CEE 577: Surface Water Quality Modeling

Lecture #41
TOC & THMFP Models II
Scientific Literature

NYC: Cannonsville Case Study
Cannonsville Reservoir Study

- Algal & THM Precursor Models
  - Doerr, Stepczuk and others
- Cannonsville Reservoir
  - Part of Catskill-Delaware Supply for NYC
  - Dimictic; Eutrophic (impounded in 1965)
    - $P_{avg} = 30 \mu g/L$
  - Characteristics for 1995
    - Hydraulics
      - $H_{mean} = 19$ m
      - $V = 373 \times 10^6$ m$^3$
      - $t_{mean} = 4.7$ months
      - $SA = 19.3 \times 10^6$ m$^2$
      - $DA = 1160 \times 10^6$ m$^2$
    - Loading
      - $TOC = ? \times 10^3$ kg/yr
      - $P = ? \times 10^3$ kg/yr

For more, see the literature at:  
https://www.ecs.umass.edu/eve/research/nyc_chloramines/literature.html

Inflow
- West Branch of Delaware River (WBDR)
  - 80%
- Three outflows
  - Over spillway
  - Withdrawal to aqueduct
    - 10, 20**, or 37 m below spillway
  - Release at base of dam
• Individual models

Forcing Functions

• Lower flows in 1995, resulted in lower loadings
PAR

- Photosynthetically-active radiation
- Often defined as the light between 400 and 700 nm

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<table>
<thead>
<tr>
<th>No.</th>
<th>Coefficient</th>
<th>Symbol</th>
<th>Value/Units</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>maximum specific growth rate for phytoplankton</td>
<td>$K_{max}$</td>
<td>1.7 d$^{-1}$</td>
<td>Auer and Forrer 1998</td>
</tr>
<tr>
<td>2.</td>
<td>phytoplankton respiration rate</td>
<td>$k_r$</td>
<td>0.29 d$^{-1}$</td>
<td>Auer and Forrer 1998</td>
</tr>
<tr>
<td>3.</td>
<td>light half saturation coefficient for phytoplankton growth</td>
<td>$K_l$</td>
<td>55 µg L$^{-1}$ m$^{-3}$</td>
<td>Auer and Forrer 1998</td>
</tr>
<tr>
<td>4.</td>
<td>background extinction coefficient</td>
<td>$k_p$</td>
<td>$-0.018$ W m$^{-2}$ s$^{-1}$</td>
<td>Effler et al. 1999b</td>
</tr>
<tr>
<td>5.</td>
<td>multiplier for Chl component of extinction</td>
<td>$k_{hal}$</td>
<td>0.02 m$^{-3}$ Chl</td>
<td>Effler et al. 1999b</td>
</tr>
<tr>
<td>6.</td>
<td>decay coefficient for ANLP</td>
<td>$k_{hal}$</td>
<td>0.20 d$^{-1}$</td>
<td>Auer et al. 1998</td>
</tr>
<tr>
<td>7.</td>
<td>sediment release rate SRP</td>
<td>SRP$_{sed}$</td>
<td>$0.4$ mg m$^{-2}$ d$^{-1}$</td>
<td>Erickson and Auer 1998</td>
</tr>
<tr>
<td>8.</td>
<td>phosphorus half saturation constant for phytoplankton growth</td>
<td>$K_{P_{hal}}$</td>
<td>0.5 µg P L$^{-1}$</td>
<td>Auer and Forrer 1998</td>
</tr>
<tr>
<td>9.</td>
<td>bioavailable fraction of non-living PP load</td>
<td>anlp</td>
<td>25%</td>
<td>Auer et al. 1998</td>
</tr>
<tr>
<td>10.</td>
<td>Chl settling velocity</td>
<td>$v_{set}$</td>
<td>0.17 m d$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>11.</td>
<td>settling velocity ANLP and UANLP</td>
<td>$v_{set}$</td>
<td>0.94 m d$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>12.</td>
<td>settling velocity NLNP</td>
<td>$v_{set}$</td>
<td>0.66 m d$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>13.</td>
<td>SOD at 20 ºC</td>
<td>SOD$_{20}$</td>
<td>1.06 g m$^{-3}$ d$^{-1}$</td>
<td>Erickson and Auer 1998</td>
</tr>
<tr>
<td>14.</td>
<td>organic C to Chl ratio</td>
<td>$A_{Chl}$</td>
<td>80 µg C µg Chl$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>15.</td>
<td>organic C to N ratio of phytoplankton</td>
<td>$A_{N}$</td>
<td>6.75 µg C µg N$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
</tbody>
</table>

* when bottom NO$_3$ > 0.01 µg N L$^{-1}$
* When bottom is anoxic and NO$_3$ < 0.01 µg N L$^{-1}$
* WEP = water exposed elevation (ft)
SOD

- For

In-situ device

Table 4—Results of sediment oxygen demand experiments.

<table>
<thead>
<tr>
<th>Date of Collection, 1995</th>
<th>Station</th>
<th># of cores *</th>
<th># of trials *</th>
<th>Mean ± s.d. $SO_2$ (gO$_2$/m$^2$ d$^{-1}$)</th>
<th>Mean ± s.d. $SOD$ (gO$_2$/m$^3$ d$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-6 July</td>
<td>2</td>
<td>3</td>
<td>5</td>
<td>0.64 ± 0.09</td>
<td>1.90 ± 0.18</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>0.44 ± 0.05</td>
<td>0.93 ± 0.06</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>2</td>
<td>5</td>
<td>0.46 ± 0.06</td>
<td>0.98 ± 0.10</td>
</tr>
<tr>
<td>29-30 August</td>
<td>2</td>
<td>1</td>
<td>5</td>
<td>0.65 ± 0.07</td>
<td>1.04 ± 0.10</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>1</td>
<td>5</td>
<td>0.46 ± 0.08</td>
<td>1.02 ± 0.17</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>1</td>
<td>3</td>
<td>0.45 ± 0.05</td>
<td>0.90 ± 0.10</td>
</tr>
<tr>
<td>Overall</td>
<td>11</td>
<td>20</td>
<td></td>
<td>0.50 ± 0.11</td>
<td>1.06 ± 0.23</td>
</tr>
</tbody>
</table>

* total number of cores per station.
* total number of trials for cores collected at the same station and sampling time.

Figure 5—The relationship between chemical oxygen demand (COD) and sediment oxygen demand (SOD).
Model Performance

- Weekly measurement in water column
- Objective: monthly average within 2 standard deviations

Performance II

- Systematic depletions of:
  - Epilimnetic NO_x
  - Hypolimnetic DO

- Over-prediction of ammonia?
Performance: DO

- Progressive depletion of DO in hypolimnion
Verification

- Problem with limited data in 1994
Verification

Performance: Withdrawal
Cannonsville THMs: General Info

- Major Papers
  - Stepczuk, Martin, Longabucco, Bloomfield & Effler, 1998
    - “Allochthonous Contributions of THM Precursors in a Eutrophic Reservoir”, *J. Lake & Res. Mgmt.*, 14(2/3)344-355
  - Stepczuk, Martin, Effler, Bloomfield & Auer, 1998
    - “Spatial and Temporal Patterns of THM Precursors in a Eutrophic Reservoir”, *J. Lake & Res. Mgmt.*, 14(2/3)356-366
  - Stepczuk, Owens, Effler, Bloomfield & Auer, 1998

- THMFP Method
  - Method 5710B of Standard Methods
  - pH 7.0, 7 days, 25 C, dosed to get >1.0 mg/L residual
  - Average CV was 4% for field replicates

1995 Data

- Severe Drought
- Net production of precursors in Epilimnion is evident from THMFP data
Mass Balance Model: THMFP

\[ \Delta M = W - E + S \]
\[ S = \Delta M - W + E \]

- Terms
  - \( W \) = allochthonous mass loading
    - From tributaries
  - \( E \) = mass export by outflow
    - Spill + release + water supply withdrawal
  - \( S \) = net autochthonous production
    - Gross production - decay

Stepczuk et al., 1998, J. Lake & Res. Mgmt., 14(2/3)367-378

Mass Balance Model: DOC

- Mid-summer drop in \( S \)
  - Not seen with THMFP
- Lower average S:W ratio
  - 1.7 for THMFP
  - 0.7 for TOC

Stepczuk et al., 1998, J. Lake & Res. Mgmt., 14(2/3)367-378
Mass Balance Model: \( S \)

- Monthly changes in \( S \)
  - Incremental not cumulative
  - No apparent correlation between net production of THMFP and DOC
  - Raises questions about use of TOC as a surrogate for THMFP

\[ V_1 \frac{dc_1}{dt} = W_1 - Q_1 c_1 + E_{12}' (c_2 - c_1) - V_1 S_1 \]
\[ V_2 \frac{dc_2}{dt} = W_2 + Q_2 c_2 + E_{12}' (c_1 - c_2) - V_2 S_2 \]

2-Layer model
- Spatial resolution
  - Epilimnion
    - Designated “1” or “E”
  - Hypolimnion
    - Designated “2” or “H”
- Loading (W)
  - Measured stream data for epilimnion
- Outflow (Q)
  - Separated based on withdrawal location
- Mixing (E)
  - From temperature data
- Net production (S)
  - Not directly observed

Stepczuk et al., 1998, J. Lake & Res. Mgmt., 14(2/3)367-378
Estimation of vertical Dispersion Coefficient

- Use analogous 2-layer temperature model

\[ V_2 \left( \frac{\Delta T_2}{\Delta t} \right) = E_{12} A_{12} (T_1 - T_2) \]

\[ E_{12} = \frac{|T_2^{(t-1)} - T_2^{(t)}| V_2 z_{12}}{(T_1 - T_2) \Delta t A_{12}} \]

- Apply measured temperature profiles to get \( E \)


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Fitting \( S \) to Data

- Adjust \( S \) to match model predictions to data
- Keep \( S \) at zero

\( S_1 \) & \( S_2 \) determined by fitting curves to data

\( S_1 \) & \( S_2 \) equal to 0
Select of S (cont.)

- Intermediate option
  - Fit $S_1$ to data
  - Set $S_2$ to zero
- Justification for $S_2 = 0$
  - No algal growth in hypolimnion
  - Allochthonous THMFP originally trapped in hypolimnion is recalcitrant

Mechanistic Model for S

- Sub-model for algal FP production
  \[
  \frac{d(THMFP)}{dt} = \alpha_{THMFP} \mu A
  \]
  \[
  = \alpha_{THMFP} \mu A (FN)(F_{L_z})A
  \]

- Depends on:
  - Algal concentration ($A$)
    - from measured Chl ($C_T$)
  - Light Function
    - From Microcosm studies
    - Data fit data to Steele’s Equation
  - \[ F_{L_z} = \frac{I_z}{K_L} \exp(1 - \frac{I_z}{K_L}) \]

Stepczuk et al., 1998, J. Lake & Res. Mgmt., 14(2/3)356-368

Stepczuk et al., 1998, J. Lake & Res. Mgmt., 14(2/3)367-378
Mechanistic Model for $S$

- Sub-model for degradation of THMFP
  - Independent 1st order loss terms for autochthonous and allochthonous forms

\[
\frac{d(\text{THMFP}_{\text{autochthonous}})}{dt} = -k_{L(au)} \text{THMFP}_{\text{autochthonous}}
\]

\[
\frac{d(\text{THMFP}_{\text{allochthonous}})}{dt} = -k_{L(al)} \text{THMFP}_{\text{allochthonous}}
\]

Mechanistic Model

- Results based on:
  - Two Scenarios
    - No decay of any THMFP in hypolimnion
    - No decay of allochthonous THMFP
  - Fitted $K_L$ values

- Stepczuk et al., 1998, J. Lake & Res. Mgmt., 14(2/3)367-378

- Epilimnion: $k_{L(al)}=k_{L(au)}=0.08d^{-1}$
- Hypolimnion: $k_{L(al)}=0.00; k_{L(au)}=0.15d^{-1}$
2-Layer model

- Spatial resolution
  - Epilimnion
    - Designated “1” or “E”
  - Hypolimnion
    - Designated “2” or “H”

\[
V_1 \frac{dc_1}{dt} = W_1 - Q_1 c_1 + E_{12}'(c_2 - c_1) - V_1 S_1
\]

\[
V_2 \frac{dc_1}{dt} = W_2 + Q_2 c_2 + E_{12}'(c_1 - c_2) - V_2 S_2
\]

Stepczuk et al., 1998, J. Lake & Res. Mgmt., 14(2/3)367-378

- To next lecture