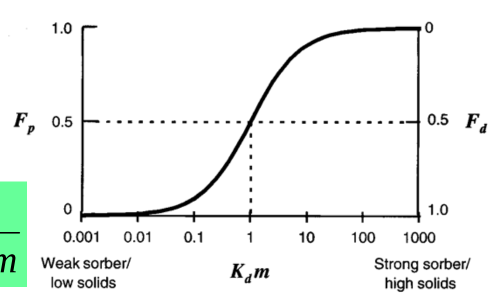
$$c_T = c_d + c_p = c_d + mK_d c_d$$

Toxics: Linear sorption modeling

- Now define

$$f_d \equiv \frac{c_d}{c_T} = \frac{c_d}{c_d + mK_d c_d}$$

- adsorption model



$$f_d = \frac{1}{1 + K_d m} \qquad f_p = \frac{K_d m}{1 + K_d m}$$

$$c_d = f_d c_T \qquad c_p = f_p c_T \qquad f_d + f_p = 1$$

Estimation of partition coeffici

$$f_d = \frac{1}{1 + K_d m}$$

- Relationship to organic fraction

$$K_d = f_{oc} K_{oc}$$

$$\left(\frac{mg-tox./g-C}{mg-tox./m^3} \right) or \left(\frac{m^3}{g-C} \right)$$

- and properties of organic fraction

$$K_{oc} = 6.17x10^{-7} K_{ow}$$

Octanol:water partition coefficient

- combining, we get:

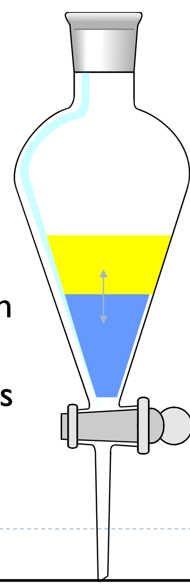
$$K_d = 6.17x10^{-7} f_{oc} K_{ow}$$

$$\left(\frac{mg-tox./m^3-Oct.}{mg-tox./m^3-H_2O} \right)$$

Karickhoff et al., 1979; Wat. Res. 13:241

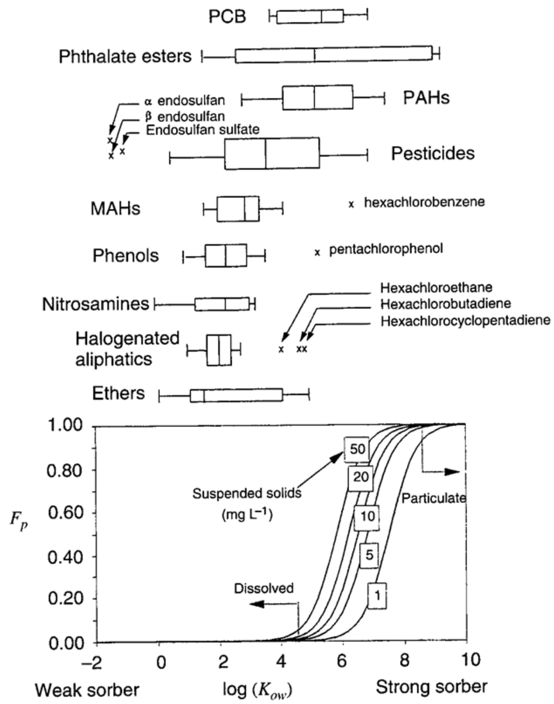
Octanol:water partitioning

- 2 liquid phases in a separatory funnel that don't mix
  - octanol
  - water
- Add contaminant to flask
- Shake and allow contaminant to reach equilibrium between the two
- Measure concentration in each (K_{ow} is the ratio)



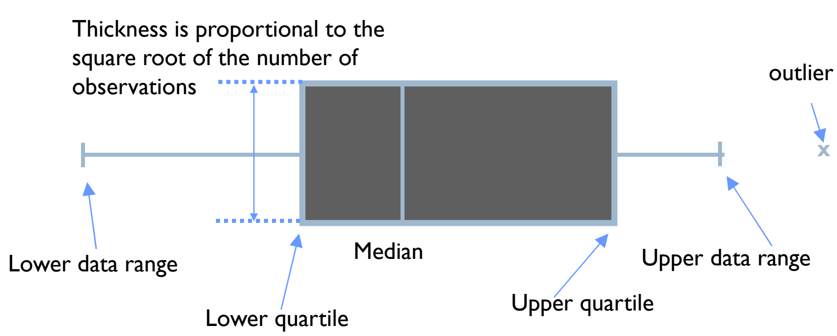
Observations

- Summary of K_{ow} and TSS effects
- From Chapra, pg. 722



Box and Whisker Plots

- Useful for summarizing non-ideal data distributions



- To next lecture