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CEE 577: Surface Water Quality Modeling

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 parafins
  - 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}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

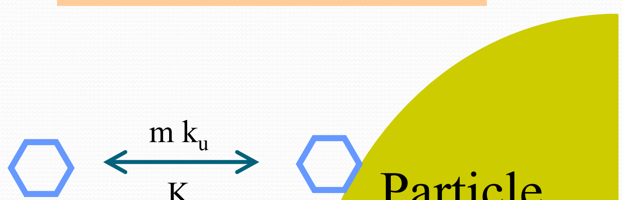
$c_d' \equiv$ dissolved toxicant

$c_p \equiv$ particulate toxicant

and: $c_d = \phi c_d'$

so: $c_T = c_p + c_d$

- Definitions



- dissolved to particulate equilibrium

$$c_d' \longleftrightarrow c_p$$

Langmuir Isotherm

- At Equilibrium
  - Rate of adsorption = rate of desorption

$$R_{ad} = R_{de}$$

$$k_{ad} M_s c_d \left(\nu_m - \nu\right) = k_{de} M_s \nu$$

  - So, solving for the sorbed concentration (ν)

$$\nu = \frac{\nu_m c_d}{\frac{k_{de}}{k_{ad}} + c_d}$$

Limiting Cases

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

$$\nu = \frac{\nu_m c_d}{\frac{k_{de}}{k_{ad}} + c_d} \approx \frac{\nu_m c_d}{\frac{k_{de}}{k_{ad}}} = \frac{\nu_m k_{ad}}{k_{de}} c_d$$

$$\nu = K_d c_d$$

  - So the bulk particulate concentration is:

$$c_p = m\nu = mK_d c_d$$

  - And the total toxicant is:

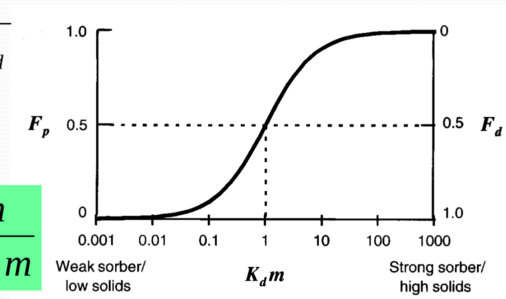
$$c_T = c_d + c_p = c_d + mK_d c_d$$

Toxics: Linear sorption modeling

- Now define

$$f_d \equiv \frac{c_d}{c_T} = \frac{c_d}{c_d + mK_d c_d}$$

- adsorption model

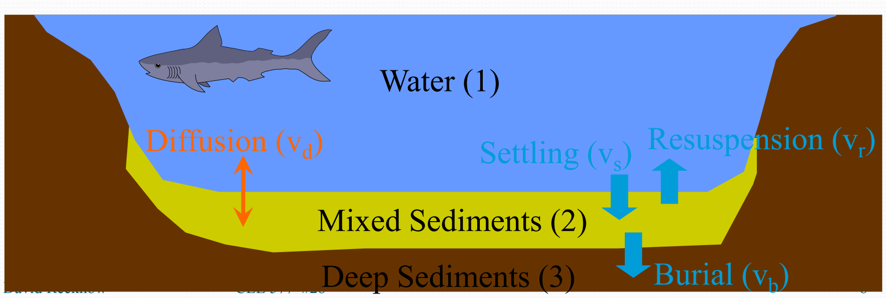


$$f_d = \frac{1}{1 + K_d m} \qquad f_p = \frac{K_d m}{1 + K_d m}$$

$$c_d = f_d c_T \qquad c_p = f_p c_T \qquad f_d + f_p = 1$$

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

Can be expressed as: Qm_{in}

- In water column

$$V_1 \frac{dm_1}{dt} = W_m - Qm_1 - v_s A m_1 + v_r A m_2$$

- in mixed sediments

$$V_2 \frac{dm_2}{dt} = v_s A m_1 - v_r A m_2 - v_b A m_2$$

Solids: Steady State Solution

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

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

Toxicant Mass Balance

New Chapra approach

Can be expressed as: Qc_{in}

- In the water column

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

- 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