CEE 577: Surface Water Quality Modeling

Lecture #30

Toxics: Sorption & Volatilization

(Chapra, L41)
Estimation of partition coefficients

- Relationship to organic fraction
  \[ K_d = f_{oc} K_{oc} \]

- and properties of organic fraction
  \[ K_{oc} = 6.17 \times 10^{-7} K_{ow} \]

- combining, we get:
  \[ K_d = 6.17 \times 10^{-7} f_{oc} K_{ow} \]

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

Thickness is proportional to the square root of the number of observations.
• **To next lecture**