3 Environment impacts (assessment)

- Site investigation (Chap. 2 & 3)
  - QA/QC (Chap. 3)
  - Sampling (Chap. 3)
- Background concentrations (Chap. 3)
- Contaminant-soil interactions
  - Bioavailability
  - Sorption/desorption (Dr. Uttam Saha)
  - Speciation/bioavailability/remediation (Dr. Don Sparks)
- Shining light on biogeochemical processes in the earth’s critical zone
- Assessment
  - Fate and transport (Appendix c)
    - Dr. Dean Rhue (W): Tracking arsenic in soils/landscapes
    - Dr. Bin Gao (F): Colloids-facilitated contaminant transport
  - Risk assessment (Chap. 5-6 & Appendix B, F-J)
  - Toxicology
    - Dr. Bitton-M

Fate and Transport

- Fate
  - Where the contaminant moves
- Transport
  - How the contaminant moves
- Factors affecting fate & transport
  - Properties of contaminant
  - Properties of matrix-soil, water, & air
  - Environment-temperature & precipitation

Soil composition

Important factors-contaminant

- Water solubility-water/solid (Ws)
  - Solid contaminants are less mobile than liquid
  - One of the most important
- Volatilization-water/gas (H)
  - Important for mass transfer to atmosphere
  - Henry’s law constant (H) and vapor pressure
    - A measure of the extent of chemical partitioning between air and water at equilibrium
    - Relative tendency of a chemical to volatilize from water (water solubility) to air (vapor pressure)
    - \( H = \frac{C_{\text{air}}}{C_{\text{water}}} \)

Important factors

- Partition coefficient
  - Water/air (\( K_{\text{wa}} \)): volatility
    - \( K_{\text{wa}} = \frac{C_{\text{water}}}{C_{\text{air}}} = 1/H \)
  - Octanol/water (\( K_{\text{ow}} \)): bioaccumulation
    - \( K_{\text{ow}} = \frac{C_{\text{octanol}}}{C_{\text{water}}} \)
    - Hydrophobic: \( K_{\text{ow}} < 10 \) or log \( K_{\text{ow}} < 1 \)
    - Hydrophilic: \( K_{\text{ow}} > 100 \) or log \( K_{\text{ow}} < 2 \)
Relationship of molecular structure to $K_{OW}$

- Chlorinated benzenes
- Hydrophobic: $log K_{OW} > 2$

**Important factors**

- Partition coefficient
  - Water/air ($K_w$): volatility
    - $K_w = C_{water}/C_{air} = 1/H$
  - Octanol/water ($K_{OW}$): bioaccumulation
    - $K_{OW} = C_{octanol}/C_{water}$
    - Hydrophilic: $K_{OW} < 10$
    - Hydrophobic: $K_{OW} > 100$
  - Soil/water ($K_d$): mobility
    - $K_d = C_{soil}/C_{water}$
    - Chemical & soil specific
  - Organic carbon adsorption ($K_{OC}$): adsorption
    - $K_{OC} = K_d/C_{OC}$
    - Chemical specific

Relationship of molecular structure to $K_{OW}$

- Benzene
- Naphthalene
- Benzanthracene
- Anthracene
- Benzopyrene
- Hydrophobic: $log K_{OW} > 2$

Pesticide | No. of values | Mean $K_d$
--- | --- | ---
COOH acid |  |  |
2,4-D | 23 | 0.49
Imazaquin | 37 | 0.81
Imazaquinpyr | 24 | 1.13
Picolam | 51 | 0.47
2,4,5-T | 8 | 1.24
NISO$_2$ acid |  |  |
Chlorimuron | 8 | 1.10
Chlorsulfuron | 15 | 0.69
Flumesulam | 36 | 2.88
Fomesafen | 5 | 4.52
Sulfometuron-methyl | 15 | 0.97
Triflusulfuron-methyl | 5 | 0.78

Webber et al., 2004
**Important factors**

- **Bioconcentration factor (BCF): bioaccumulation**
  - \( \text{BCF} = \frac{C_{\text{tissue}}}{C_{\text{water}}} \) (similar to \( K_{\text{ow}} \))
  - \( \text{BCF} = \frac{C_{\text{tissue}}}{C_{\text{soil}}} \)
  - Concerns: \( \text{BCF} > 100 \)

**Bioconcentration factors of fish (EPA, 1990)**

<table>
<thead>
<tr>
<th>Chemical</th>
<th>BCF (L kg(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aldrin</td>
<td>28</td>
</tr>
<tr>
<td>Benzene</td>
<td>44</td>
</tr>
<tr>
<td>Ni</td>
<td>47</td>
</tr>
<tr>
<td>Cd</td>
<td>81</td>
</tr>
<tr>
<td>Cu</td>
<td>200</td>
</tr>
<tr>
<td>Chloradane</td>
<td>14,000</td>
</tr>
<tr>
<td>DDT</td>
<td>54,000</td>
</tr>
<tr>
<td>PCBs</td>
<td>100,000</td>
</tr>
</tbody>
</table>

**Important parameters**

- **Water solubility-water/solid (Ws)**
- **Volatilization-water/gas (H=C\(_{\text{air}}\)/C\(_{\text{water}}\))**
- **Partition coefficient**
  - Volatility: water/air (\( K_W = C_{\text{water}}/C_{\text{air}} \))
  - Bioaccumulation: octanol/water (\( K_{\text{ow}} = C_{\text{octanol}}/C_{\text{water}} \))
  - Mobility: soil/water
    (\( K_d = C_{\text{soil}}/C_{\text{water}} \) & \( K_{\text{GC}} = K_d/C_{\text{octanol}} \))
- **Bioaccumulation: bioconcentration factor**
  (\( \text{BCF} = \frac{C_{\text{tissue}}}{C_{\text{soil}}} \) or \( = \frac{C_{\text{tissue}}}{C_{\text{water}}} \))
- **Mobility in groundwater: retardation factor**
  (\( R = 1 + D_b \times K_d / \text{porosity} \))