Updated: 16 April 2013

Print version

CEE 577: Surface Water Quality Modeling

Lecture #30

Toxics: Sorption & Volatilization

(Chapra, L41)

Estimation of partition coefficients

- 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

$$K_{oc} = 6.17 x 10^{-7} K_{ow}$$

Octanol:water partition coefficient

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

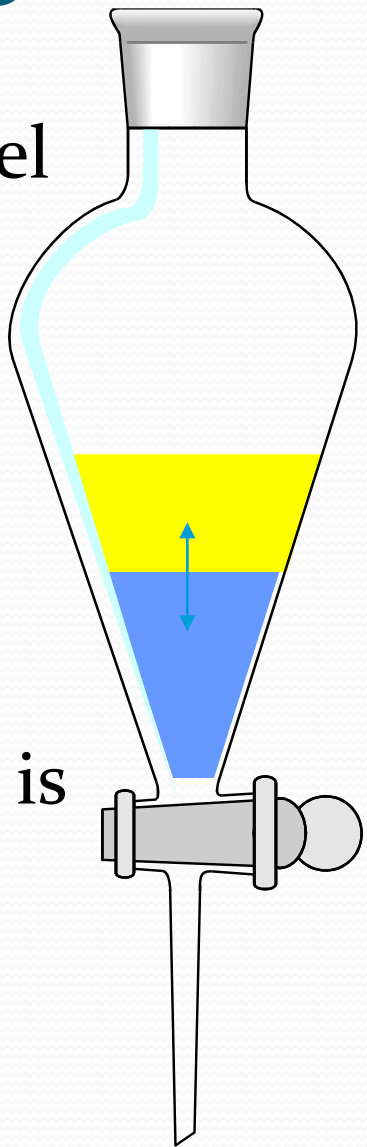
- combining, we get:

$$K_d = 6.17 x 10^{-7} f_{oc} K_{ow}$$

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

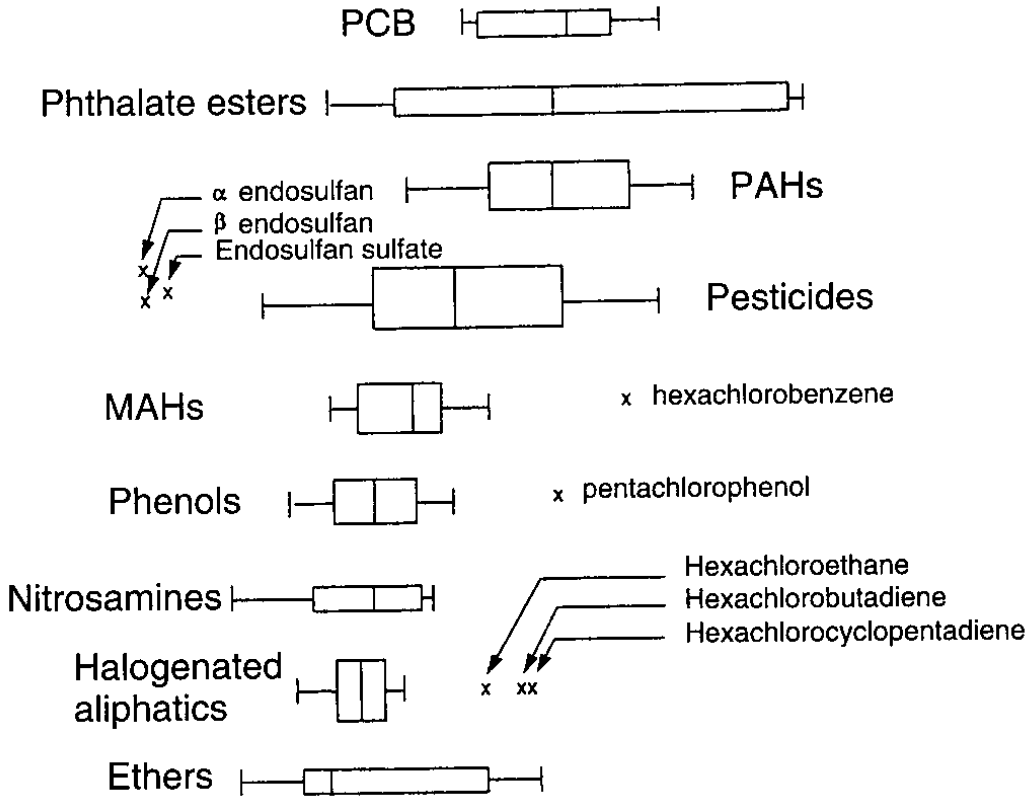
Octanol:water partitioning

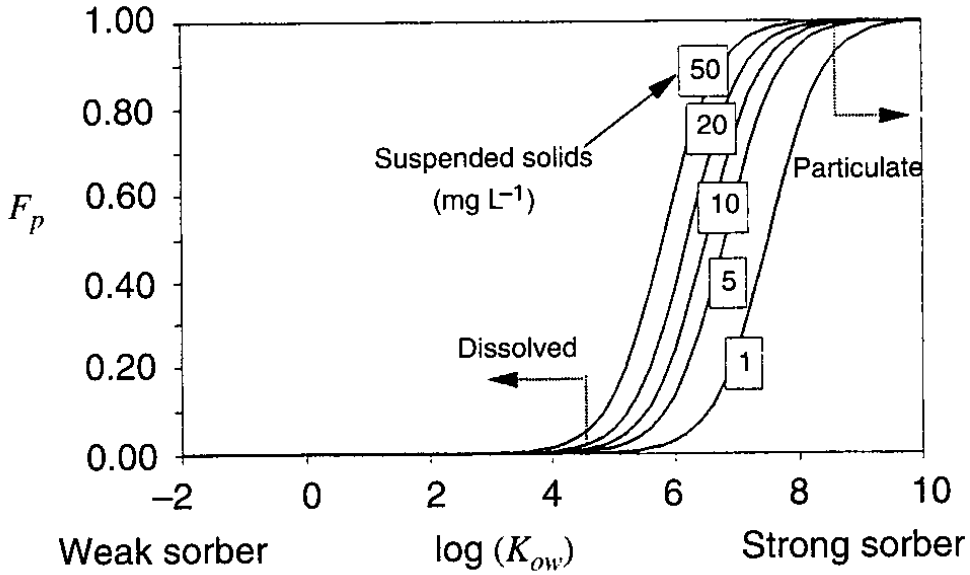
- 2 liquid phases in a separatory funnel that don't mix
  - octanol
  - water
- Add contaminant to flask
- Shake and allow contaminant to reach equilibrium between the two
- Measure concentration in each (K_{ow} is the ratio)



Observations

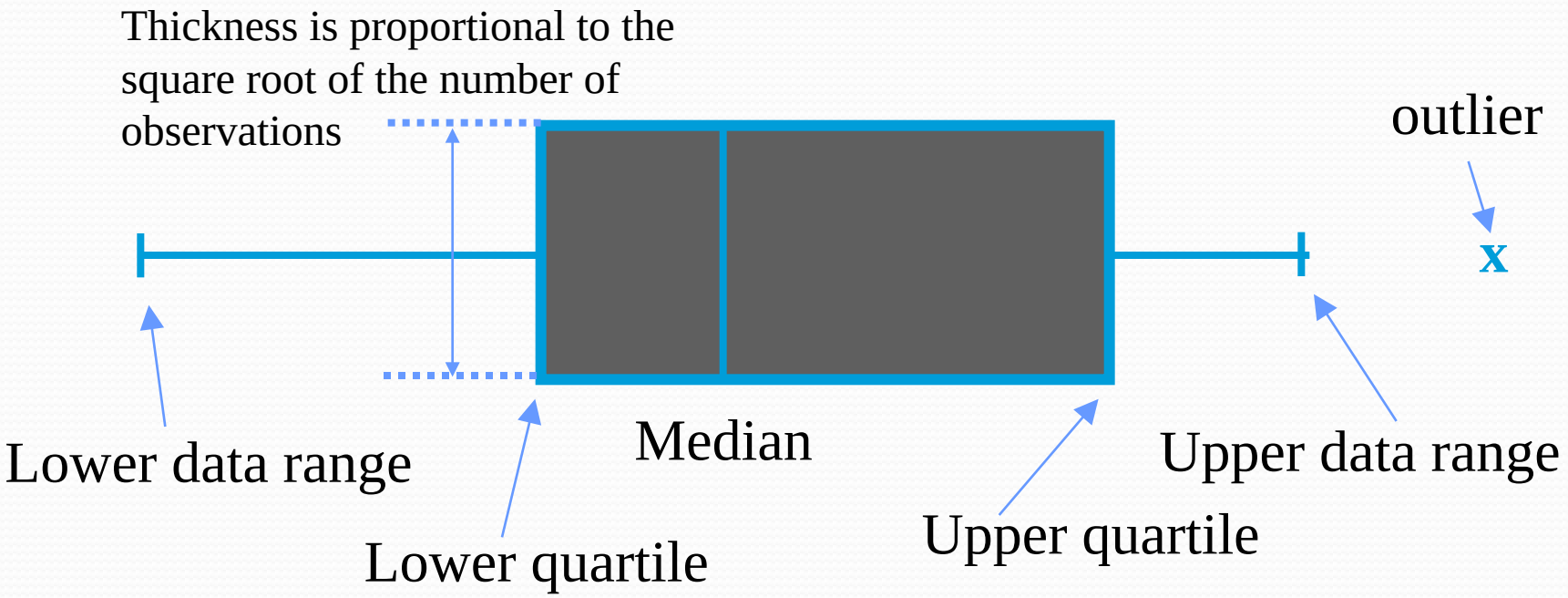
- Summary of K_{ow} and TSS effects
- From Chapra, pg. 722





Box and Whisker Plots

- Useful for summarizing non-ideal data distributions



- To next lecture