LECTURE #14

INSTREAM WATER QUALITY – BIOCHEMICAL REACTIONS

Utah State University

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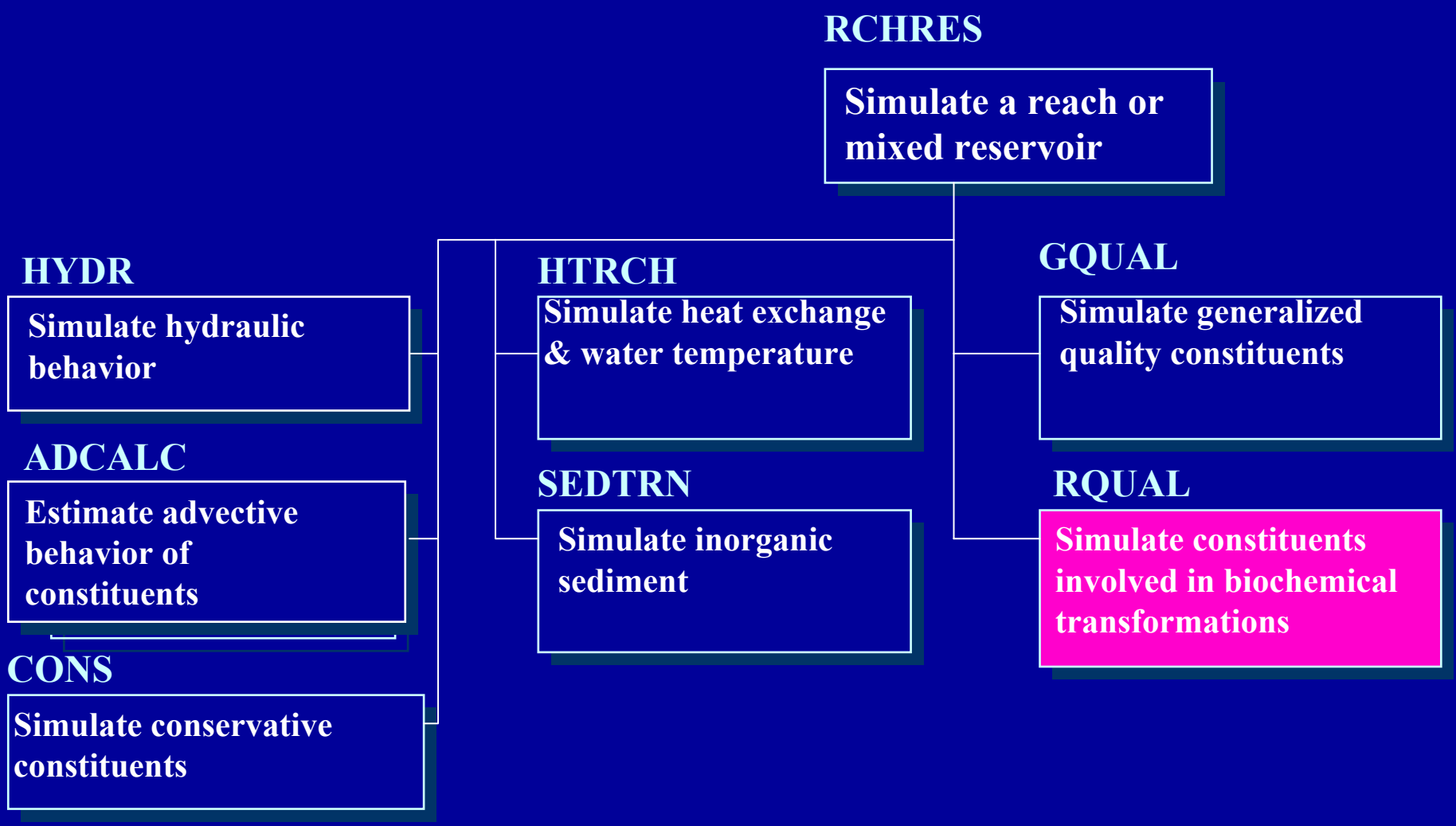
RCHRES STRUCTURE CHART



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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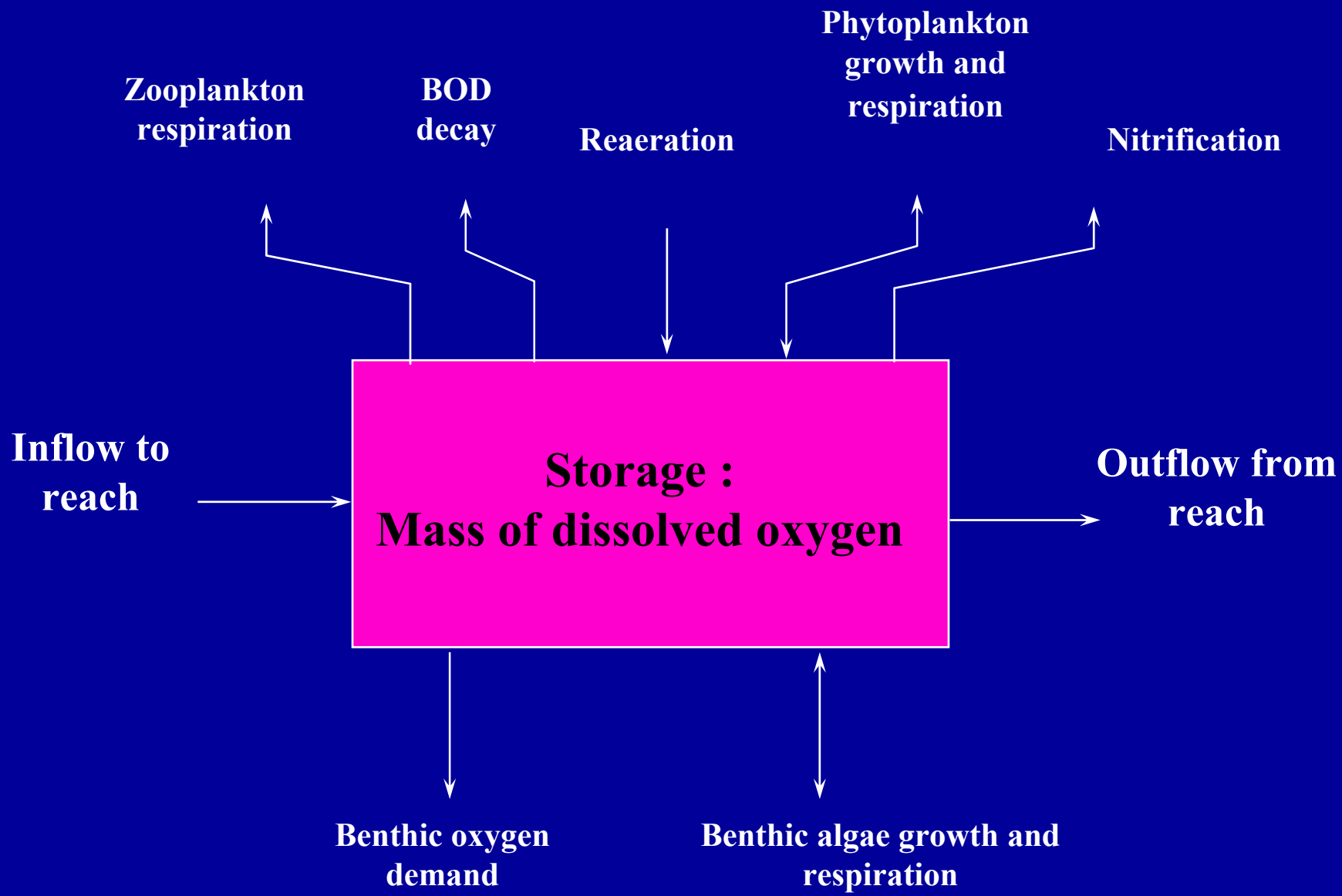
DISSOLVED OXYGEN MASS BALANCE



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 method
   - Based on velocity and slope
   - Temperature correction
   - Escape coefficient
2. Covar method
   - Power function of velocity and depth
   - Temperature correction
   - Escape coefficient
   - Three sets of coefficients & exponents based on depth and velocity regimes (Owens, Churchill, O'Connor-Dobbins)
3. User-specified, similar to Covar method

Lakes

- Function of depth and wind speed
- User-defined circulation correction factor

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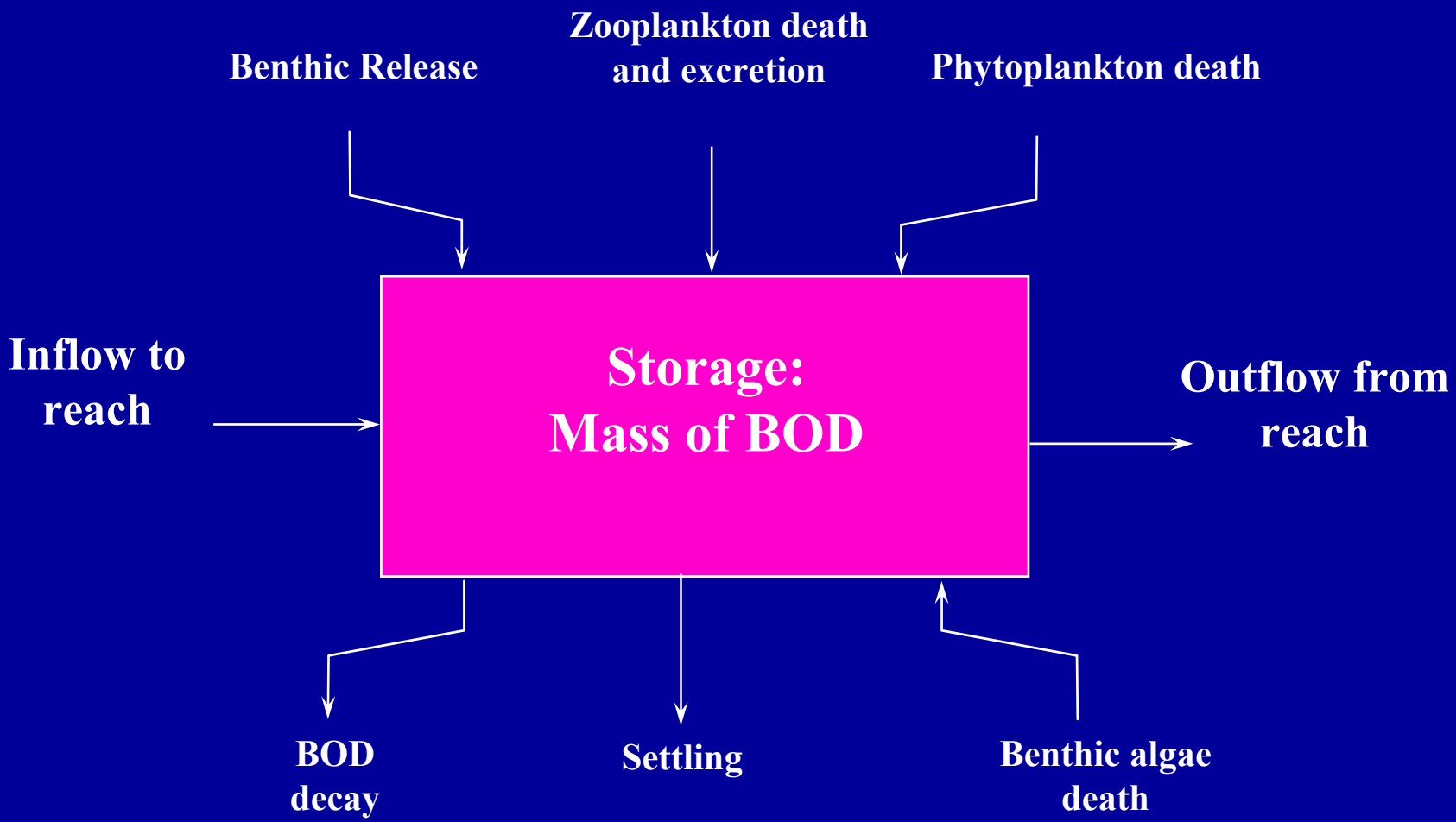
BOD MASS BALANCE



BOD DECAY

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

where:

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

θ = **Temperature correction coefficient**

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

T_w = **Water temperature (°C)**

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BENTHIC PROCESSES

- **Benthic oxygen demand (optional)**
  - Exponential function of DO
  - Benthic oxygen demand at 20 ^{o} C
  - Temperature correction
- **Benthic release of BOD (optional)**
  - Release rate under aerobic conditions
  - Release rate under low oxygen conditions
  - Exponential function of DO
  - Affected by scouring condition

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OXYGEN/BOD PARAMETERS

REAK - Escape coefficient in reaeration equations

TCGINV - Temperature correction coeff. for reaeration

EXPREV - Exponent to velocity in user-specified reaeration equation

EXPRED - Exponent to depth in user-specified reaeration equation

CFOREA - Lake reaeration correction factor; accounts for good or poor circulation

KBOD20 - BOD decay rate at 20 ^{o}C (hr^{-1})

TCBOD - Temperature correction coeff. for BOD decay

KODSET - BOD settling rate (m/hr or ft/hr)

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NUTRX: INORGANIC NUTRIENTS

- **CONSTITUENTS**
  - NO_3
  - NO_2
  - TAM, particulate TAM
  - PO_4, particulate PO_4
- **PROCESSES**
  - Decomposition of BOD material to PO_4 and TAM or NO_3
  - Nitrification of TAM to NO_3
  - Denitrification of NO_3 to N_2
  - Adsorption of TAM and PO_4 to sediment
  - Benthic release of TAM and PO_4

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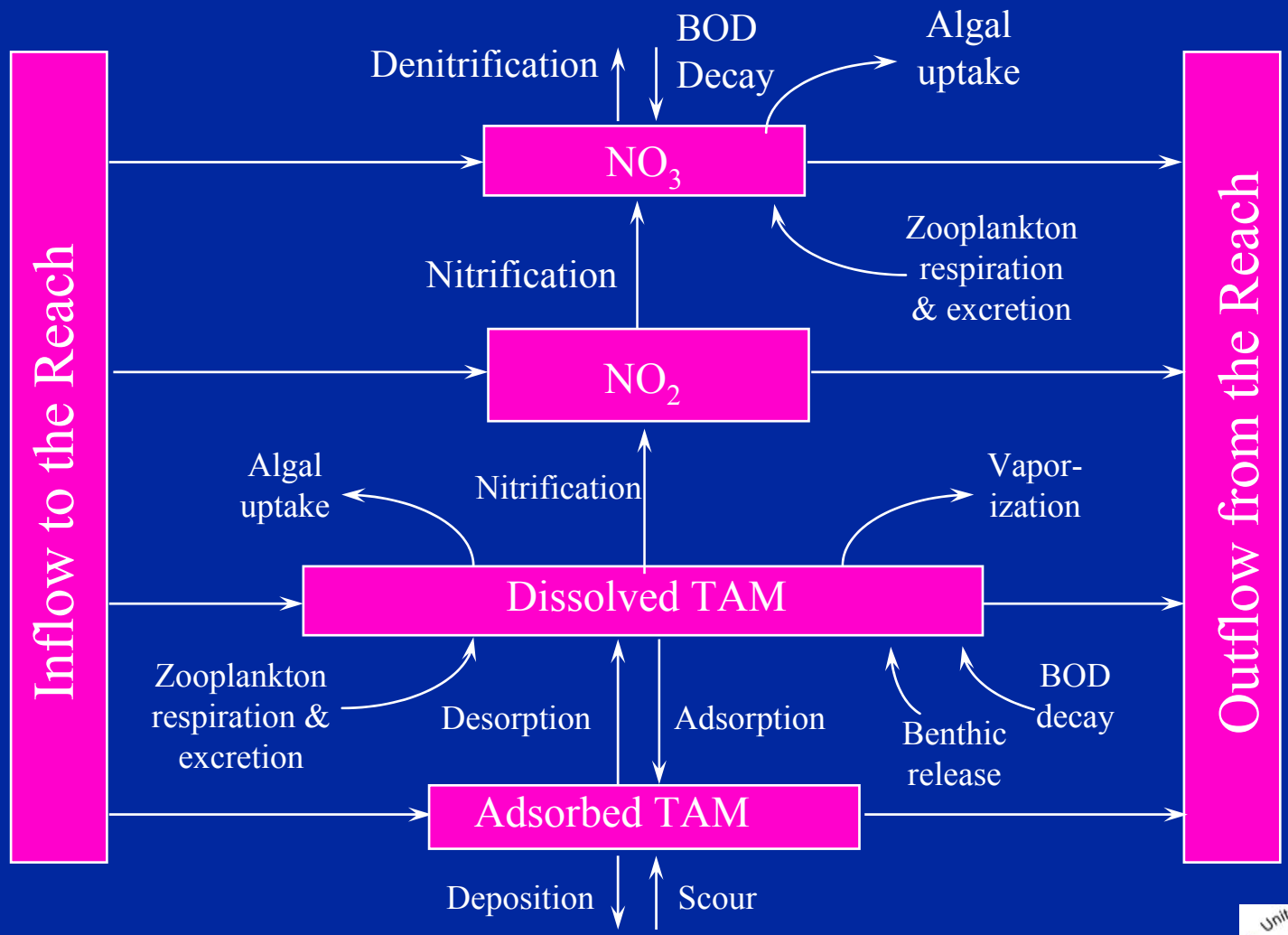
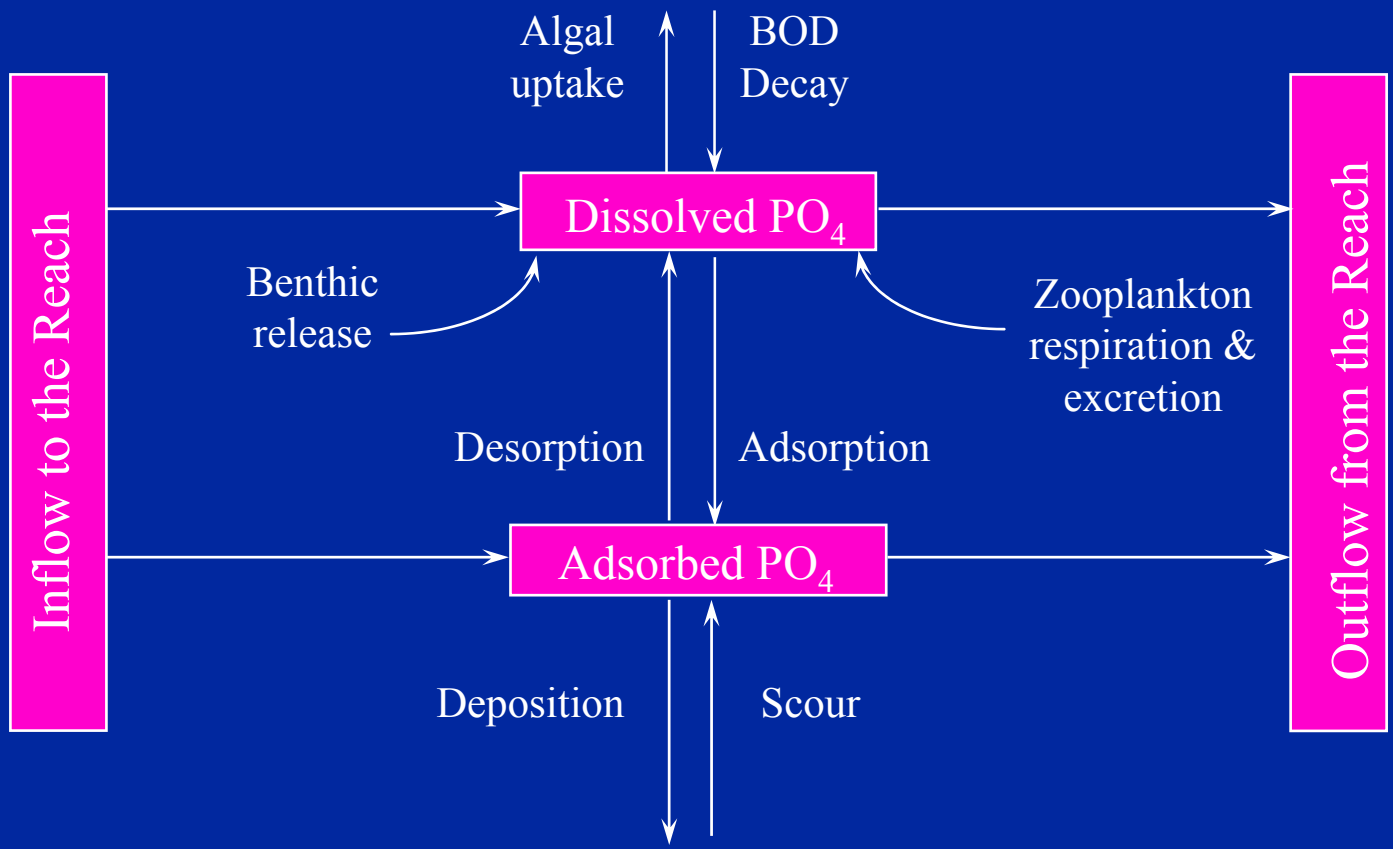
INORGANIC NITROGEN SOURCES, SINKS AND TRANSFORMATIONS



INORGANIC PHOSPHORUS SOURCES, SINKS AND TRANSFORMATIONS



NITRIFICATION AND DENITRIFICATION

- **Nitrification:** TAM $\longrightarrow$ 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)
  - Process occurs below threshold DO (DENOXT)

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SEDIMENT- NUTRIENT INTERACTIONS

Particulate P and N - Optional

- Equilibrium adsorption of PO_4 and TAM to three sediment fractions (sand, silt, clay) in the water column
- Deposition/resuspension of sediment is computed in Section SEDTRN
- Resuspended sediment has a constant user-defined concentration of N and P
- Nutrient resuspension is limited by mass of sediment in bed

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NUTRIENT PARAMETERS

KTAM20	- Nitrification rate of TAM at 20 ^{o}C
KNO220	- Nitrification rate of NO_2 at 20 ^{o}C
KNO320	- Denitrification rate at 20 ^{o}C
DENOXT	- Dissolved oxygen threshold concentration for denitrification (mg/l)
ADNHPM ADPOPM	- Adsorption coefficients for TAM and PO_4 adsorbed to inorganic sediment (mg/l)
BNH4 BPO4	- Concentrations of TAM and PO_4 adsorbed to scoured bed sediments
BRTAM	- Benthic release rates of TAM under aerobic and anaerobic conditions (mg/m^2/hr)
BRPO4	- Benthic release rates of PO_4 under aerobic and anaerobic conditions (mg/m^2/hr)

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NUTRIENT PARAMETERS: COMPOSITION OF BIOMASS

CVBPC - Ratio of C to P in biomass (molar)

CVBPN - Ratio of N to P in biomass (molar)

BPCNTC - Percentage of biomass weight consisting of C

CVBO - Mg dissolved oxygen associated with 1 mg biomass

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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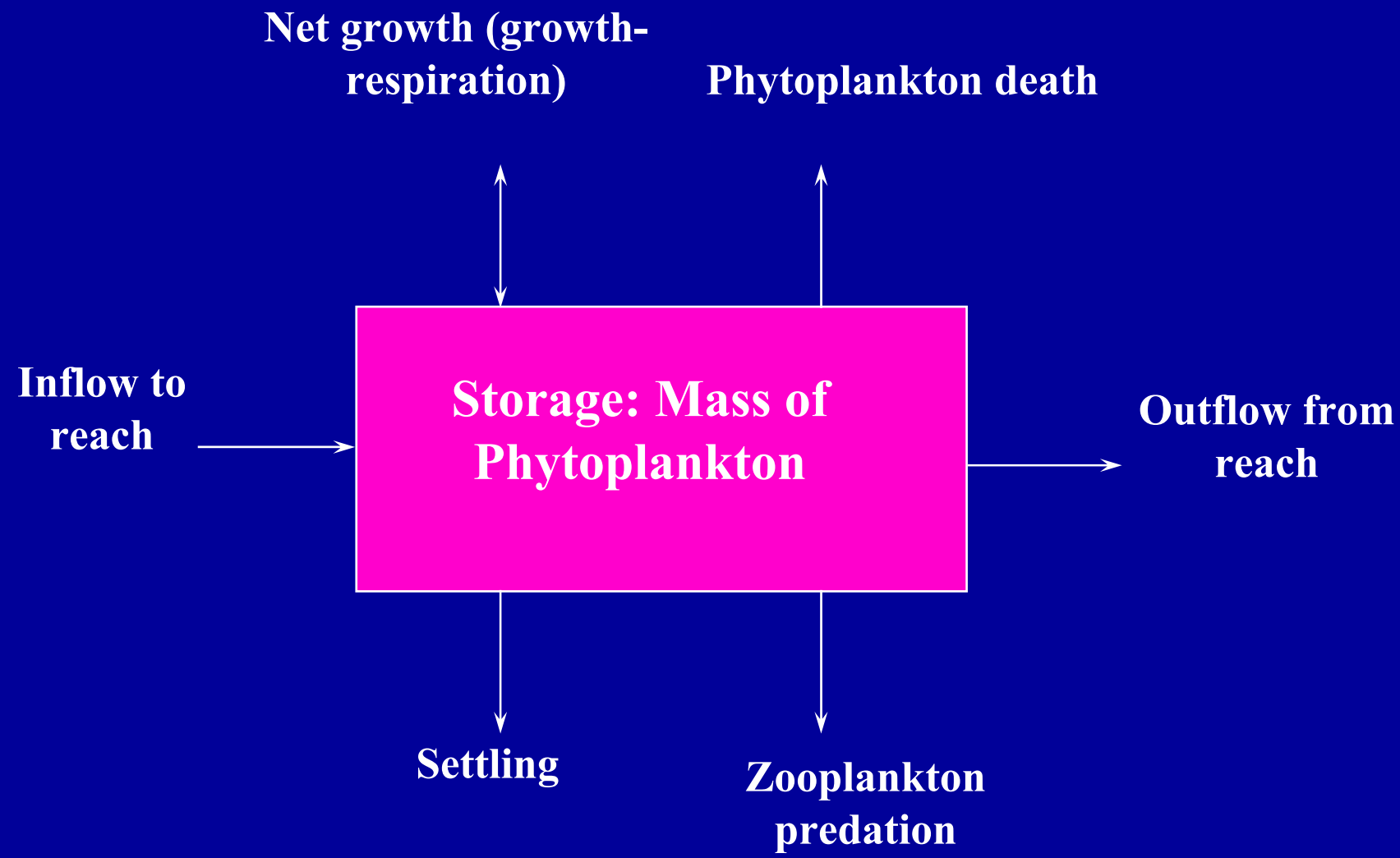
PHYTOPLANKTON MASS BALANCE



PHYTOPLANKTON SIMULATION

- **Single species**
  - Default composition: C:N:P = 106:16:1
- **Advection and settling**
  - Settling rate: PHYSET
  - Advection routine: minimum concentration of phytoplankton
- **Light**
  - Solar radiation reduced by surface shading and reflection
  - Light extinction = base (water) + sediment + phytoplankton
  - Euphotic depth and light available to phytoplankton computed
  - 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 rate
  - Low death rate (ALDL) when nutrients are plentiful
  - High death rate (ALDH) when nutrients are scarce or phytoplankton concentration is high
  - Increment to death rate during anaerobic conditions

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PHYTOPLANKTON PARAMETERS: 1

MALGR - maximum algal unit growth rate (/hr)

CMMLT - Michaelis-Menton constant for light-limited growth (ly/min)

CMMN - nitrate Michaelis-Menton constant for N-limited growth (mg/l)

CMMNP - nitrate Michaelis-Menton constant for P-limited growth (mg/l)

CMMP - phosphate Michaelis-Menton constant for P-limited growth (mg/l)

TALGRH - temperature above which algal growth ceases (C)

TALGRL - temperature below which algal growth ceases (C)

TALGRM - temperature below which algal growth is retarded (C)

EXTB - base extinction coefficient (/m)

RATCLP - ratio of chlorophyll a to phosphorus in biomass

NONREF - non-refractory fraction of algae and zooplankton biomass

ALNPR - fraction of nitrogen required for algal growth satisfied by NO_3

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PHYTOPLANKTON PARAMETERS: 2

- **ALR20** - unit algal respiration rate at 20C (/hr)
- **ALDH** - high algal unit death rate (/hr)
- **ALDL** - low algal unit death rate (/hr)
- **OXALD** - increment to phytoplankton death rate due to anaerobic conditions (/hr)
- **NALDH** - inorganic N concentration below which high algal death rate occurs (mg/l N)
- **PALDH** - inorganic P concentration below which high algal death rate occurs (mg/l P)
- **CLALDH** - chlorophyll a concentration above which high algal death rate occurs (ug/l)
- **SEED** - minimum concentration of plankton not subject to advection
- **MXSTAY** - concentration of plankton not subject to advection at low flow
- **OREF** - flow rate where plankton concentration not subject to advection is midway between SEED and MXSTAY
- **PHYSET** - settling rate of phytoplankton

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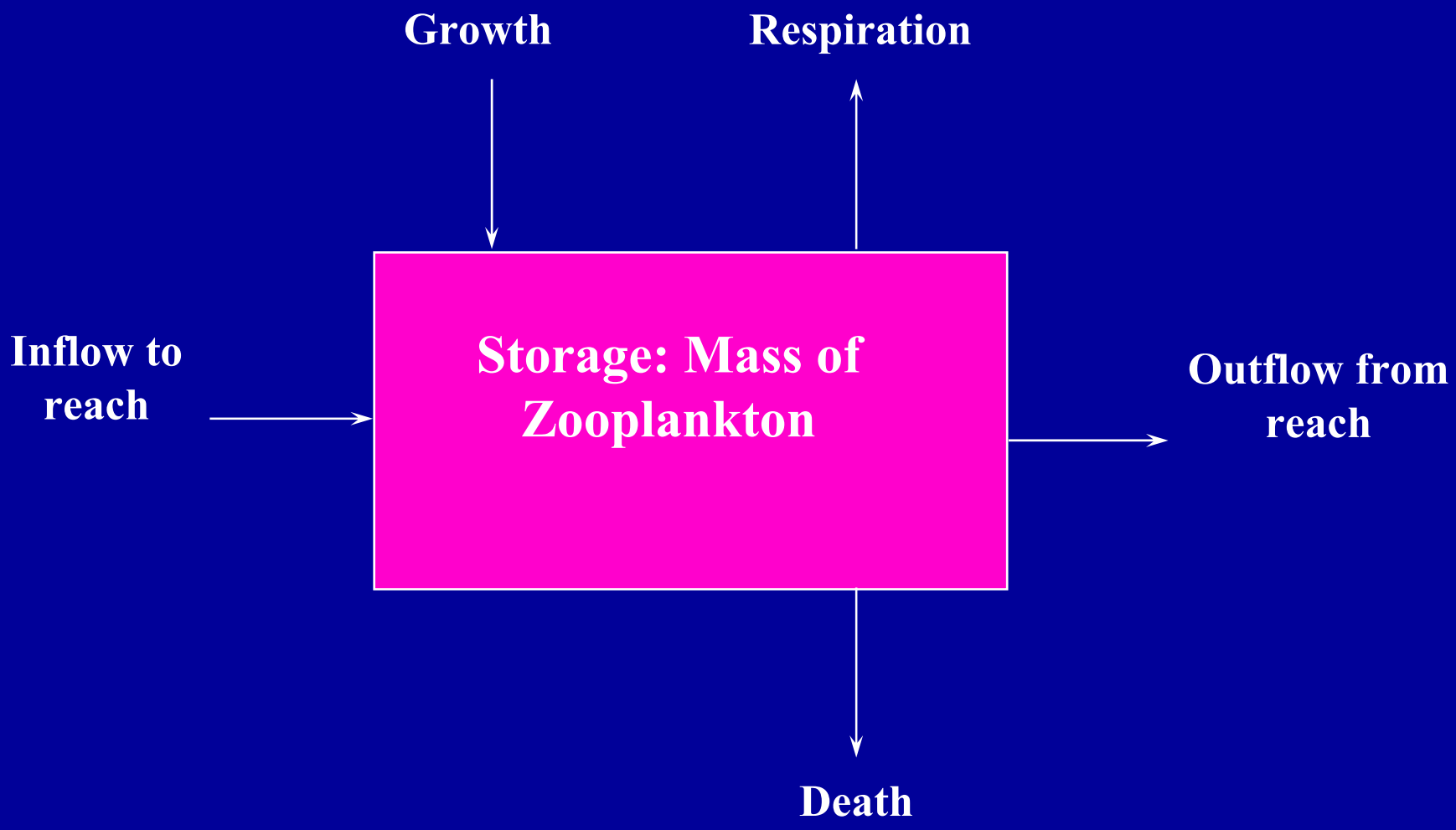
ZOOPLANKTON MASS BALANCE



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

ZFOOD - quality of zooplankton food (1, 2, 3)

MZOEAT - maximum zooplankton unit ingestion rate (mg phyto/mg zoo/hr)

ZFIL20 - zooplankton filtering rate at 20C (l/mg zoo/hr)

ZRES20 - zooplankton unit respiration rate at 20C (/hr)

ZD - natural zooplankton unit death rate (/hr)

OXZD - increment to zooplankton death rate in anaerobic conditions (/hr)

TCZFIL - temperature correction coefficient for filtering (-)

TCZRES - temperature correction coefficient for respiration (-)

ZEXDEL - fraction of non-refractory excretion immediately decomposed when the ingestion rate is greater than MZOEAT (-)

ZOMASS - average weight of a zooplankton organism (mg)

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BENTHIC ALGAE

- **Attached to rocks and other stationary material**

- **Simulated using same composition, processes and methods as phytoplankton except:**
  - 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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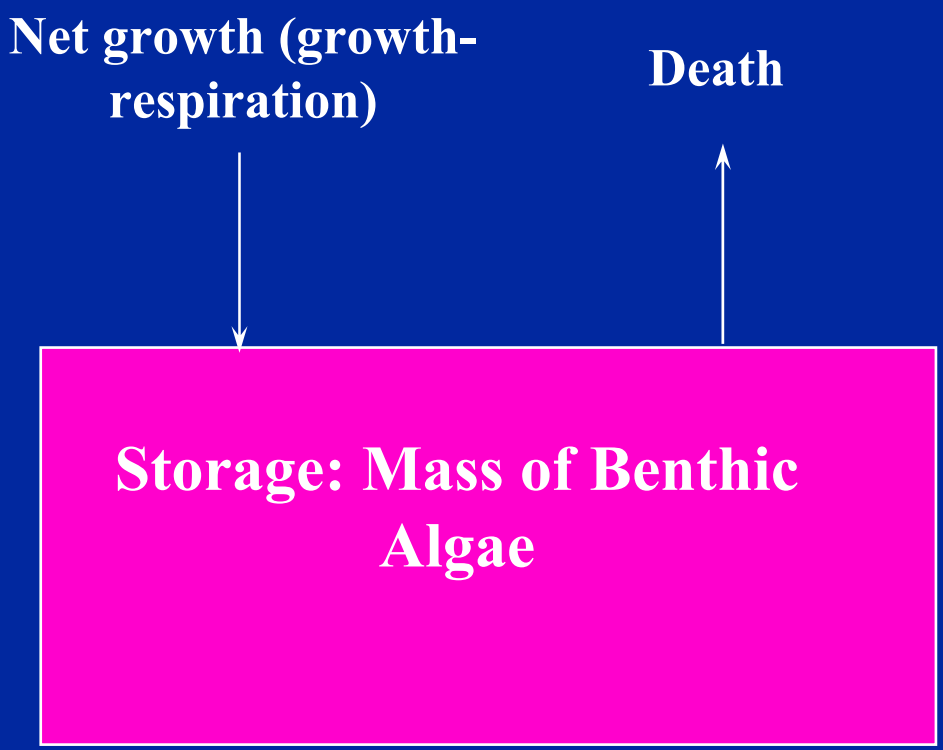
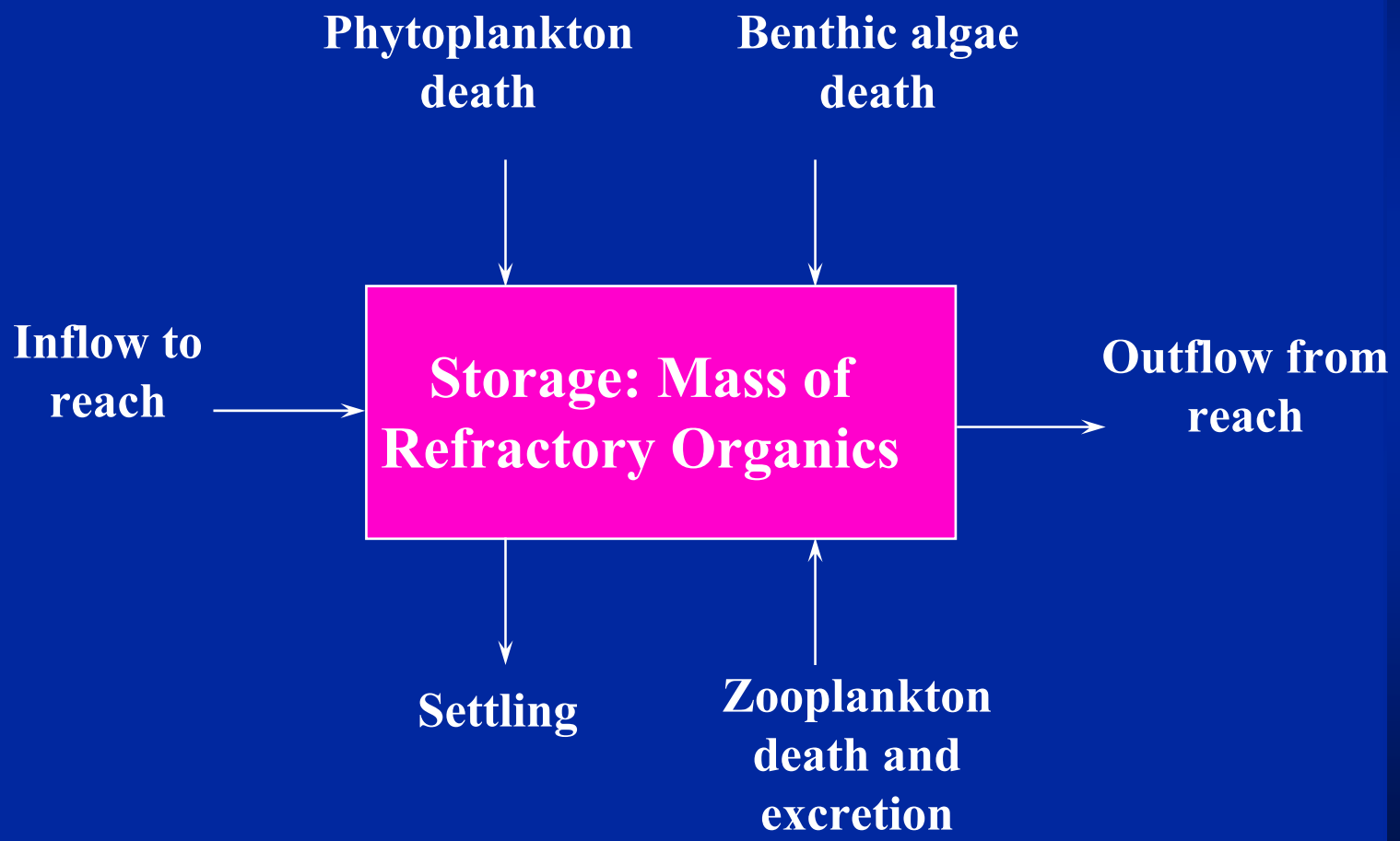
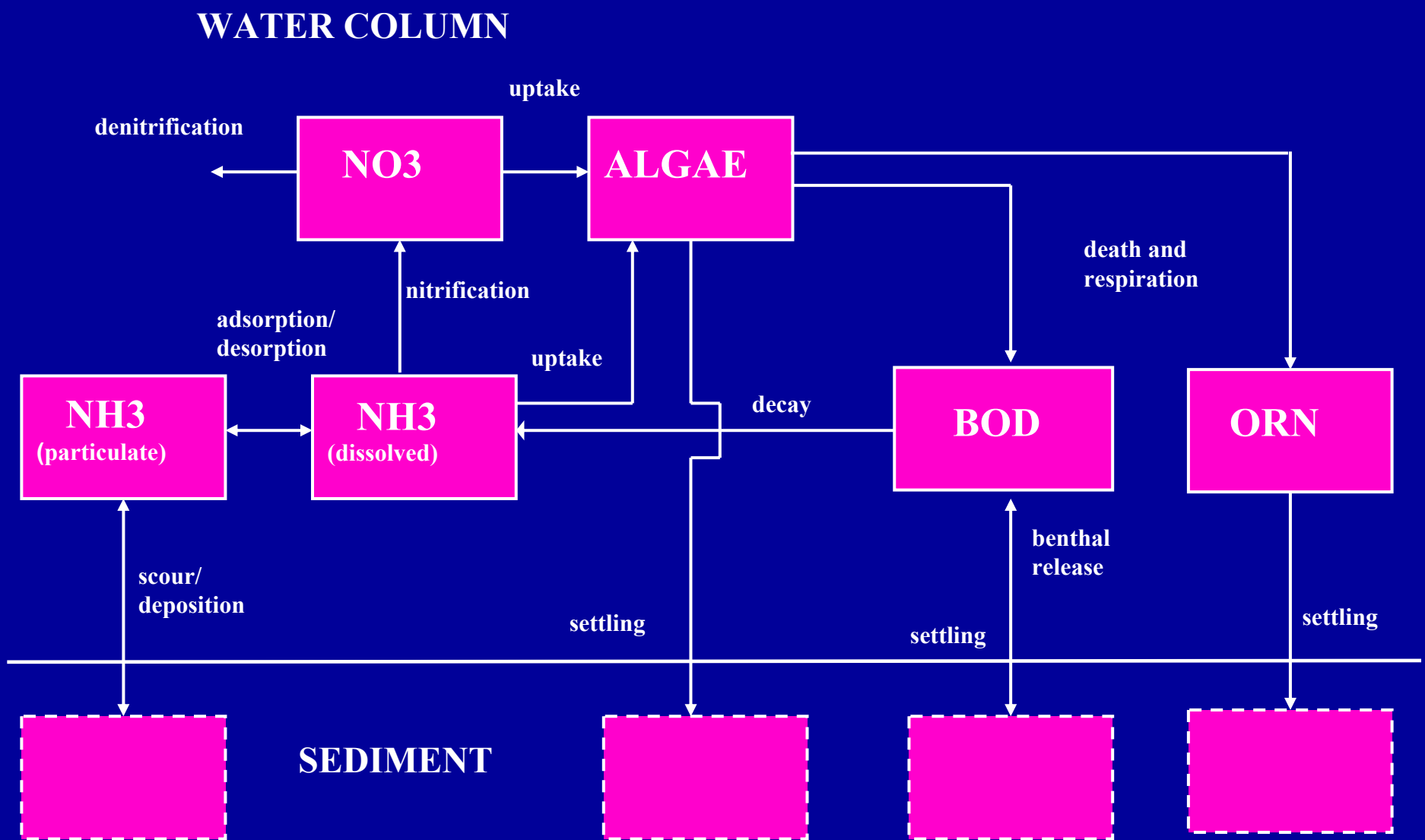
BENTHIC ALGAE MASS BALANCE



REFRACTORY ORGANICS (N,P,C) MASS BALANCE



SUMMARY OF NITROGEN CYCLE



PHCARB: pH & INORGANIC CARBON

- Computes pH based on total inorganic carbon (TIC), alkalinity, and CO_2 equilibrium
- Alkalinity simulated as a conservative (CONS)
- CO_2 input from atmosphere proportional to oxygen reaeration

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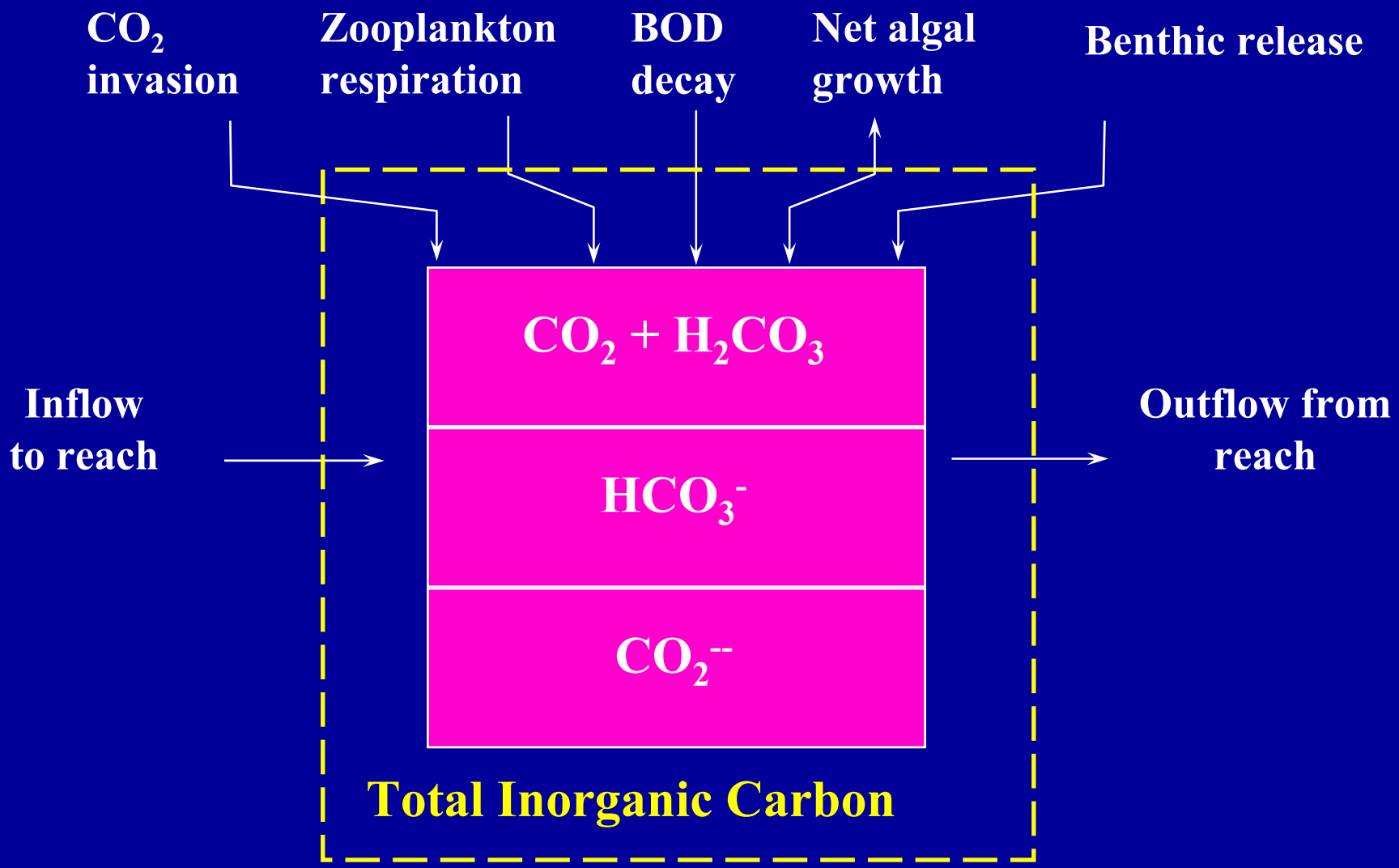
INORGANIC CARBON MASS BALANCE



PHCARB PARAMETERS

CFCINV- Ratio of CO_2 invasion rate to oxygen reaeration rate

BRCO2- Benthic release rates of CO_2 for aerobic and anaerobic conditions ($mg/m^2/hr$)

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