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Print version

CEE 577: Surface Water Quality Modeling

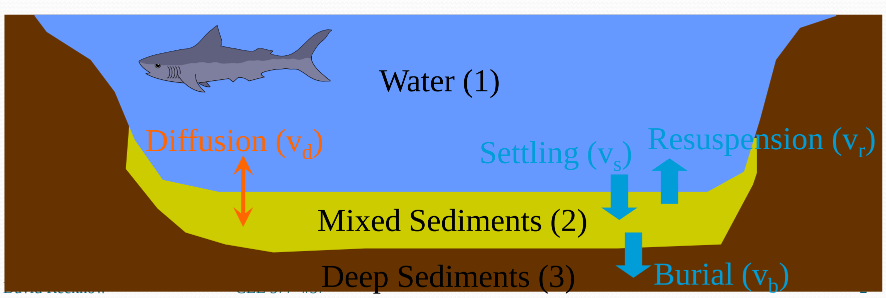
Lecture #37

Toxics: Rivers

(Chapra, L44)

Review: 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

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

New Chapra approach

Toxicant Mass Balance

Can be expressed as: Qc_{in}

- In the water column

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

- In the mixed sediments

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

Steady State Solution

- Water column

$$c_1 = \frac{Qc_{in}}{Q + k_1V_1 + v_v A f_{d1} + (1 - F_r')(v_s f_{p1} + v_d f_{d1})A}$$

- Mixed Sediments

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

Steady State Solution

- Formulate total loss velocity

$$v_T = k_1 H_1 + v_v f_{d1} + (v_s f_{p1} + v_d f_{d1})(1 - F_r')$$

- which can be in the form of a total rate

$$K_T = {}^{v_T}\!/_{H_1} \qquad \text{And since:} \qquad H_1 = {}^{V_1}\!/_{A}$$

- At SS

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

- So this reduces to:

$$c_1 = \frac{Qc_{in}}{Q + K_T V_1} \qquad \text{or} \qquad c_1 = \frac{W}{\lambda V_1} \qquad \text{Where:} \quad \lambda = \frac{Q}{V_1} + K_T$$

Sediment Feedback & k

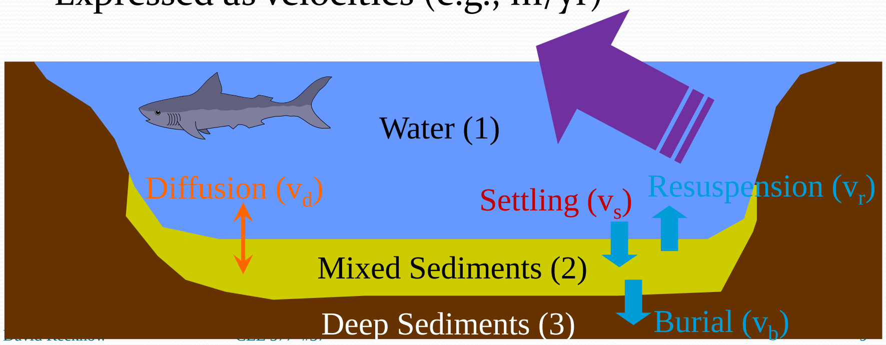
- **The ratio of sediment feedback to total sediment purging**

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

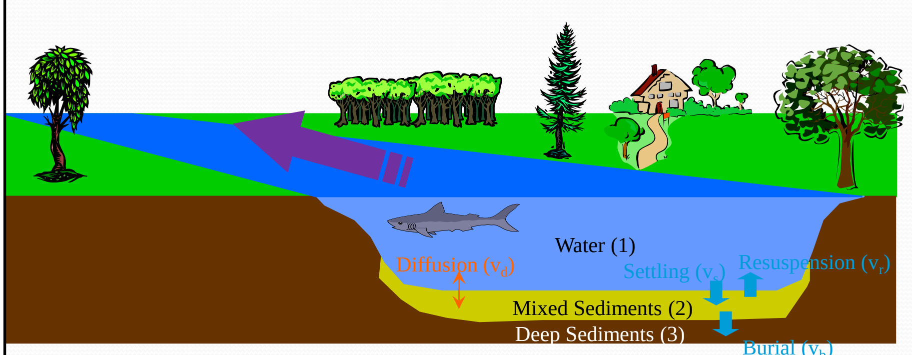
- The first-order constants k1 and k2 incorporate various decay processes
  - Biodegradation
  - Hydrolysis
  - photolysis

Toxics Model: CSTR to a PRF

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



- Combine with advective flow



Solids: Mass Balance

Earlier lake model

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

Divide by V, and replace loadings with advective term

- In water column

$$\cancel{\frac{dm_1}{dt}}^{0} = -U \frac{dm_1}{dx} - \frac{v_s}{H_1} m_1 + \frac{v_r}{H_1} m_2$$

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

Divide by A

- in mixed sediments

$$H_2 \cancel{\frac{dm_2}{dt}}^{0} = v_s m_1 - v_r m_2 - v_b m_2$$

Solids: Steady State Solution

- Assuming that the sediments do not move downstream
- mass balance on m_2 and therefore relationship between m_2 and m_1 are identical for lake and river

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

Toxicant Mass Balance

Earlier lake model

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

Divide by V, and replace loadings with advective term

- In the water column

$$\frac{dc_1}{dt} = -U\frac{dc_1}{dx} + \frac{v_d}{H_1}\left(f_{d2}c_2 - f_{d1}c_1\right) - k_{T1}c_1 - \frac{v_v}{H_1} f_{d1}c_1 - \frac{v_s}{H_1} f_{p1}c_1 + \frac{v_r}{H_1}c_2$$

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

- In the mixed sediments

Divide by A

$$H_2 \frac{dc_2}{dt} = v_d\left(f_{d1}c_1 - f_{d2}c_2\right) - k_{T2}H_2c_2 + v_s f_{p1}c_1 - v_r c_2 - v_b c_2$$

New Chapra approach

Steady State Solution

- Formulate total loss velocity

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

- which can be in the form of a total rate

$$K_T = {}^{v_T}\!/_{H_1}$$

  - and the ratio of sediment feedback to total sediment purging remains:

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

Steady State Solution

Earlier lake model

$$c_1 = \frac{Qc_{in}}{Q + k_1V_1 + v_v AF_{d1} + (1-F_r')(v_sF_{p1} + v_dF_{d1})A}$$

- The water column solution is:

$$c_1 = c_{1o}e^{-\frac{K_T x}{U}}$$

$$c_1 = \frac{Qc_{in}}{Q + K_TV_1}$$

- and as before the sediment solution is:

$$c_2 = \frac{v_sF_{p1} + v_dF_{d1}}{\underbrace{k_2H_2 + v_r + v_b + v_dF_{d2}}_{R_{21}}}c_1$$

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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

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Simplified Versions (cont.)

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

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

(0) (0)

  - Useful for modeling toxic metals

Solutions (cont.)

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

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

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

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

Overview of solutions to toxic model

For Lakes:

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

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

For Rivers:

$$C_{T1} = C_{T1o} e^{-K_{T1} x/U}$$

$C_{T1o} \rightarrow \frac{W}{Q}$

- To next lecture