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CEE 577: Surface Water Quality Modeling

Lecture #35

Toxics: Simplified Forms

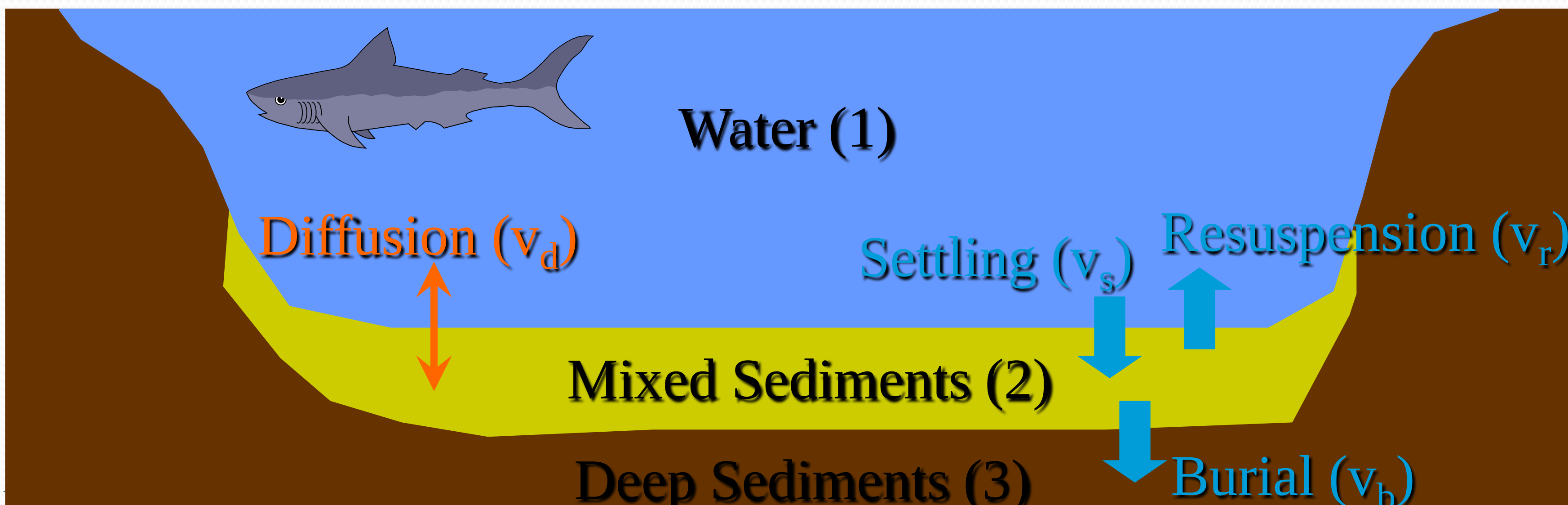
(Chapra, L42, L43 & L44)

Special Considerations for Metals

- In general they are not subject to decomposition
  - e.g., biodegradation, hydrolysis, photolysis
  - exception: radionuclides undergo radioactive decay
- Most do not volatilize (Hg is an exception)
- They speciate into may forms which differ in toxicity and behavior
- Natural background and non-point loadings may be quite high

Toxics Model: CSTR with sediments

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



Toxicant Mass Balance: Adapted for Metals

- In the water column

No volatilization for metals

$$V_1 \frac{dc_1}{dt} = W_T - Qc_1 + v_d A\left(f_{d2}c_2 - f_{d1}c_1\right) - k_{T1}V_1c_1 - \cancel{v_v A f_{d1}c_1} - v_s A f_{p1}c_1 + v_r A c_2$$

- In the mixed sediments

$$V_2 \frac{dc_2}{dt} = v_d A\left(f_{d1}c_1 - f_{d2}c_2\right) - k_{T2}V_2c_2 + v_s A f_{p1}c_1 - v_r A c_2 - v_b A c_2$$

radioactive decay only

Steady State Solution: Adapted for Metals

$$c_1 = \frac{Qc_{in}}{Q + k_1 V_1 + \cancel{v_v A F_{d1}} + (1 - F_r')(v_s F_{p1} + v_d F_{d1}) A}$$

No volatilization for metals

$$c_2 = \frac{v_s F_{p1} + v_d F_{d1}}{k_2 H_2 + v_r + v_b + v_d F_{d2}} c_1$$

radioactive decay only

The ratio of sediment feedback to total sediment purging

$$F_r' = \frac{v_r + v_d F_{d2}}{v_r + v_b + v_d F_{d2} + k_2 H_2}$$

radioactive decay only

Overview of solutions to toxic model

For Lakes:

$$C_{T1} = \frac{W}{\lambda V}$$

Where:

$$\lambda = \frac{Q}{V} + K_{T1}$$

For Rivers:

$$C_{T1} = \underbrace{C_{T1o}}_{\frac{W}{Q}} e^{-K_{T1} x/U}$$

Solutions (cont.)

$$K_{T1} = k_1 + \frac{v_v}{H_1} f_{d1} + \left(1 - F_r'\right)\left(\frac{v_s}{H_1} f_{p1} + \frac{v_d}{H_1} f_{d1}\right)$$

Where: $$F_r' = \frac{v_r + v_d F_{d2}}{v_r + v_b + v_d F_{d2} + k_2 H_2}$$

The ratio of sediment feedback to total sediment purging

$$k_1 = k_{d1} f_{d1} + k_{p1} f_{p1}$$

$$k_2 = k_{d2} f_{d2} + k_{p2} f_{p2}$$

Toxicant Concentration in the Mixed Sediments

Either Lake or River Model:

$$c_2 = \frac{v_s F_{p1} + v_d F_{d1}}{k_2 H_2 + v_r + v_b + v_d F_{d2}} c_1$$

Simplified Versions

- Level 0
  - no movement from sediment to water column
    - $v_r = 0$, $v_d = 0$
    - therefore, $F'_r = 0$

$$K_{T1} = k_1 + \frac{v_v}{H_1} f_{d1} + \frac{v_s}{H_1} f_{p1}$$

  - Now c_2 has no effect on c_1 and we return to a one compartment model
    - all time-variable solutions can be applied

Simplified Versions (cont.)

- Level 1
  - no volatilization, no decomposition
    - $v_v = 0$, $k_1 = 0$, $k_2 = 0$

$$K_{T1} = k_1 + \frac{v_v}{H_1} f_{d1} + \left(1 - F_r'\right)\left(\frac{v_s}{H_1} f_{p1} + \frac{v_d}{H_1} f_{d1}\right)$$

$$0 \qquad 0$$

  - Useful for modeling toxic metals

Homework #6 part I

- Chapra Lecture 40 problem: 40.1
  - Thomann and DiToro (1983) presented the following data related to the solids budget for the Western Basin of Lake Erie:
    - Volume = 23×10^9 m^2
    - Area = 3030×10^6 m^2
    - Solid loading = 11.4×10^{12} g/yr
    - Suspended Solids = 20 mg/L
    - Flow = 167×10^9 m^3/yr
  - They assumed that the solids settle at a rate of 2.5 m/d (912.5 m/yr), and tha the sediments have ρ=2.4 g/mL and ϕ-0.9. Determine the burial and resuspension velocities.

Homework #6 part II

- Chapra Lecture 40 problem: 40.2
  - Suppose that a toxic substance that is subject to volatilization (v_v = 100 m/yr) is discharged to Lake Huron with an inflow concentration of 100 µg/L. In the absence of sediment feedback, determine the concentration for three cases: (a) weak sorber (K_d = 0.002 m^3/g), (b) moderate sorber (K_d = 0.1), and (c) strong sorber (K_d = 2). Other necessary information should be taken from Examples 40.1 and 40.2.

Homework #6 part III

- Chapra Lecture 40 problem: 40.3a
  - A substance (K_d = 0.02 m^3/d; M = 300) is discharged into a lake (c_{in} = 100 μg/L) having the following characteristics:

Volume = $1x10^6$ m^3	Mean depth = 5 m
Residence time = 1 year	Suspended solids = 10 mg/L
Settling velocity = 50 m/yr	Sediment deposition = 100 g/m^3/yr
Sediment porosity = 0.85	Sediment density = 2.5 g/cm^3

    - (a) It the resuspension is negligible, compute the steady-state concentration for three levels of volatilization:
      - (i) high soluble (ν_v = 0)
      - (ii) moderately soluble (ν_v = 10 m/yr)
      - (iii) nearly insoluble (ν_v = 100 m/yr)

- To next lecture