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, Stepoczuk 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
    - $H_{mean} = 19 \, m$
    - $V = 373 \times 10^6 \, m^3$
    - $\tau_{mean} = 4.7 \, \text{months}$
    - $SA = 19.3 \times 10^6 \, m^2$
    - $DA = 1160 \times 10^6 \, m^2$
  - Loading
    - $TOC = ? \times 10^2 \, kg/yr$
    - $P = ? \times 10^3 \, kg/yr$

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**

(d) 

(e)
Forcing Functions

- Lower flows in 1995 resulted in lower loadings
PAR

- Photosynthetically-active radiation
  - Often defined as the light between 400 and 700 nm
Table 3.—Model coefficients independently determined to support the nutrient-phytoplankton model for Cannonsville Reservoir.

<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>$\mu_{max}$</td>
<td>1.7 d$^{-1}$</td>
<td>Auer and Forrer 1998</td>
</tr>
<tr>
<td>2.</td>
<td>phytoplankton respiration rate</td>
<td>$k_{sr}$</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>53 $\mu$E$\cdot$m$^{-2}\cdot$s$^{-1}$</td>
<td>Auer and Forrer 1998</td>
</tr>
<tr>
<td>4.</td>
<td>background extinction coefficient</td>
<td>$K_w$</td>
<td>$= -0.018xWSE^1+6.67$</td>
<td>Effler et al. 1998b</td>
</tr>
<tr>
<td>5.</td>
<td>multiplier for Chl component of extinction</td>
<td>$K_c$</td>
<td>0.02 m$^2$mg$^{-1}$ Chl</td>
<td>Effler et al. 1998b</td>
</tr>
<tr>
<td>6.</td>
<td>decay coefficient for ANLPP mineralization</td>
<td>$k_{pi}$</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>$R_{sed_{SRP,b}}$</td>
<td>0* mg$\cdot$m$^{-2}\cdot$d$^{-1}$</td>
<td>Erickson and Auer 1998</td>
</tr>
<tr>
<td>8.</td>
<td>phosphorus half-saturation constant for phytoplankton growth</td>
<td>$K_{SRP}$</td>
<td>0.5 $\mu$gP$\cdot$L$^{-3}$</td>
<td>Auer and Forrer 1998</td>
</tr>
<tr>
<td>9.</td>
<td>biavailable fraction of non-living PP load</td>
<td>availpp</td>
<td>25%</td>
<td>Auer et al. 1998</td>
</tr>
<tr>
<td>10.</td>
<td>Chl settling velocity</td>
<td>$v_{el_{Chl}}$</td>
<td>0.17 m$\cdot$d$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>11.</td>
<td>settling velocity ANLPP and UNLPP</td>
<td>$v_{el_{PP}}$</td>
<td>0.94 m$\cdot$d$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>12.</td>
<td>settling velocity NLPN</td>
<td>$v_{el_{PN}}$</td>
<td>0.46 m$\cdot$d$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>13.</td>
<td>SOD, at 20 °C</td>
<td>$SOD_{20}$</td>
<td>1.06 g$\cdot$m$^{-2}\cdot$d$^{-1}$</td>
<td>Erickson and Auer 1998</td>
</tr>
<tr>
<td>14.</td>
<td>organic C to Chl ratio</td>
<td>$a_{CCl}$</td>
<td>80 $\mu$gC$\cdot$gChl$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
<tr>
<td>15.</td>
<td>organic C to N ratio of phytoplankton</td>
<td>$a_{CN}$</td>
<td>6.25 $\mu$gC$\cdot$gN$^{-1}$</td>
<td>Effler and Brooks 1998</td>
</tr>
</tbody>
</table>

* when bottom $NO_2 > 0.01 \mu$gN$\cdot$L$^{-1}$.
† when bottom is anoxic and $NO_2 < 0.01 \mu$gN$\cdot$L$^{-1}$.
$WSE =$ water surface elevation (m).
Table 4.—Results of sediment oxygen demand experiments.

<table>
<thead>
<tr>
<th>Date of Core Collection, 1995</th>
<th>Station</th>
<th># of cores</th>
<th># of trials</th>
<th>Mean ± s.d. SOD$_{\text{a}}$ (gO$_2$ \cdot m$^{-2}$ \cdot d$^{-1}$)</th>
<th>Mean ± s.d. SOD$_{\text{b}}$ (gO$_2$ \cdot m$^{-2}$ \cdot 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>1.36 ± 0.18</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>0.44 ± 0.03</td>
<td>0.93 ± 0.06</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>2</td>
<td>3</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>3</td>
<td>0.45 ± 0.07</td>
<td>1.04 ± 0.10</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>1</td>
<td>3</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>0.96 ± 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>

$^a$ total number of cores per station.

$^b$ total number of trials for cores collected at the same station and sampling time.
SOD continued

- In-situ device

![Image of an in-situ device]

**Figure 5.** The relationship between chemical oxygen demand (COD) and sediment oxygen demand (SOD).

\[
\text{SOD} = 2.63 \ln(\text{COD}) - 9.0
\]

\[
R^2 = 0.68
\]
Model Performance

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

- Systematic depletions of:
  - Epilimnetic NO\textsubscript{x}
  - Hypolimnetic DO

- Over-prediction of ammonia?
Performance: DO

- Progressive depletion of DO in hypolimnion
Verification

- Problem with limited data in 1994
Verification
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
  - 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

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

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

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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

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

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

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

- Use analogous 2-layer temperature model

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

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

- Apply measured temperature profiles to get E

Owens, 1998, J. Lake & Res. Mgmt., 14(2/3)152-161
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

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

- Sub-model for algal FP production

\[
\frac{d(THMFP)}{dt} = \alpha_{THMFP} \mu A \\
= \alpha_{THMFP} \mu_{\text{max}} (FN)(FL_z) A
\]

- Depends on:
  - Algal concentration (A)
    - from measured Chl (C_T)
  - Light Function
    - From Microcosm studies
    - Data fit data to Steele’s Equation

\[
FL_z = \frac{I_z}{K_L} \exp \left(1 - \frac{I_z}{K_L}\right)
\]

\[
K_L = 150 \frac{\mu E}{m^2 s}
\]

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

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

\[
d\left( THMFP_{autochthonous} \right) = -k_{L(au)} THMFP_{autochthonous} \\
d\left( THMFP_{allochthonous} \right) = -k_{L(al)} THMFP_{allochthonous}
\]
Mechanistic Model

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

2-Layer model

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

\[
\begin{align*}
V_1 \frac{dc_1}{dt} &= W_1 - Q_1 c_1 + E'_{12} (c_2 - c_1) - V_1 S_1 \\
V_2 \frac{dc_1}{dt} &= W_2 + Q_2 c_2 + E'_{12} (c_1 - c_2) - V_2 S_2
\end{align*}
\]

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

\( S_1 \) & \( S_2 \) determined by fitting curves to data
• To next lecture