LECTURE #14

INSTREAM WATER QUALITY – BIOCHEMICAL REACTIONS
RCHRES STRUCTURE CHART

RCHRES
- Simulate a reach or mixed reservoir

HYDR
- Simulate hydraulic behavior

ADCALC
- Estimate advective behavior of constituents

CONS
- Simulate conservative constituents

HTRCH
- Simulate heat exchange & water temperature

SEDTRN
- Simulate inorganic sediment

GQUAL
- Simulate generalized quality constituents

RQUAL
- Simulate constituents involved in biochemical transformations
RQUAL STRUCTURE CHART

**RQUAL**
Simulate constituents involved in biochemical transformations

**OXRX**
Simulate dissolved oxygen and BOD

**NUTRX**
Simulate inorganic nutrients (N and P)

**PLANK**
Simulate plankton and refractory organics

**PHCARB**
Simulate pH and inorganic carbon
OXRX: DISSOLVED OXYGEN AND BOD PROCESSES

- Reaeration
- BOD decay/oxygen depletion
- Settling of BOD material
- Benthic oxygen demand
- Benthic release of BOD
DISSOLVED OXYGEN MASS BALANCE

Storage:
Mass of dissolved oxygen

Inflow to reach:
- Zooplankton respiration
- BOD decay
- Reaeration
- Phytoplankton growth and respiration
- Benthic algae growth and respiration
- Benthic oxygen demand
- Nitrification

Outflow from reach:
- Zooplankton respiration
- BOD decay
- Reaeration
- Phytoplankton growth and respiration
- Benthic algae growth and respiration
- Benthic oxygen demand
- Nitrification
OXYGEN REAERATION AND SATURATION

Function of DO deficit and reaeration coefficient

\[ DO_{reaeration} = K_{reaeration} \cdot (DO_{sat} - DO) \]

where:

- \( K_{reaeration} \) = Reaeration coefficient (hr\(^{-1}\))
- \( DO_{sat} \) = Oxygen saturation level for current water temperature (mg/L)
- \( DO \) = Dissolved oxygen concentration (mg/L)

\[ DO_{sat} = 14.65 + T_w \cdot f \cdot \left( -0.4102 + T_w \cdot (0.007991 - 0.7777 \cdot 10^{-4} \cdot T_w) \right) \]

where:

- \( T_w \) = Water temperature (°C)
- \( f \) = Correction factor based on reach elevation
OXYGEN REAERATION: OPTIONAL METHODS

Streams

1. Tsivoglou-Wallace equation
   • Function of velocity and slope
   • Temperature correction
   • Rate coefficient

2. Covar equation
   • Function of velocity and depth
   • Temperature correction
   • Rate coefficient
   • Three sets of coefficients & exponents based on depth and velocity regimes

3. User-specified parameters (Covar equation)

Lakes

• Function of depth and wind speed
• User-defined correction factor
BOD MASS BALANCE

- Inflow to reach
- Storage of BOD
- Outflow from reach

- Benthic Release
- Zooplankton death and excretion
- Phytoplankton death

- BOD decay
- Settling
- Benthic algae death
BOD DECAY

\[ \text{DO}_{\text{consumed}} = K_{\text{BOD}} \cdot \theta^{(T_w-20)} \cdot \text{BOD} \]

where:

\[ K_{\text{BOD}} \] = BOD decay rate at 20 °C (hr\(^{-1}\))

\[ \theta \] = Temperature correction coefficient

\[ \text{BOD} \] = BOD concentration (mg/L)

\[ T_w \] = Water temperature (°C)
BENTHIC PROCESSES (Optional)

• Benthic oxygen demand
  – Exponential function of DO
  – Benthic oxygen demand at 20 °C
  – Temperature correction

• Benthic release of BOD
  – Release rate under aerobic conditions
  – Release rate under low oxygen conditions
  – Exponential function of DO
  – Adjusted under scouring conditions
OXYGEN/BOD PARAMETERS

- Escape coefficient in reaeration equations (REAK)
- Temperature correction coefficient for reaeration (TCGINV)
- Velocity exponent in user-specified reaeration (EXPREV)
- Depth exponent in user-specified reaeration (EXPRED)
- Lake reaeration correction factor (CFOREA)
- BOD decay rate at 20 °C (hr⁻¹) (KBOD20)
- Temperature coefficient for BOD decay (TCBOD)
- BOD settling rate (m/hr or ft/hr) (KODSET)
NUTRX: INORGANIC NUTRIENTS

• **CONSTITUENTS**
  - NO$_3$ (nitrate)
  - NO$_2$ (nitrite)
  - NH$_3$ (ammonia), particulate NH$_3$
  - PO$_4$ (orthophosphate) particulate PO$_4$

• **PROCESSES**
  - Decomposition of BOD material to PO$_4$ and NH$_3$ (or NO$_3$)
  - Nitrification of NH$_3$ to NO$_3$
  - Denitrification of NO$_3$ to N$_2$
  - Adsorption of NH$_3$ and PO$_4$ to sediment
  - Benthic release of NH$_3$ and PO$_4$
INORGANIC NITROGEN SOURCES, SINKS AND TRANSFORMATIONS

Inflow to the Reach

- Dissolved TAM
  - Algal uptake
  - Zooplankton respiration & excretion

- Adsorbed TAM
  - Deposition
  - Scour
  - Desorption
  - Adsorption

- NO₂
  - Nitrification
  - Algal uptake
  - Vaporization

- NO₃
  - Denitrification
  - BOD decay

Outflow from the Reach

- NO₂
  - Nitrification
  - Zooplankton respiration & excretion

- NO₃
  - Algal uptake

- Dissolved TAM
  - BOD decay
  - Benthic release
INORGANIC PHOSPHORUS SOURCES, SINKS AND TRANSFORMATIONS

Inflow to the Reach

- Algal uptake
- Benthic release
- Deposition

Dissolved PO₄

- Desorption
- Adsorption
- Scour

Adsorbed PO₄

Outflow from the Reach

- BOD Decay
- Zooplankton respiration & excretion
NITRIFICATION AND DENITRIFICATION

• **Nitrification:** $\text{NH}_3 \rightarrow \text{NO}_2 \rightarrow \text{NO}_3$
  - First-order in ammonia concentration
  - Nitrification rate coefficient ($\text{TAMNIT}$)
  - Temperature correction ($\text{TCNIT}$)
  - Consumes oxygen

• **Denitrification:** $\text{NO}_3 \rightarrow \text{N}_2$
  - First-order in nitrate
  - Denitrification rate coefficient ($\text{KNO320}$)
  - Temperature correction ($\text{TCDEN}$)
  - Only occurs below threshold DO ($\text{DENOXT}$)
Particulate PO$_4$ and NH$_3$ - Optional

- Adsorption of PO$_4$ and NH$_3$ to three sediment fractions (sand, silt, clay) in the water column

- Deposition/resuspension of sediment is computed in SEDTRN section

- Resuspended sediment has constant, user-defined concentrations of NH$_3$ and PO$_4$

- Nutrient resuspension is limited by mass of sediment in bed
NUTRIENT PARAMETERS

- Nitrification rate of NH$_3$ at 20 °C (KTAM20)
- Nitrification rate of NO$_2$ at 20 °C (KNO220)
- Denitrification rate at 20 °C (KNO320)
- Dissolved oxygen threshold for denitrification (DENOXT)
- Adsorption coefficients for NH$_3$ and PO$_4$ adsorbed to inorganic sediment (ADNHPM, ADPOPM)
- Concentrations of NH$_3$ and PO$_4$ adsorbed to resuspended bed sediments (BNH4, BPO4)
- Benthic release rates of NH$_3$ under aerobic and anaerobic conditions (mg/m$^2$/hr) (BRTAM)
- Benthic release rates of PO$_4$ under aerobic and anaerobic conditions (mg/m$^2$/hr) (BRPO4)
NUTRIENT PARAMETERS: COMPOSITION OF BIOMASS

- Ratio of C to P in biomass (molar) \((CVBPC)\)
- Ratio of N to P in biomass (molar) \((CVBPN)\)
- Percentage of biomass weight consisting of C \((BPCNTC)\)
- Mass (mg) of dissolved oxygen associated with 1 mg biomass \((CVBO)\)

Default biomass composition: \(C:N:P = 106:16:1\)
PLANK: PLANKTON PROCESSES

• Phytoplankton
  – Growth, respiration, death
  – Settling from water column
  – Predation by zooplankton

• Zooplankton
  – Growth, respiration, death

• Benthic algae
  – Growth, respiration, death

• Refractory organics (N, P, C)
  – Results from decomposition of algal material
  – Settling
 PHYTOPLANKTON MASS BALANCE 

Inflow to reach

Net growth (growth-respiration)  Phytoplankton death

Storage of Phytoplankton

Settling

Zooplankton predation

Outflow from reach

20 of 35
PHYTOPLANKTON SIMULATION

• Single species
  – Default composition: C:N:P = 106:16:1

• Advection and settling
  – Settling rate: PHYSET
  – Advection routine: maintains minimum concentration of phytoplankton in reach

• Light
  – Solar radiation reduced by surface shading and reflection
  – Light extinction = base/water + sediment + phytoplankton
  – Euphotic depth and light available to phytoplankton
  – Light correction factor (< 1 if euphotic depth < average depth)
PHOTOPHANTON SIMULATION

• Growth simulation by Michaelis-Menton kinetics

\[ G_i = \frac{G_{\text{max,T}} \cdot X_i}{C_{x_i} + X_i} \]

where

- \( G_i \) = Growth rate based on nutrient or light limitation
- \( G_{\text{max,T}} \) = Temperature-corrected maximum growth rate
- \( X_i \) = Nutrient concentration or light intensity
- \( C_{x_i} \) = Michaelis-Menten constant for nutrient or light limited growth

• Growth rate = minimum \( G_i \) (where \( i = \text{nitrogen, phosphorus, light} \))
PHYTOPLANKTON SIMULATION

- **Respiration**
  - First-order, temperature-corrected rate

- **Death**
  - First-order
  - Low death rate (**ALDL**) when nutrients are plentiful
  - High death rate (**ALDH**) when nutrients are scarce or phytoplankton concentration is high
  - Increased during anaerobic conditions
PHYTOPLANKTON PARAMETERS: 1

- Maximum algal unit growth rate (MALGR)
- Michaelis-Menten constant for light-limited growth (CMMLT)
- Nitrate Michaelis-Menten constant for N-limited growth (CMMN)
- Nitrate Michaelis-Menten constant for P-limited growth (CMMP)
- Phosphate Michaelis-Menten constant for P-limited growth (CMNP)
- Temperature above which algal growth ceases (TALGRH)
- Temperature below which algal growth ceases (TALGRL)
- Temperature below which algal growth is retarded (TALGRM)
- Base extinction coefficient (EXTB)
- Ratio of chlorophyll a to phosphorus in biomass (RATCLP)
- Non-refractory fraction of algae and zooplankton biomass (NONREF)
- Fraction of nitrogen required for algal growth satisfied by NO₃ (ALNPR)
PHYTOPLANKTON PARAMETERS: 2

- Unit algal respiration rate at 20C (ALR20)
- High algal unit death rate (ALDH)
- Low algal unit death rate (ALDL)
- Increment to phytoplankton death rate due to anaerobic conditions (OXALD)
- Inorganic N concentration below which high death rate occurs (NALDH)
- Inorganic P concentration below which high death rate occurs (PALDH)
- Chlorophyll a concentration above which high death rate occurs (CLALDH)
- Minimum concentration of plankton not subject to advection (SEED)
- Concentration of plankton not subject to advection at low flow (MXSTAY)
- Flow rate where plankton concentration not subject to advection is midway between SEED and MXSTAY (OREF)
- Settling rate of phytoplankton (PHYSET)
**ZOPLANKTON**

- **Filtering and ingestion of phytoplankton**
  - First-order, temperature-corrected rate at low phytoplankton concentrations; constant rate at high phytoplankton concentrations

- **Assimilation**
  - Ingested phytoplankton converted to zooplankton; efficiency based on user-defined food quality

- **Respiration**
  - First-order, temperature-corrected rate; inorganic nutrients released

- **Excretion**
  - Difference between ingestion and assimilation; BOD, refractory organics, and inorganic nutrients released

- **Death**
  - First-order rate based on dissolved oxygen conditions; BOD and refractory organics released
ZOOPLOANKTON PARAMETERS

- Quality of zooplankton food (ZFOOD)
- Maximum zooplankton unit ingestion rate (mg phyto/mg zoo/hr) (MZOEAT)
- Zooplankton filtering rate at 20C (l/mg zoo/hr) (ZFIL20)
- Zooplankton unit respiration rate at 20C (/hr) (ZRES20)
- Zooplankton unit death rate (/hr) (ZD)
- Increment to zooplankton death rate in anaerobic conditions (/hr) (OxzD)
- Temperature correction coefficient for filtering (-) (TCZFIL)
- Temperature correction coefficient for respiration (-) (TCZRES)
- Fraction of non-refractory excretion immediately decomposed when the ingestion rate is greater than MZOEAT (-) (ZEXDEL)
- Average weight of a zooplankton organism (mg) (ZOMASS)
BENTHIC ALGAE

• Attached to rocks and other stationary material
• Two optional methods:

Method 1. - Simulated using same composition, processes and methods as phytoplankton
  – no advection
  – different method for estimating death
  – parameters:

  MBAL - maximum benthic algae density (mg biomass/m²)
  CFBALG - ratio of benthic algae to phytoplankton growth rate
  CFBALR - ratio of benthic algae to phytoplankton respiration rate
BENTHIC ALGAE

Method 2. - Simulated using separate kinetic equations independent of phytoplankton

- based on DSSAMt model (Caupp, et al., 1998)
- four species of algae, including N-fixing (blue-green)
- nutrient-, light-, temperature-, and density-limited growth
- respiration
- removal by invertebrate grazing and scour
REFRACTORY ORGANICS (N,P,C)
MASS BALANCE

Inflow to reach

Storage of Refractory Organics

Phytoplankton death

Benthic algae death

Settling

Zooplankton death and excretion

Outflow from reach
SUMMARY OF NITROGEN CYCLE

WATER COLUMN

NO3 → ALGAE

NH3 (dissolved) ➔ adsorption/desorption

NH3 (particulate) ➔ scour/deposition

BOD ➔ settling

ORN ➔ settling

NO3 ➔ nitrification

ALGAE ➔ death and respiration

BOD ➔ benthal release

ORN ➔ settling

32 of 35
PHCARB: pH & INORGANIC CARBON

- Computes pH based on total inorganic carbon, alkalinity, and CO₂ equilibrium

- Alkalinity is simulated as a conservative in CONS section

- CO₂ input from atmosphere is proportional to the oxygen reaeration rate
INORGANIC CARBON MASS BALANCE

CO₂ invasion
Zooplankton respiration
BOD decay
Net algal growth
Benthic release

Inflow to reach

CO₂ + H₂CO₃

HCO₃⁻

CO₂⁻⁻

Total Inorganic Carbon

Outflow from reach

34 of 35
PHCARB PARAMETERS

Ratio of $\text{CO}_2$ invasion rate to oxygen reaeration rate ($\text{CFCINV}$)

Benthic release rates of $\text{CO}_2$ for aerobic and anaerobic conditions ($\text{BRCO2}$)