Lecture #28
Toxics: Lake Models
(Chapra, L40)
TOXICS: What Are They?

- **Metals**
  - Hg, Se, Cd, Pb
- **Industrial Synthetic Organics**
  - Plasticizers: phthalates
  - solvents: tetrachloroethylene
  - waxes: chlorinated paraffins
  - others: PCB’s
- **Hydrocarbons & oil derivatives**
  - includes products of combustion: PAH’s
- **Agricultural Chemicals**
  - pesticides: DDT, kepone, mirex
- **Pharmaceuticals, etc**
  - Anti-epileptics
  - Beta-blockers
  - X-ray contrast media
  - antibiotics
- **Personal Care Products**
  - triclosan
  - musks
- **Endocrine Disrupters**
  - Steroidal estrogens
- **Radioactive Substances**
  - $^{90}\text{Sr}$, Pu, Cs
TOXICS: What makes them unique?

- Sorption properties
  - they are hydrophobic
    - they tend to bind strongly to particles
    - some volatilize
  - Concern about particulate fraction
- Biological interactions
  - they concentrate up the food chain
  - they are toxic
- They are not natural
Sorption

- Definitions

\[ c_d' \equiv \text{dissolved toxicant} \]
\[ c_p \equiv \text{particulate toxicant} \]

and:
\[ c_d = \phi c_d' \]

so:
\[ c_T = c_p + c_d \]
Langmuir Isotherm

- At Equilibrium
  - Rate of adsorption = rate of desorption
  \[ R_{ad} = R_{de} \]
  \[ k_{ad} M_s c_d (v_m - v) = k_{de} M_s v \]
  - So, solving for the sorbed concentration \((v)\)
  \[ v = \frac{v_m c_d}{\frac{k_{de}}{k_{ad}} + c_d} \]
Limiting Cases

- When $C_d$ is small, and there are lots of surface sites
  - Common situation for “toxics”

\[
\nu = \frac{\nu_m C_d}{k_{de}} + C_d \approx \frac{\nu_m C_d}{k_{de}} = \nu_m k_{ad} C_d
\]

\[
\nu = K_d C_d
\]

- So the bulk particulate concentration is:

\[
c_p = m \nu = m K_d C_d
\]

- And the total toxicant is:

\[
c_T = C_d + c_p = C_d + m K_d C_d
\]
Toxics: Linear sorption modeling

• Now define

\[ f_d = \frac{c_d}{c_T} = \frac{c_d}{c_d + mK_d c_d} \]

• adsorption model

\[ f_d = \frac{1}{1 + K_d m} \]
\[ f_p = \frac{K_d m}{1 + K_d m} \]

\[ c_d = f_d c_T \]
\[ c_p = f_p c_T \]

\[ f_d + f_p = 1 \]
Toxics Model: CSTR with sediments

- Internal Transport Processes (between compartments)
  - dissolved: diffusion
  - particulate: settling, resuspension & burial
- Expressed as velocities (e.g., m/yr)
Solids: Mass Balance

- In water column

\[ V_1 \frac{dm_1}{dt} = W_m - Qm_1 - \nu_s A_{m_1} + \nu_r A_{m_2} \]

- in mixed sediments

\[ V_2 \frac{dm_2}{dt} = \nu_s A_{m_1} - \nu_r A_{m_2} - \nu_b A_{m_2} \]

Can be expressed as: \( Q_{m_{in}} \)
Solids: Steady State Solution

- Fixed ratio of solids concentration in water column and mixed sediments

\[ m_2 \left( = (1 - \phi) \rho \right) = \frac{v_s}{v_r + v_b} m_1 \]

\( m_2 \) is the mass of solids in the water column, \( m_1 \) is the mass of mixed sediments, \( \rho \) is the density of solids, and \( \phi \) is the porosity.
Toxicant Mass Balance

In the water column

\[ V_1 \frac{dc_1}{dt} = W_T - Qc_1 + v_d A \left( f_{d2} c_2 - f_{d1} c_1 \right) - k_{T1} V_1 c_1 - v_v A f_{d1} c_1 - v_s A f_{p1} c_1 + v_r A c_2 \]

Can be expressed as: \( Qc_{\text{in}} \)

New Chapra approach

In the mixed sediments

\[ V_2 \frac{dc_2}{dt} = v_d A \left( f_{d1} c_1 - f_{d2} c_2 \right) - k_{T2} V_2 c_2 + v_s A f_{p1} c_1 - v_r A c_2 - v_b A c_2 \]
To next lecture