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CEE 577: Surface Water Quality Modeling

Lecture #30
Toxics: Sorption & Volatilization
(Chapra, L41)

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QUAL2E

- [Go to Qualze](#)

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Estimation of partition coefficients

- Relationship to organic fraction

$$K_d = f_{oc} K_{oc} \longrightarrow \left(\frac{\text{mg-tox./g-C}}{\text{mg-tox./m}^3} \right) \text{ or } \left(\frac{\text{m}^3}{\text{g-C}} \right)$$

- and properties of organic fraction

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

Octanol:water
partition
coefficient

- combining, we get:

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

$$\left(\frac{\text{mg-tox./m}^3 - \text{Oct.}}{\text{mg-tox./m}^3 - \text{H}_2\text{O}} \right)$$

Karickhoff et al., 1979; [Wat. Res. 13:241](#)

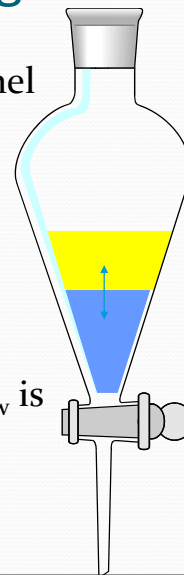
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Octanol:water partitioning

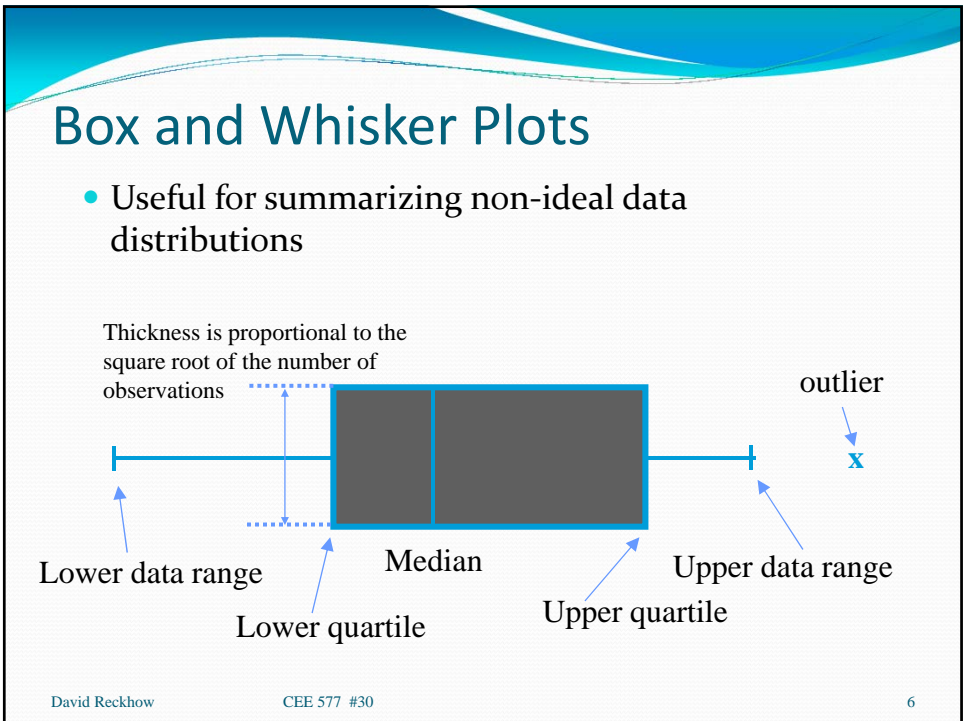
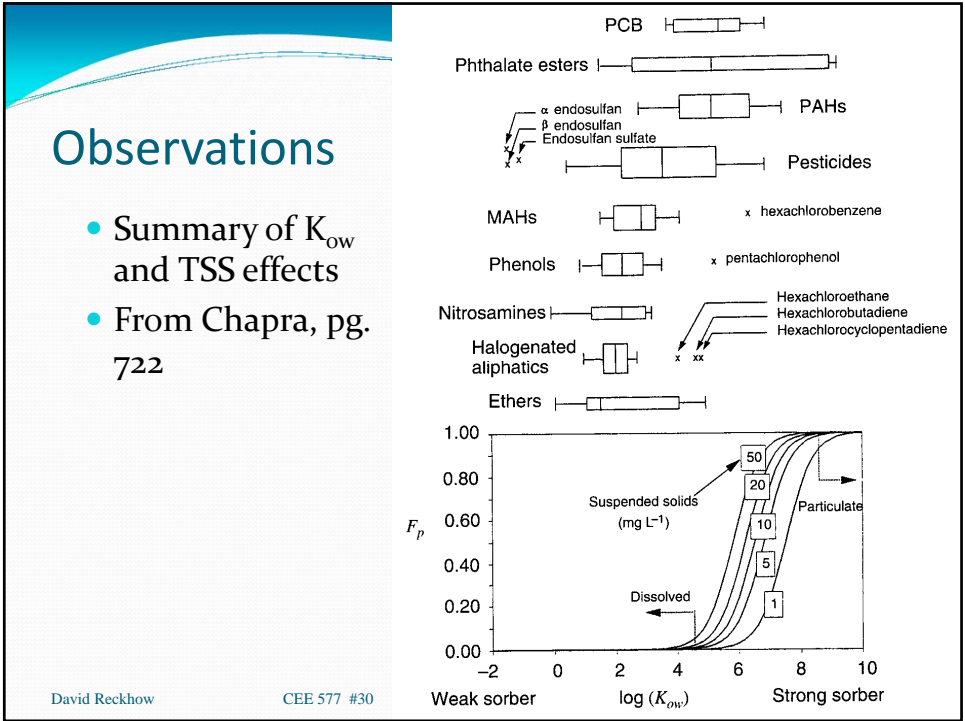
- 2 liquid phases in a separatory funnel that don't mix
 - octanol
 - water
- Add contaminant to flask
- Shake and allow contaminant to reach equilibrium between the two
- Measure concentration in each (K_{ow} is the ratio)




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- To next lecture

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