Utah State University

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LECTURE #14

INSTREAM WATER QUALITY – BIOCHEMICAL REACTIONS

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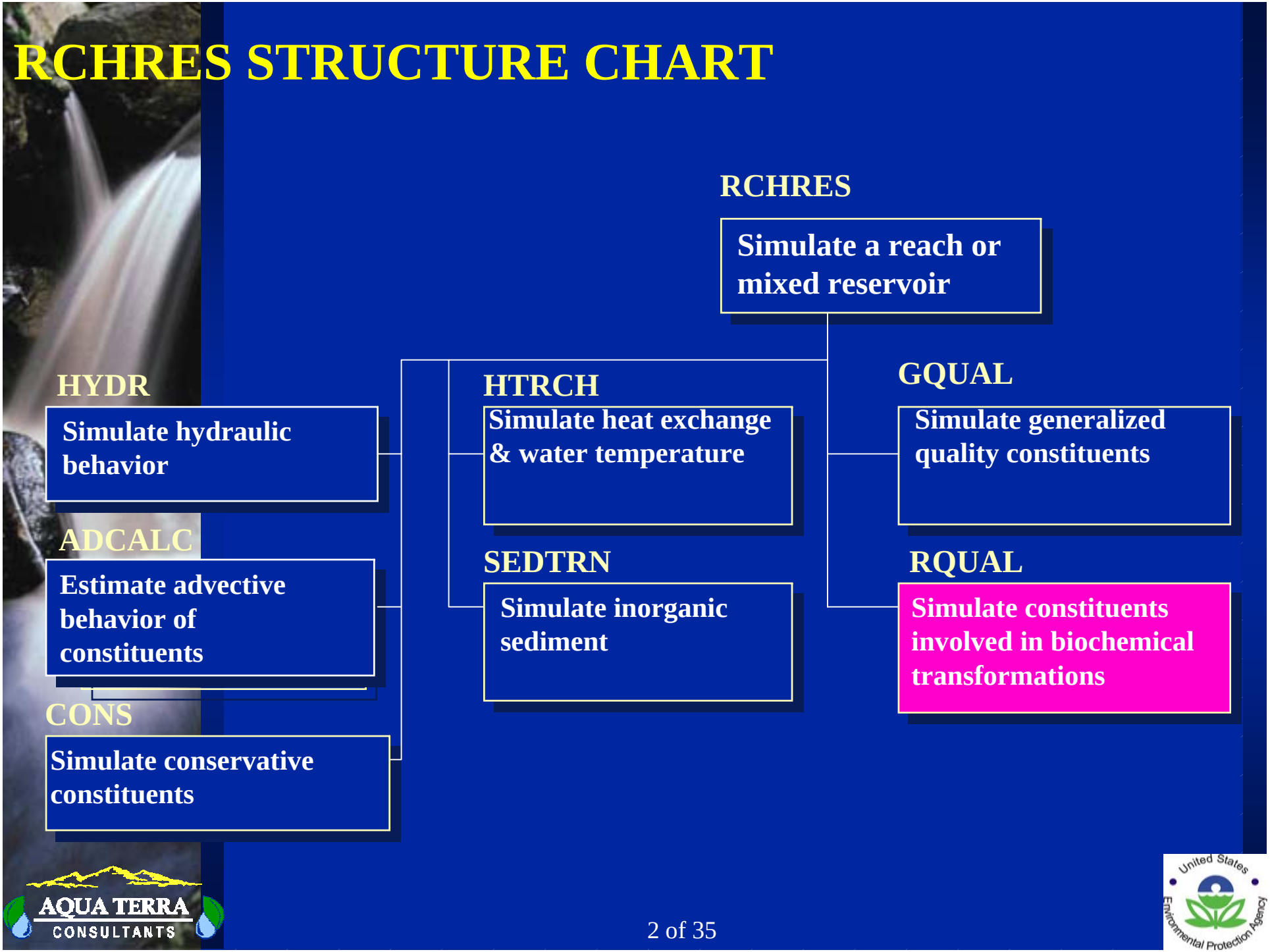
RCHRES STRUCTURE CHART



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

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OXRX: DISSOLVED OXYGEN AND BOD PROCESSES

- Reaeration
- BOD decay/oxygen depletion
- Settling of BOD material
- Benthic oxygen demand
- Benthic release of BOD

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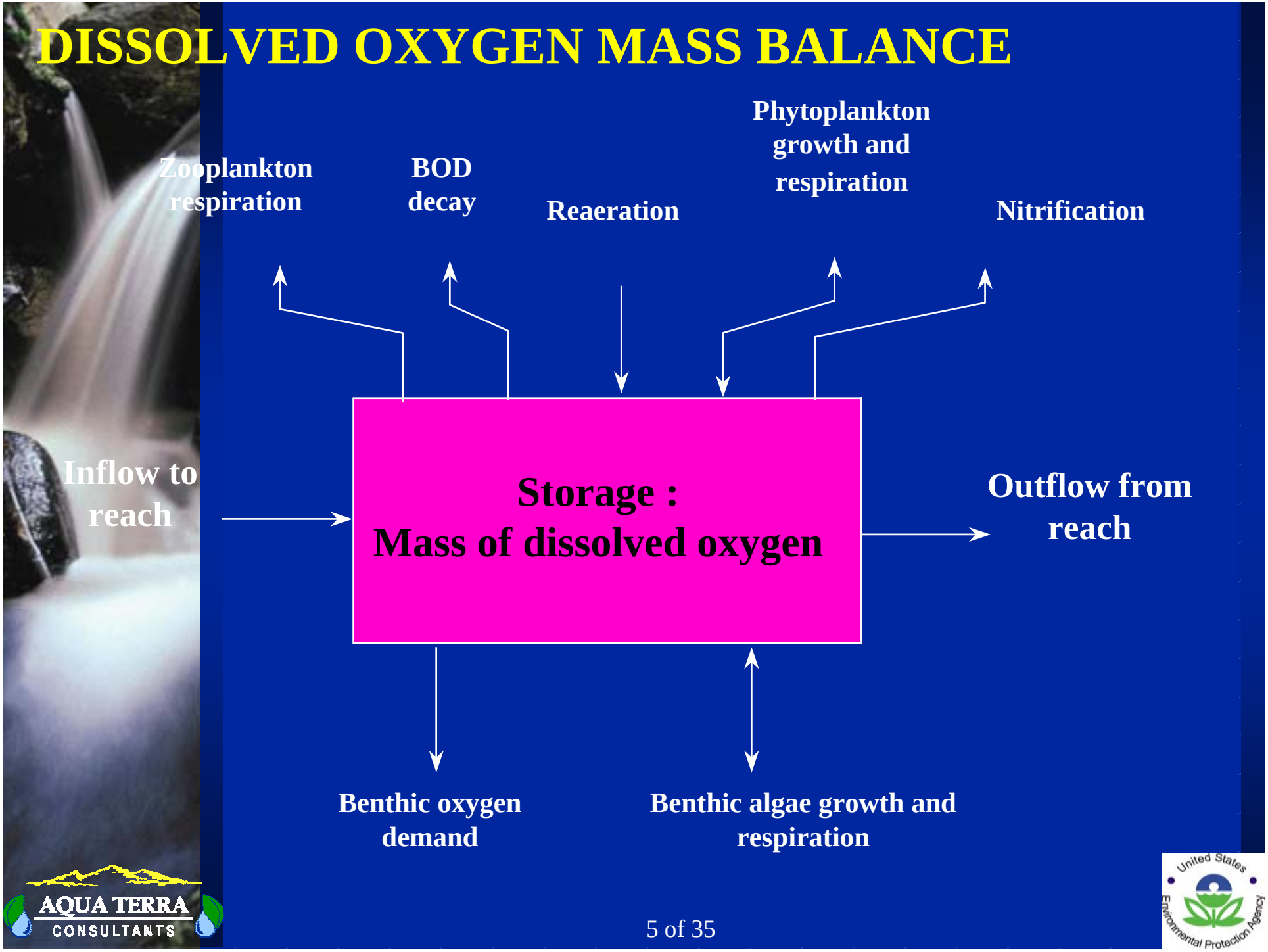
DISSOLVED OXYGEN MASS BALANCE



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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

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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

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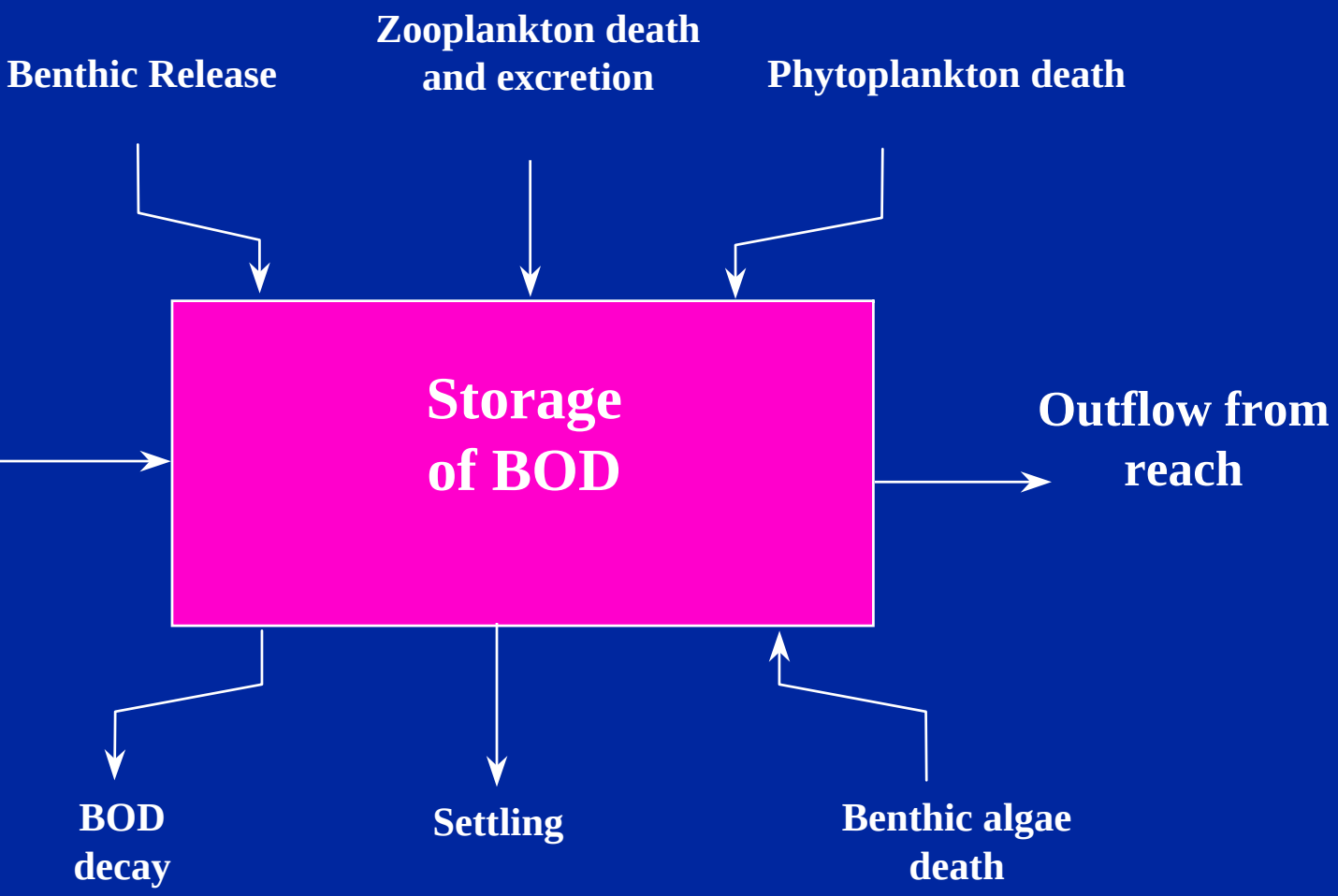
BOD MASS BALANCE



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BOD DECAY

$$DO_{consumed} = K_{BOD} \cdot \theta^{(T_w - 20)} \cdot BOD$$

where:

K_{BOD} = **BOD decay rate at 20 ^{o}C (hr^{-1})**

θ = **Temperature correction coefficient**

BOD = **BOD concentration (mg/L)**

T_w = **Water temperature (^{o}C)**

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BENTHIC PROCESSES (Optional)

- **Benthic oxygen demand**
  - Exponential function of DO
  - Benthic oxygen demand at 20 ^{o} 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

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OXYGEN/BOD PARAMETERS

- **Escape coefficient in reaeration equations (REAK)**
- **Temperature correction coefficient for reaeration (TCGINV)**
- **Velocity exponent in user-specified reaeration (EXPREV)**
- Depth e**xponent in user-specified reaeration (EXPRED)**
- **Lake reaeration correction factor (CFOREA)**
- **BOD decay rate at 20 ^{o}C (hr^{-1}) (KBOD20)**
- **Temperature coefficient for BOD decay (TCBOD)**
- **BOD settling rate (m/hr or ft/hr) (KODSET)**

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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

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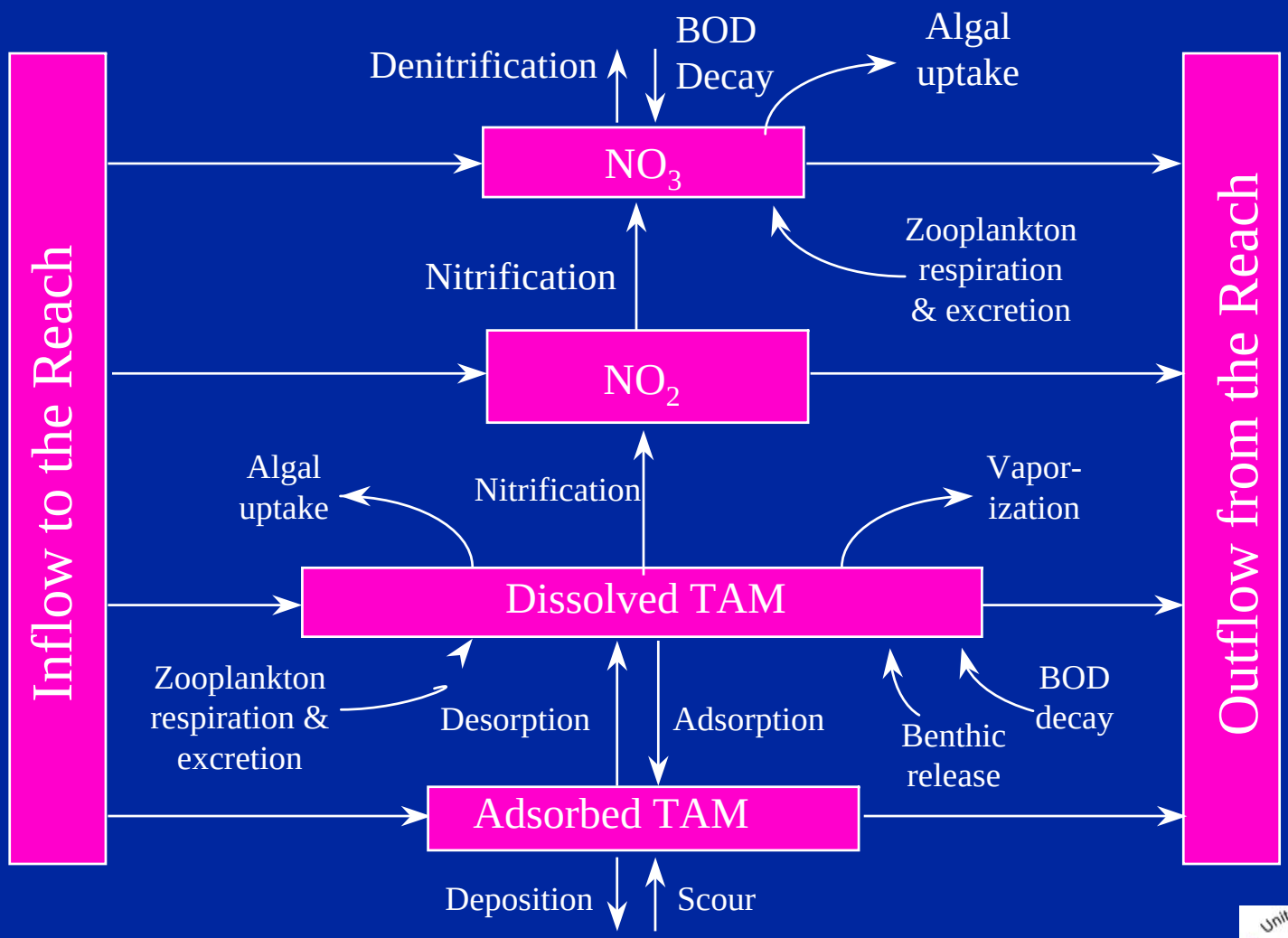
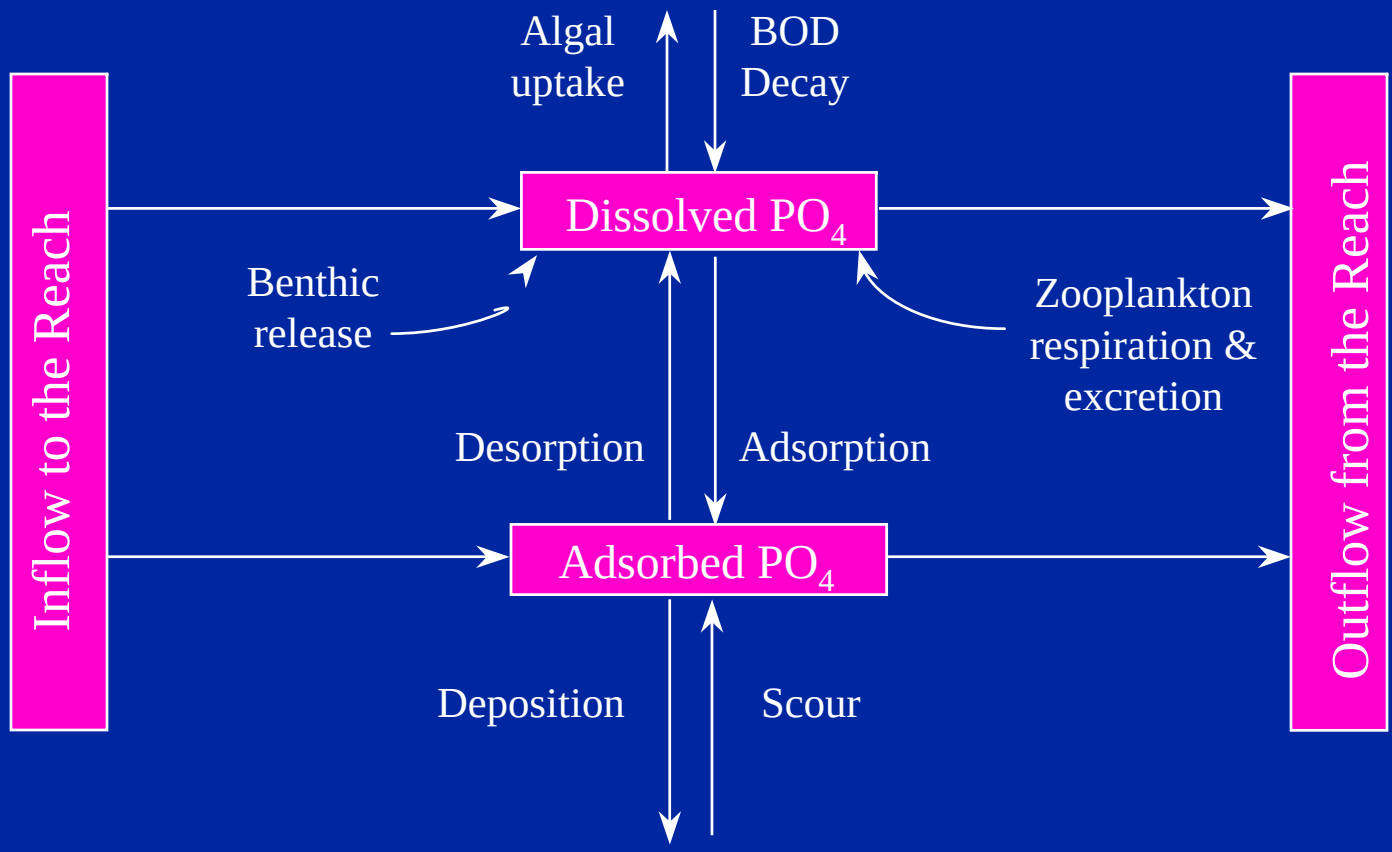
INORGANIC NITROGEN SOURCES, SINKS AND TRANSFORMATIONS



INORGANIC PHOSPHORUS SOURCES, SINKS AND TRANSFORMATIONS



NITRIFICATION AND DENITRIFICATION

- **Nitrification: $NH_3 \longrightarrow NO_2 \longrightarrow NO_3$**
  - **First-order in ammonia concentration**
  - **Nitrification rate coefficient (TAMNIT)**
  - **Temperature correction (TCNIT)**
  - **Consumes oxygen**

- **Denitrification: $NO_3 \longrightarrow N_2$**
  - **First-order in nitrate**
  - **Denitrification rate coefficient (KNO320)**
  - **Temperature correction (TCDEN)**
  - **Only occurs below threshold DO (DENOXT)**

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SEDIMENT- NUTRIENT INTERACTIONS

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

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NUTRIENT PARAMETERS

- Nitrification rate of NH_3 at 20 ^oC **(KTAM20)**
- Nitrification rate of NO_2 at 20 ^oC **(KNO220)**
- Denitrification rate at 20 ^oC **(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)**

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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

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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**

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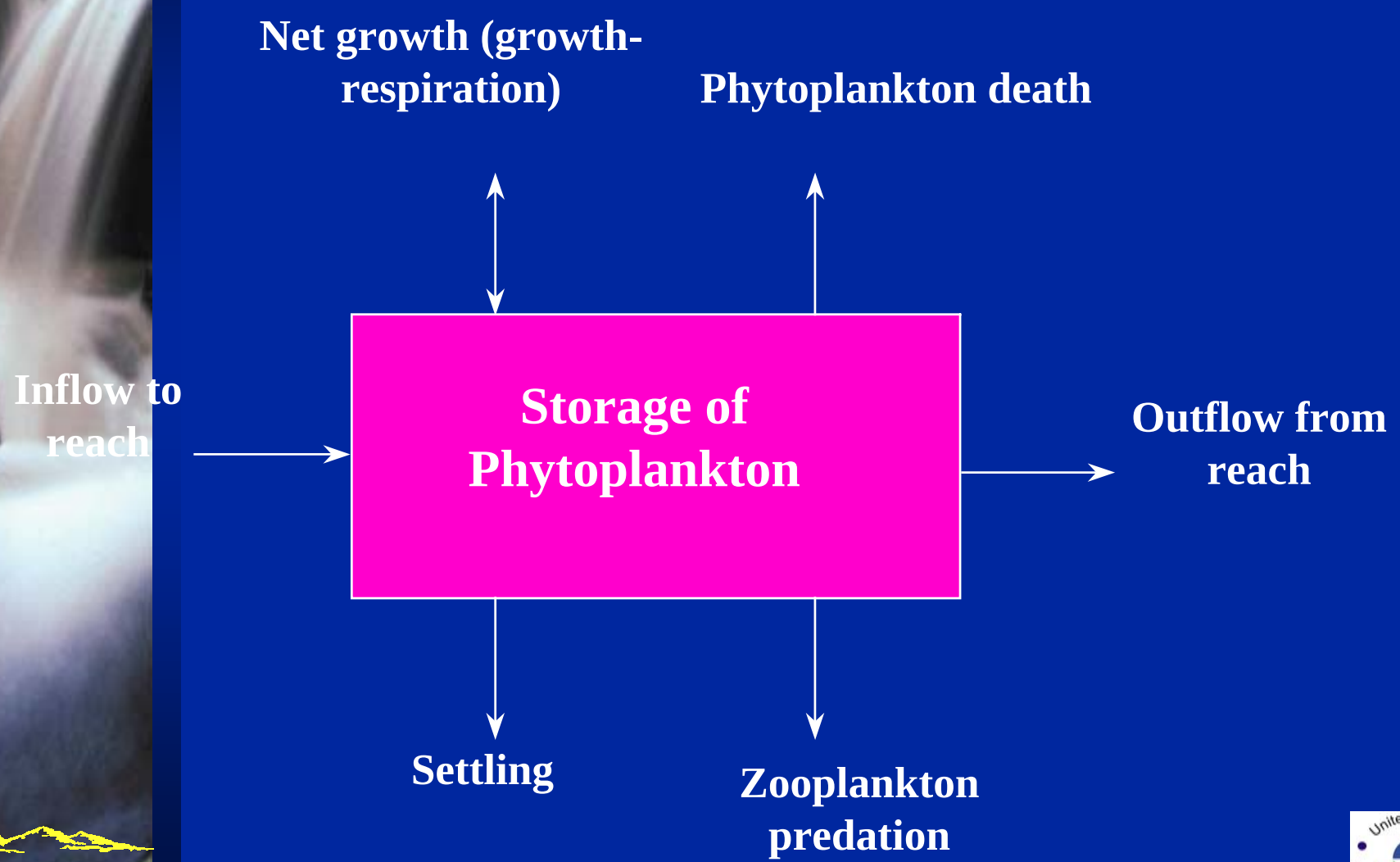
PHYTOPLANKTON MASS BALANCE



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)

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PHYTOPLANKTON SIMULATION

- **Growth simulation by Michaelis-Menton kinetics**

$$G_i = G_{max,T} * X_i/(C_{xi} + X_i)$$

where

G_i = Growth rate based on nutrient or light limitation

$G_{max,T}$ = Temperature-corrected maximum growth rate

X_i = Nutrient concentration or light intensity

C_{xi} = Michaelis-Menton constant for nutrient or light limited growth

- **Growth rate = minimum G_i (where i = nitrogen, phosphorus, light)**

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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

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PHYTOPLANKTON PARAMETERS: 1

- Maximum algal unit growth rate (MALGR)
- Michaelis-Menton constant for light-limited growth (CMMLT)
- Nitrate Michaelis-Menton constant for N-limited growth (CMMN)
- Nitrate Michaelis-Menton constant for P-limited growth (CMMNP)
- Phosphate Michaelis-Menton constant for P-limited growth (CMMP)
- 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 NO_3 (ALNPR)

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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)

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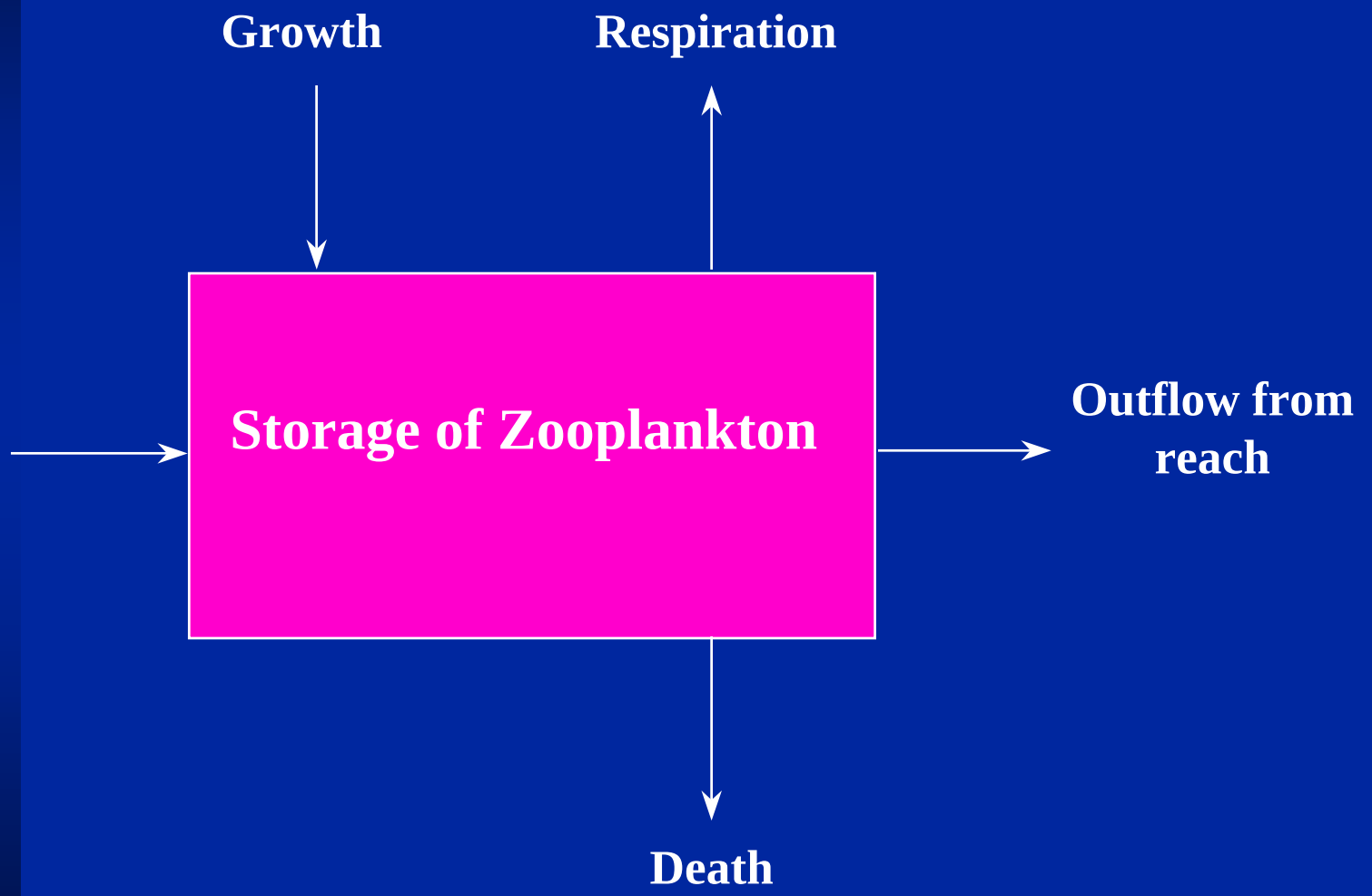
ZOOPLANKTON MASS BALANCE



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ZOOPLANKTON

- **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

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ZOOPLANKTON 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)

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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/m^2)

CFBALG - ratio of benthic algae to phytoplankton growth rate

CFBALR - ratio of benthic algae to phytoplankton respiration rate

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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

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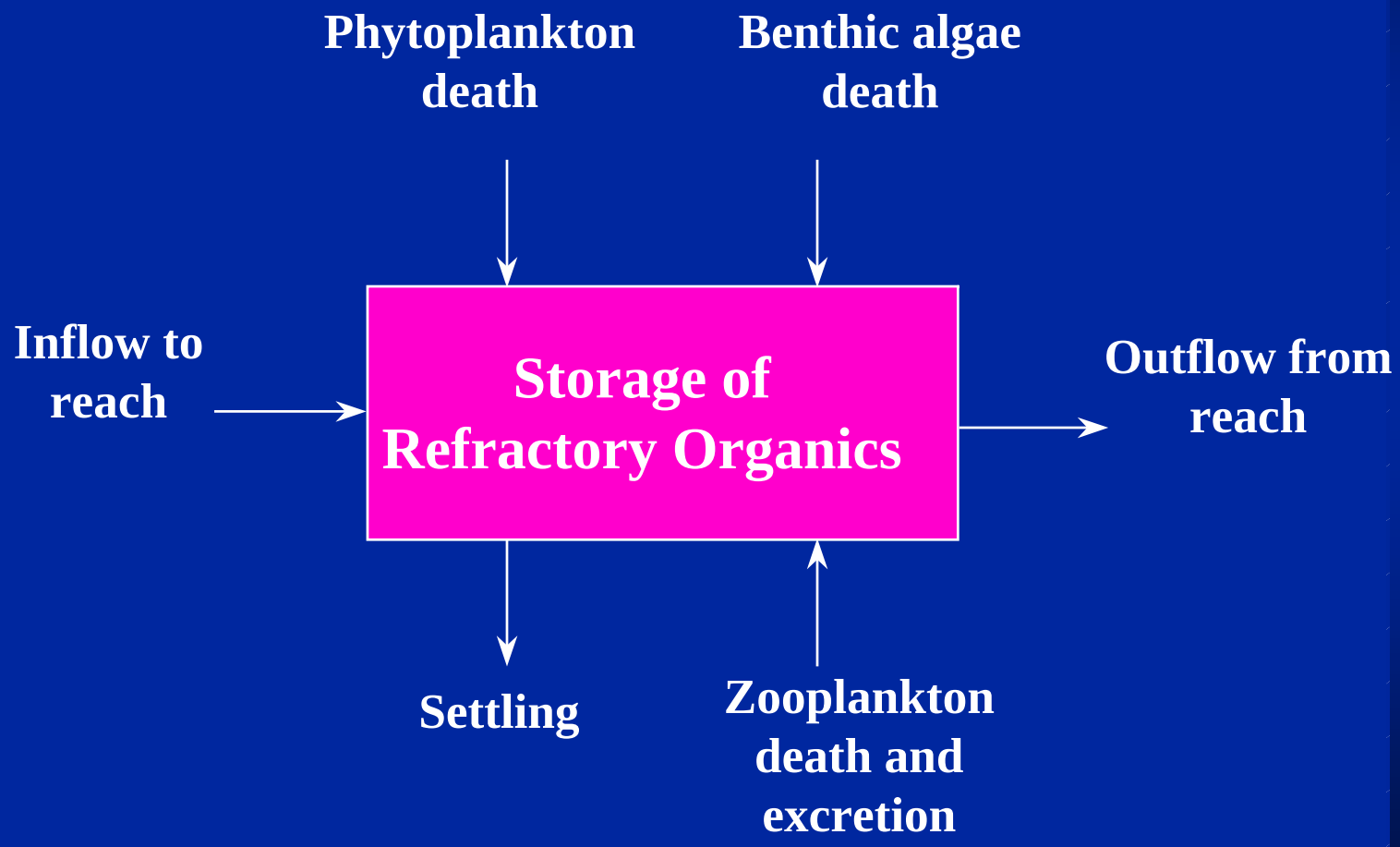
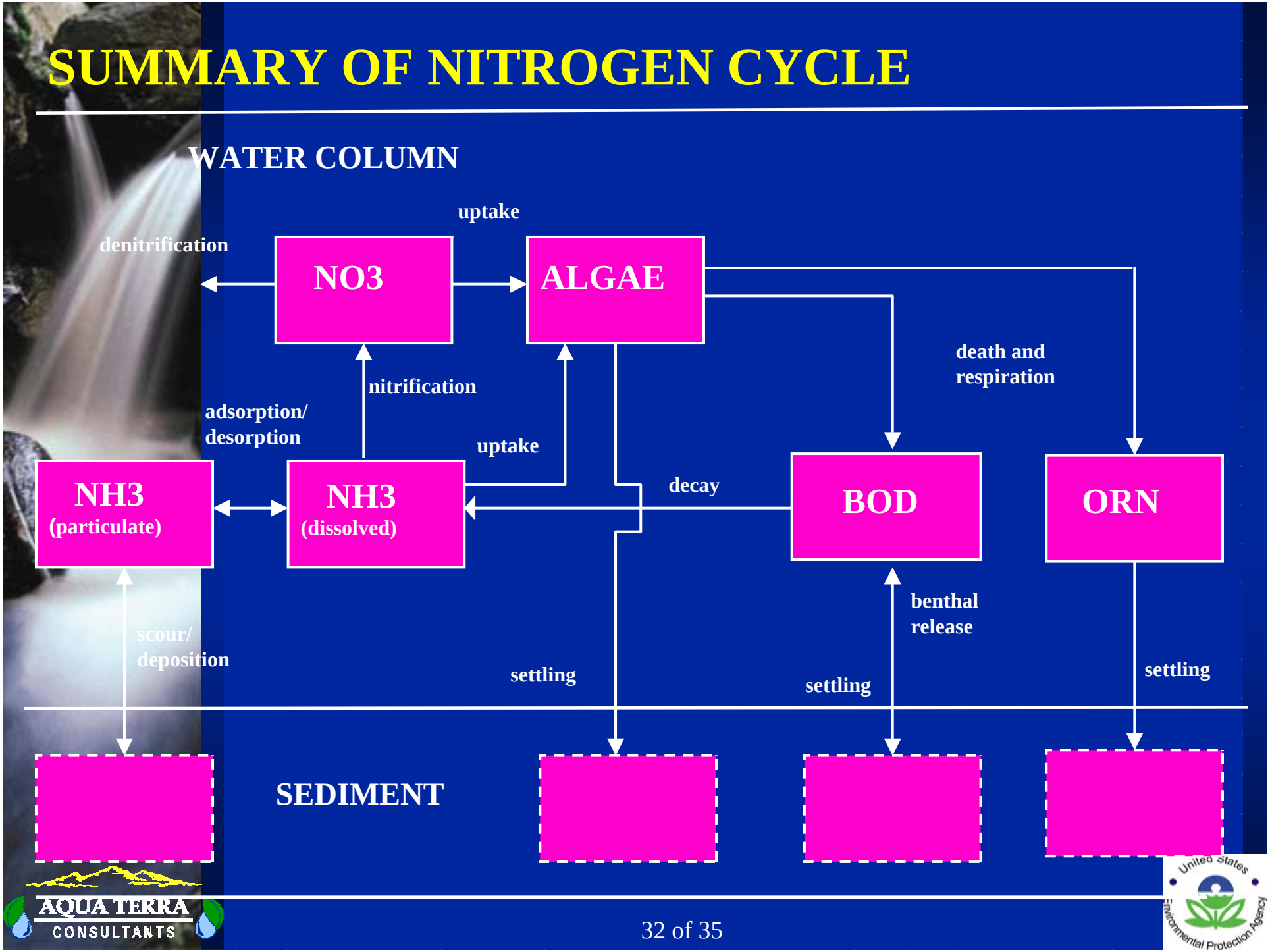
REFRACTORY ORGANICS (N,P,C) MASS BALANCE



SUMMARY OF NITROGEN CYCLE



PHCARB: pH & INORGANIC CARBON

- Computes pH based on total inorganic carbon, alkalinity, and CO_2 equilibrium
- Alkalinity is simulated as a conservative in CONS section
- CO_2 input from atmosphere is proportional to the oxygen reaeration rate

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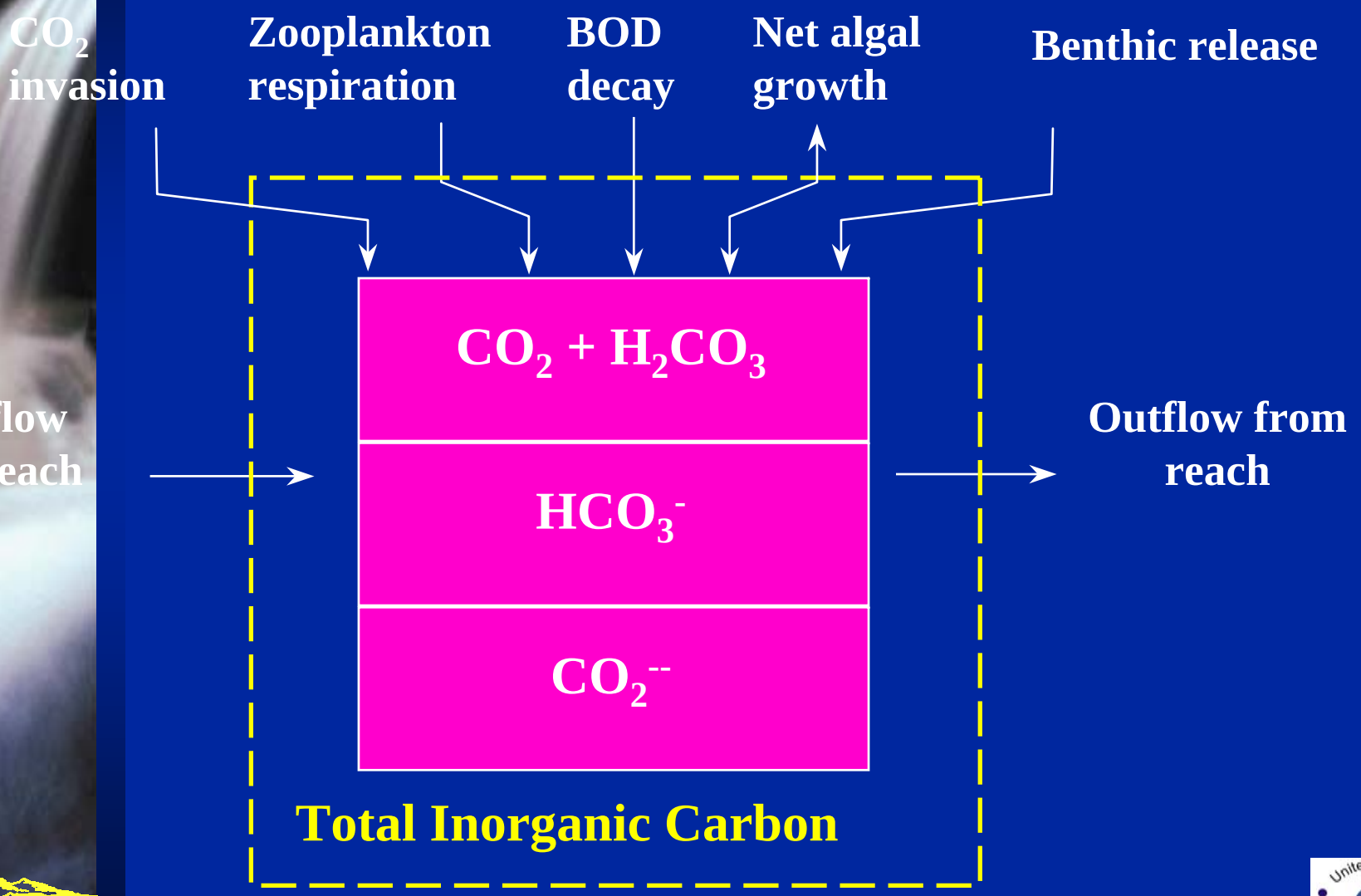
INORGANIC CARBON MASS BALANCE



PHCARB PARAMETERS

Ratio of CO_2 invasion rate to oxygen reaeration rate (CFCINV)

Benthic release rates of CO_2 for aerobic and anaerobic conditions (BRCO2)

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