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

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

Can be expressed as: \( Qm_{\text{in}} \)
Solids: Steady State Solution

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

\[ m_2 = (1 - \phi) \rho = \frac{\nu_s}{\nu_r + \nu_b} m_1 \]
Toxicant Mass Balance

- In the water column

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

- In the mixed sediments

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

Can be expressed as: \( Qc_{in} \)
Steady State Solution

- Water column

\[
c_1 = \frac{Qc_{in}}{Q + k_1 V_1 + \nu_v A f_{d1} + (1 - F'_r)(\nu_s f_{p1} + \nu_d f_{d1}) A}
\]

- Mixed Sediments

\[
c_2 = \frac{\nu_s f_{p1} + \nu_d f_{d1}}{k_2 H_2 + \nu_r + \nu_b + \nu_d f_{d2}} c_1
\]
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
  \[ K_T = \frac{v_T}{H_1} \]
  And since: \[ H_1 = \frac{V_1}{A} \]
- At SS
  \[ c_1 = \frac{Q c_{in}}{Q + k_1 V_1 + v_v A f_{d1} + (1 - F'_r)(v_s f_{p1} + v_d f_{d1}) A} \]
- So this reduces to:
  \[ c_1 = \frac{Q c_{in}}{Q + K_T V_1} \]
  or \[ c_1 = \frac{W}{\lambda V_1} \]
  Where: \[ \lambda = \frac{Q}{V_1} + K_T \]
Sediment Feedback & $k$

- The ratio of sediment feedback to total sediment purging
  
  $$F'_r = \frac{\nu_r + \nu_d f_{d2}}{\nu_r + \nu_b + \nu_d f_{d2} + k_2 H_2}$$

- The first-order constants $k_1$ and $k_2$ 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

- In water column
  \[ \frac{dm_1}{dt} = -U \frac{dm_1}{dx} - \frac{v_s}{H_1} m_1 + \frac{v_r}{H_1} m_2 \]

- In mixed sediments
  \[ H_2 \frac{dm_2}{dt} = v_s m_1 - v_r m_2 - v_b m_2 \]

Earlier lake model

\[ V_1 \frac{dm_1}{dt} = W_m - Qm_1 - v_s Am_1 + v_r Am_2 \]

Divide by \( V \), and replace loadings with advective term

\[ V_2 \frac{dm_2}{dt} = v_s Am_1 - v_r Am_2 - v_b Am_2 \]

Divide by \( A \)
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

- In the water column

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

- In the mixed sediments

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

Earlier lake model

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

New Chapra approach

Divide by V, and replace loadings with advective term

Divide by A
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
  \[ K_T = \frac{v_T}{H_1} \]
- 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

The water column solution is:

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

and as before the sediment solution is:

\[ c_2 = \frac{\nu_s F_{p1} + \nu_d F_{d1}}{k_2 H_2 + \nu_r + \nu_b + \nu_d F_{d2}} c_1 \]

Earlier lake model
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
  - $v_v = 0$, $k_1 = 0$, $k_2 = 0$

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

- Useful for modeling toxic metals
Solutions (cont.)

\[ K_{T1} = k_1 + \frac{v}{H_1} f_{d1} + \left(1 - F'_r\right) \left(\frac{v_s}{H_1} f_{p1} + \frac{v_d}{H_1} f_{d1}\right) \]

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

\[ k_1 = k_{d1} f_{d1} + k_{p1} f_{p1} \]

\[ k_2 = k_{d2} f_{d2} + k_{p2} f_{p2} \]
Overview of solutions to toxic model

For Lakes:

\[ C_{T1} = \frac{W}{\lambda V} \]

Where:

\[ \lambda = \frac{Q}{V} + K_{T1} \]

For Rivers:

\[ C_{T1} = C_{T1o}e^{-K_{T1}\frac{x}{U}} \]
To next lecture