WATER QUALITY MODELING
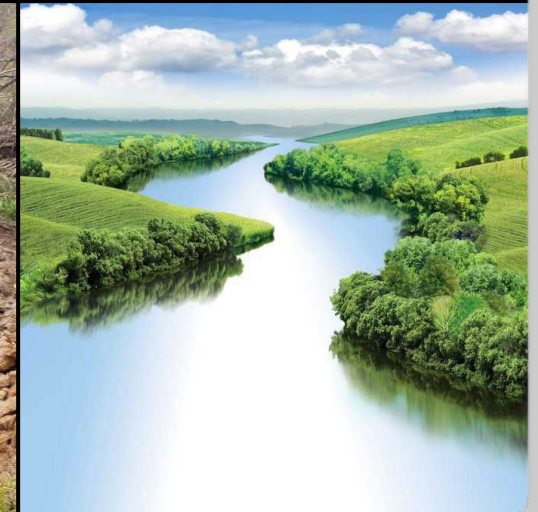
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CE-QUAL-W2 Workshop
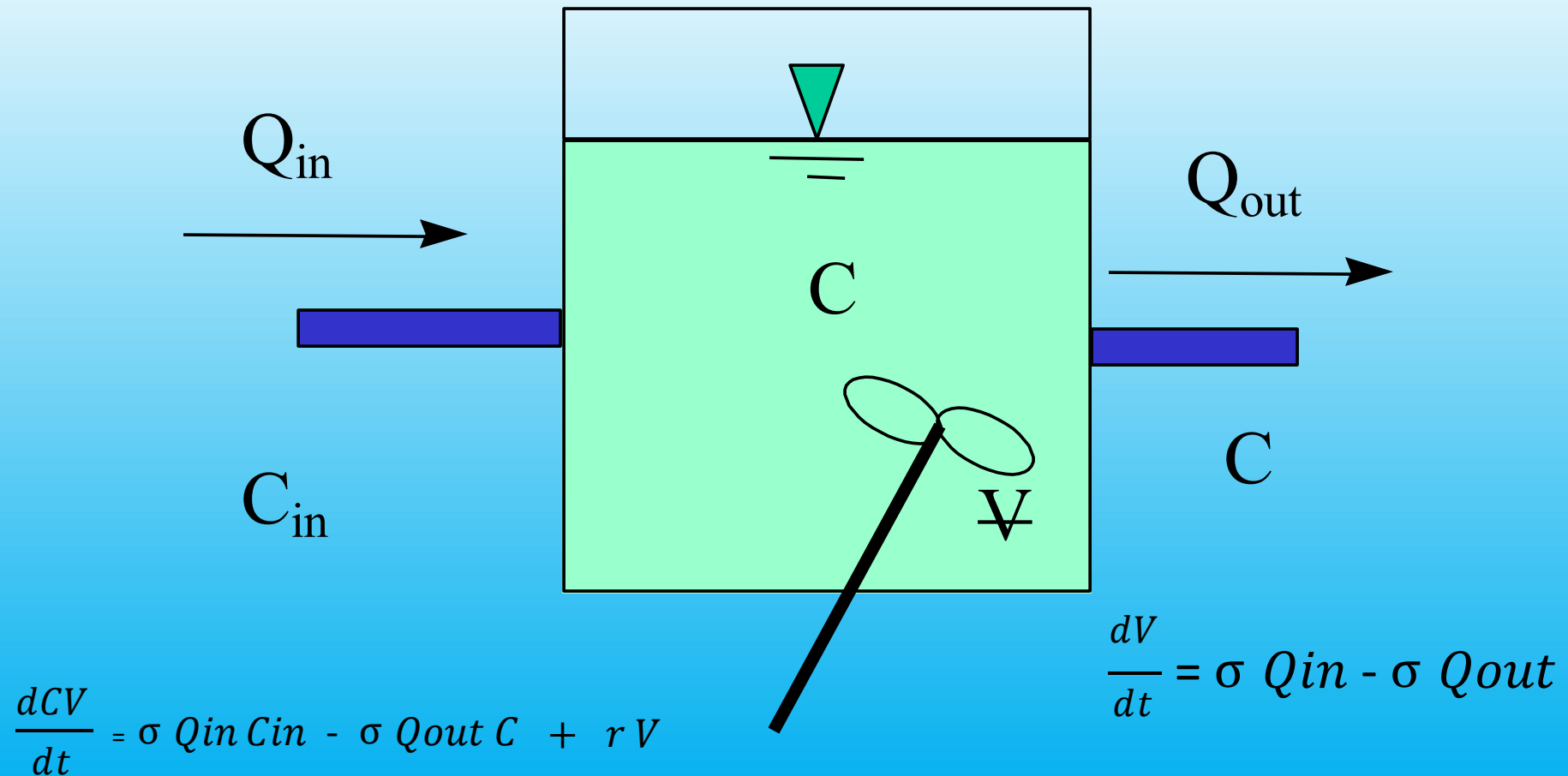
July 18-20, 2023

Outline

1. Concept/Background
2. Schematic
3. Assumptions
   - Mass Balance
   - Conservative
   - Complete Process Representation
4. Water quality capabilities
   - State variables
   - Derived variables
   - WQ processes

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Water Quality

- Water quality is agglomeration of physical, chemical, and biological components of water column that determine its overall "condition."
- Physical components include temperature and suspended solids and conservative dissolved substances.
- Chemical components include dissolved substances whose levels are impacted by physical, chemical , and biological processes.
- Biological components are living organisms whose normal biological processes are impacted by and have impacts on the conditions present in the water column.
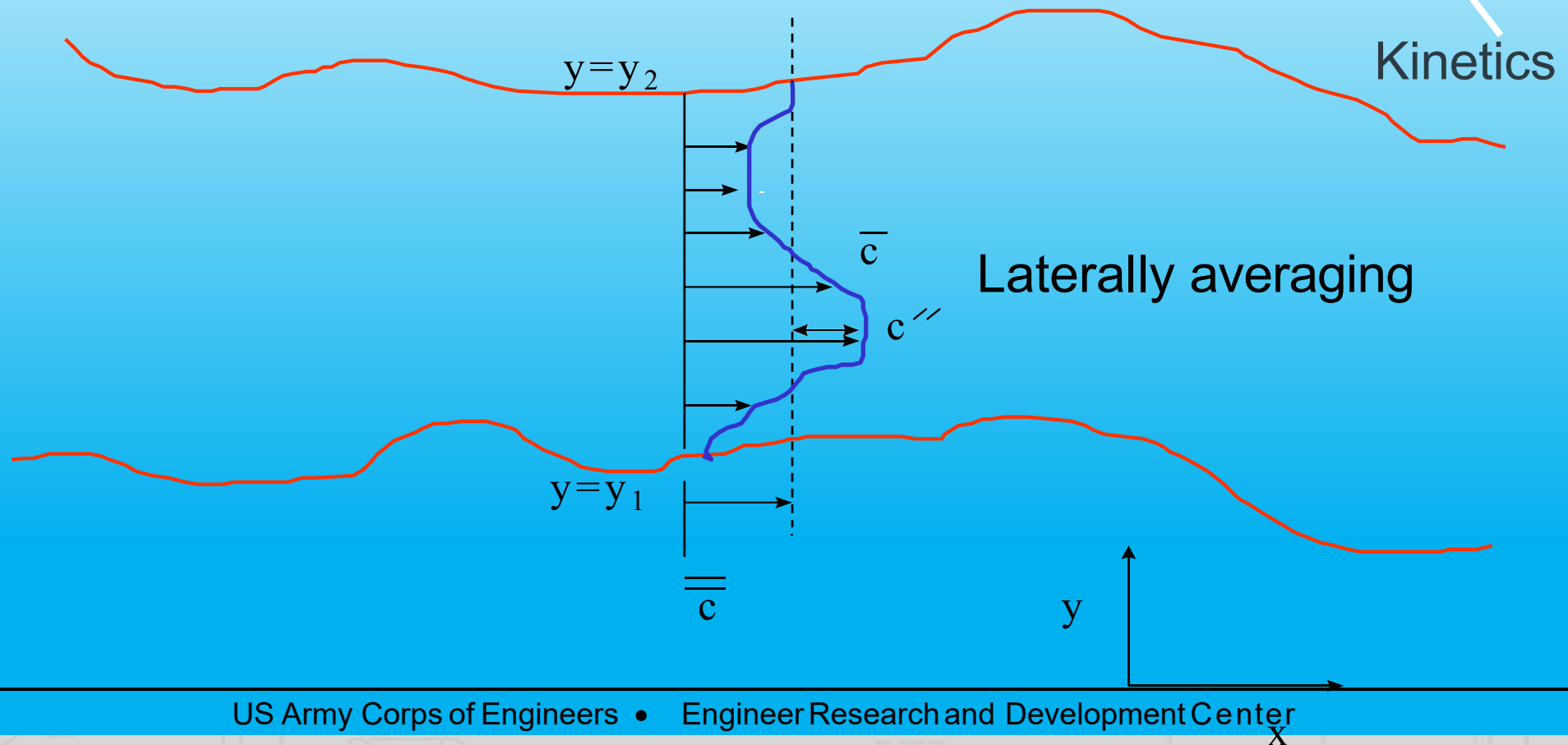
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Conceptual Water Quality Model

$$Q_{in}$$

$$Q_{out}$$

$$C$$

$$C_{in}$$

$$C$$

$$V$$

$$\frac{dCV}{dt} = \sigma\, Qin\, Cin \; - \; \sigma\, Qout\, C \; + \; r\, V$$

$$\frac{dV}{dt} = \sigma\, Qin \; - \; \sigma\, Qout$$

change in mass over time	total inflow of mass	total outflow of mass	kinetic transformations

CE-QUAL-W2 Water Quality

$$\frac{\partial B\Phi}{\partial t} + \frac{\partial UB\Phi}{\partial x} + \frac{\partial WB\Phi}{\partial z} - \frac{\partial\left(BD_x\frac{\partial\Phi}{\partial x}\right)}{\partial x} - \frac{\partial\left(BD_z\frac{\partial\Phi}{\partial z}\right)}{\partial z} = q_\Phi B + \boxed{S_\Phi B}$$

Kinetics

$y=y_2$

$\overline{c}$

c''

Laterally averaging

$y=y_1$

$\overline{\overline{c}}$

y

x

Mass Balance

- Mass of all substances in model is conserved, not created nor destroyed.
- Mass can be transformed from one form to another (i.e., Nitrogen from NH4 to NO2/NO3 to N2)
- Mass can enter and leave model by specified processes and means.
- Important that our representation of process is thorough and complete as possible

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Conservation

- The mass of all substances in model is conserved, not created nor destroyed.
- Assumption is crucial to our use of model and interpretation of its results.
- Important that our representation of process is thorough and complete as possible.
- Specified process rates should be supported by data or from technical literature.

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CE-QUAL-W2 Water Quality

- Arbitrary Constituents
- Inorganic suspended solids groups
- CH_4, H_2S
- N_2, DGP, TDG
- Labile and refractory dissolved organic matter groups (DOM, DOC, DON, DOP)
- Labile and refractory particulate organic matter fractions (POM, POC, PON, POP)
- Dissolved and particulate silica
- Alkalinity, Total inorganic carbon (TIC), PH
- Different algal groups
- NH_4-N, NO_3-N+NO_2-N
- PO_4-P
- Fe, Mn
- CBOD groups
- Sediment diagenesis model
- SYSTDG

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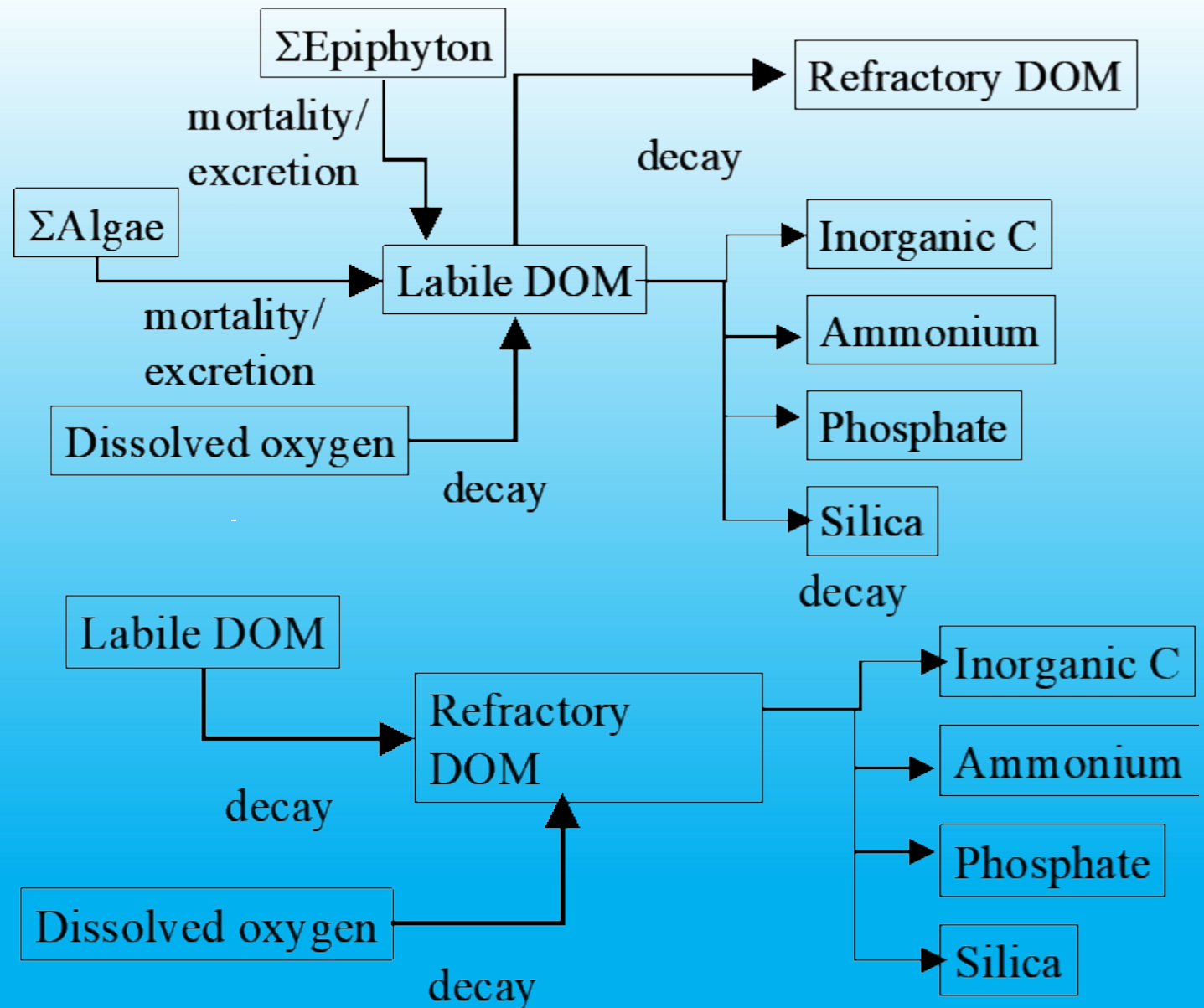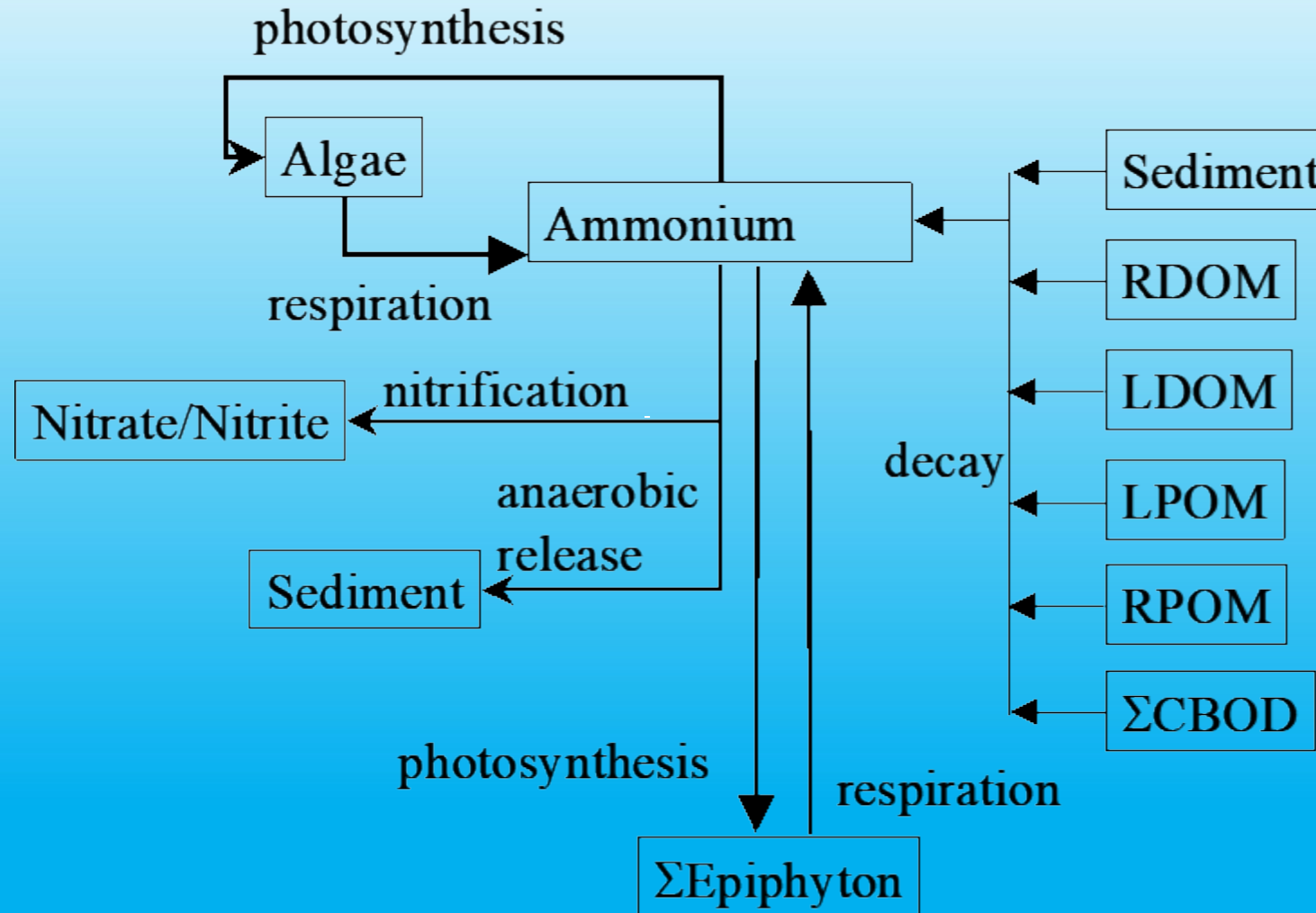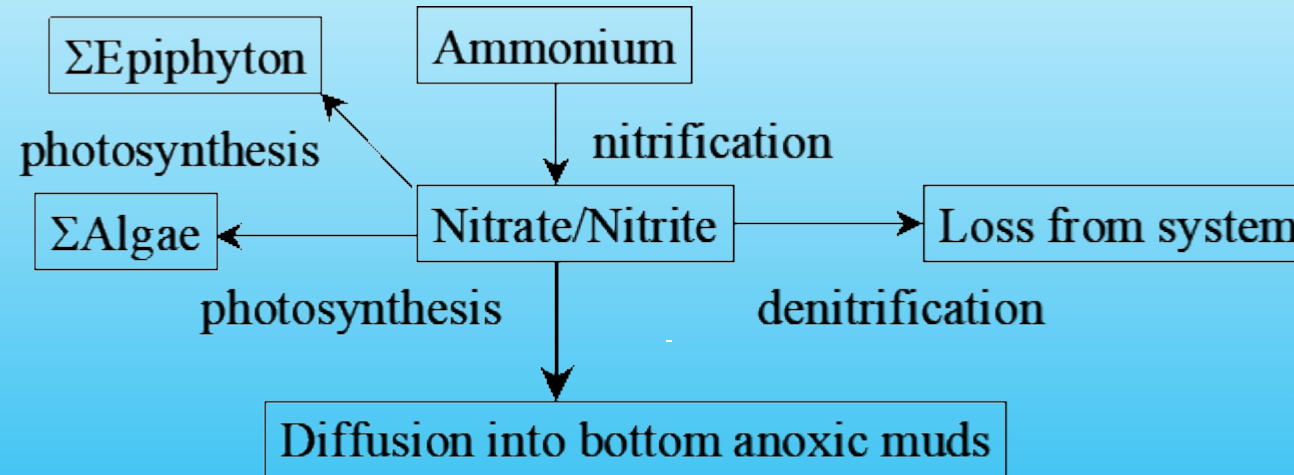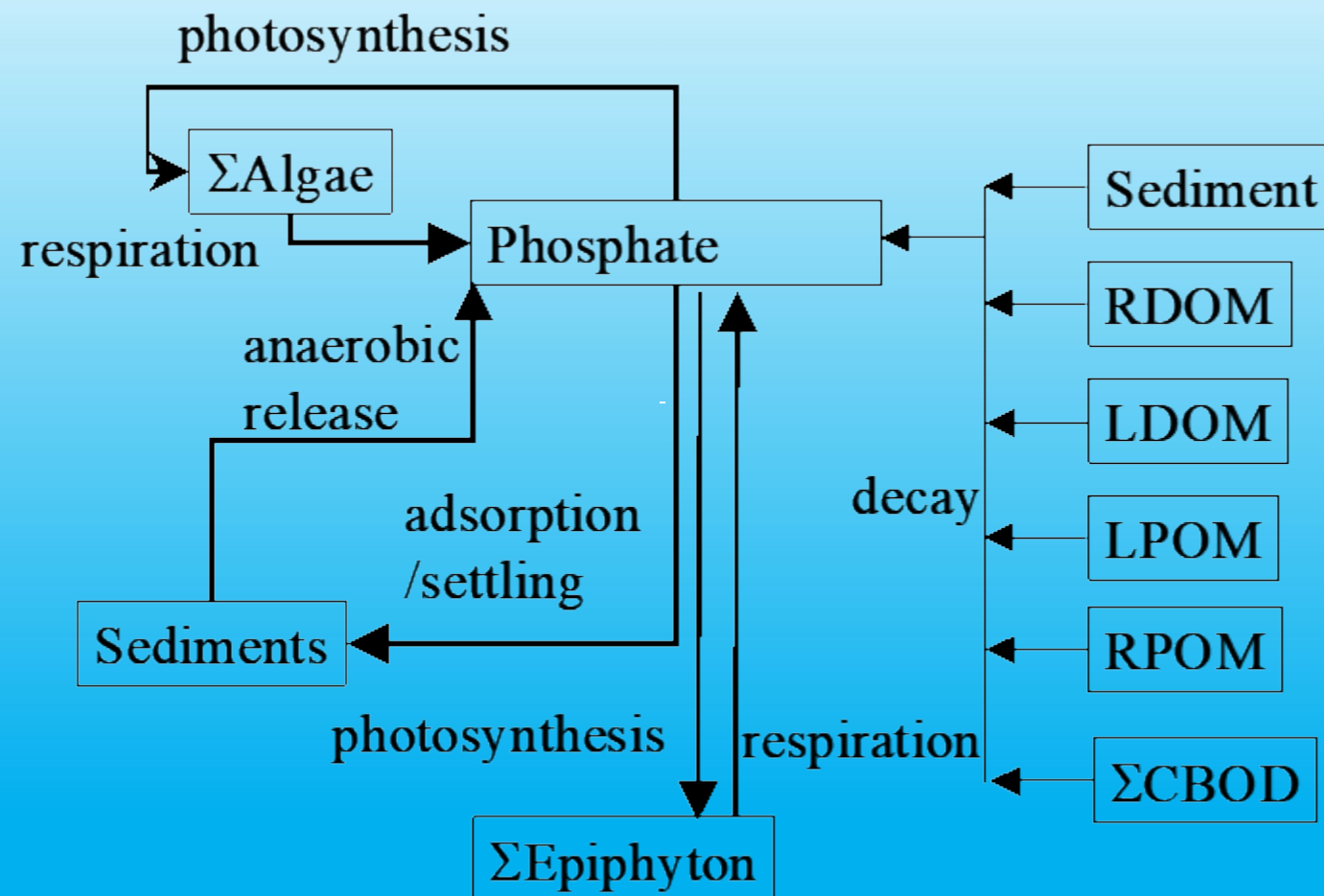
CE-QUAL-W2 DOM

CE-QUAL-W2 POM
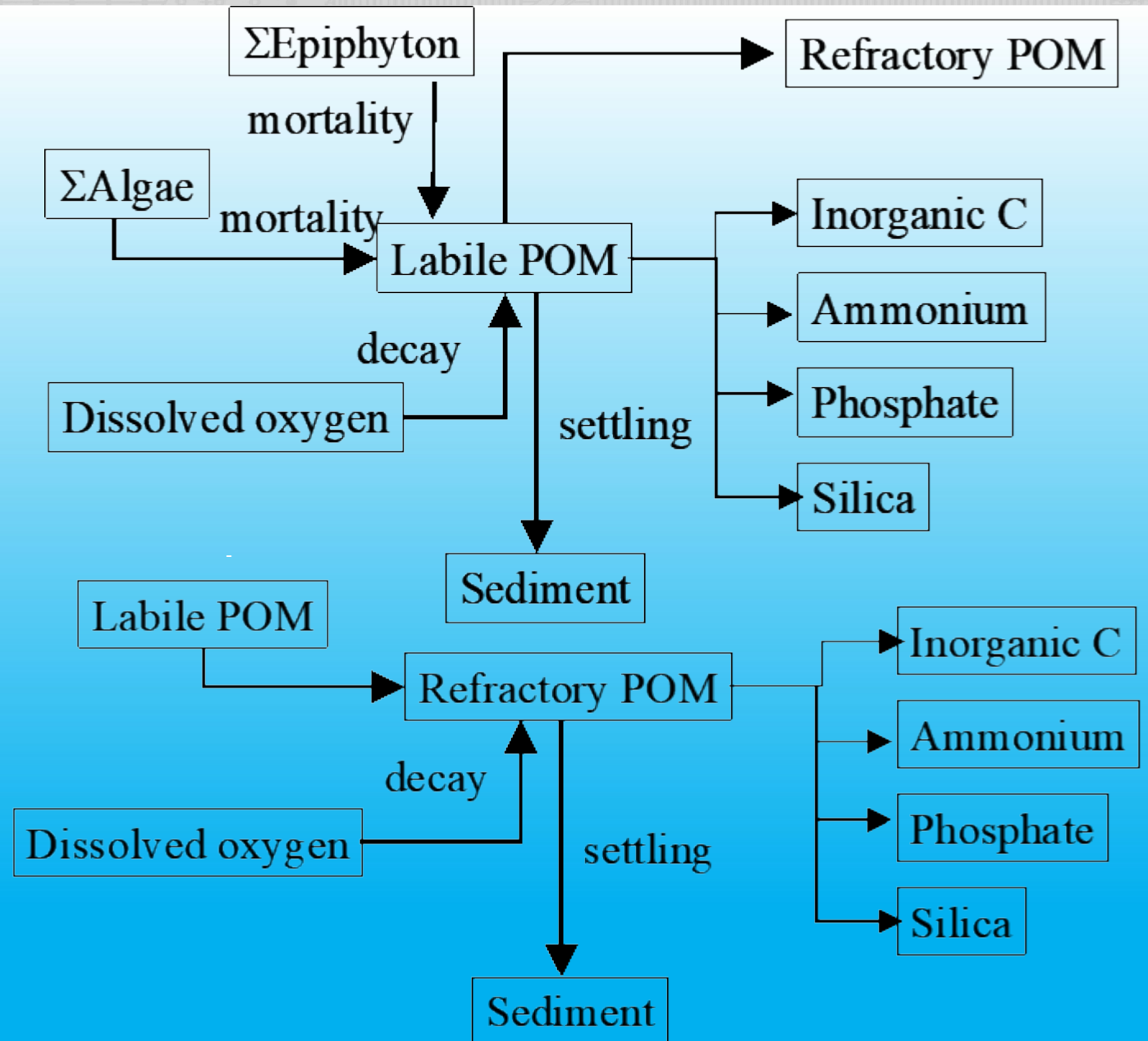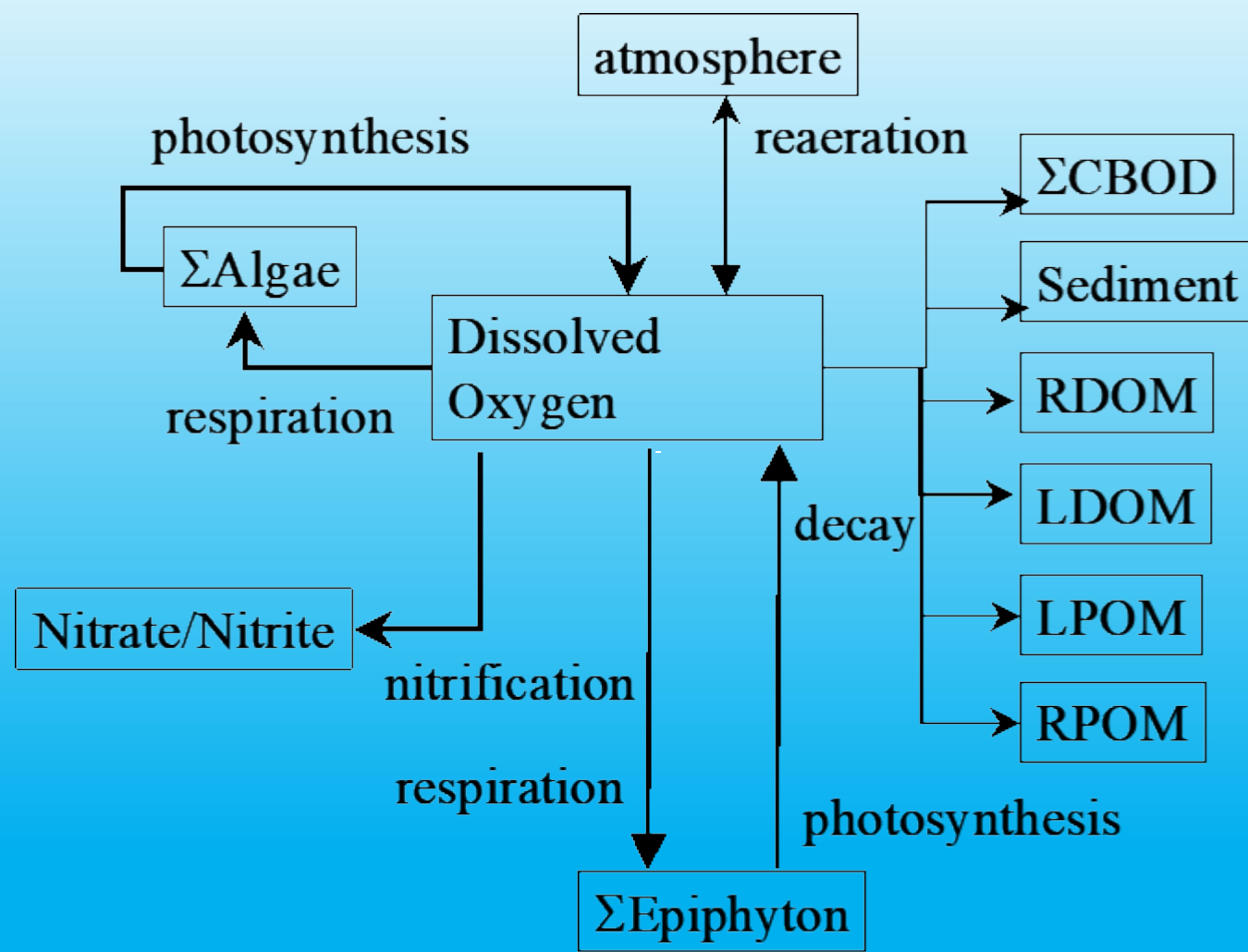
CE-QUAL-W2 Ammonium

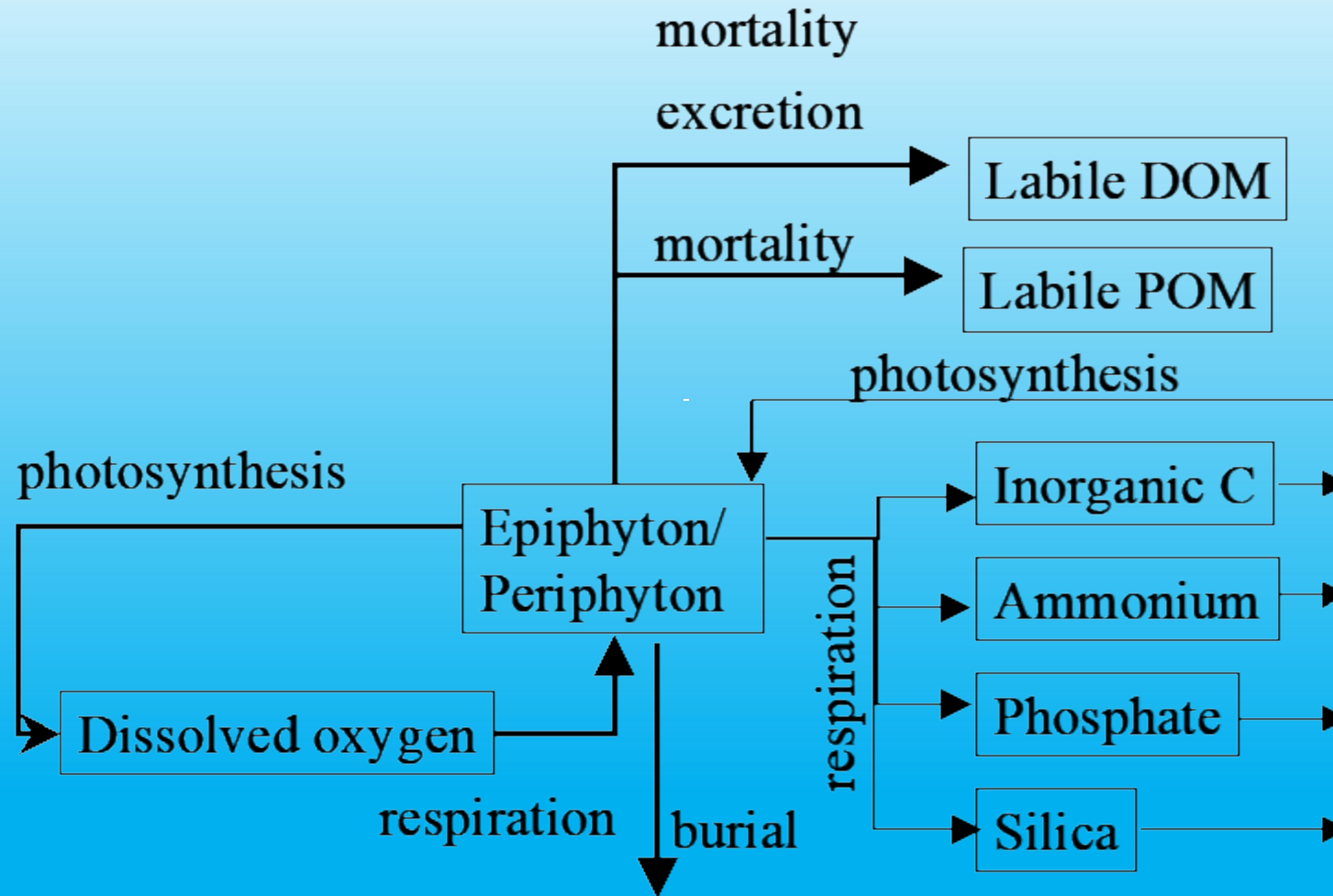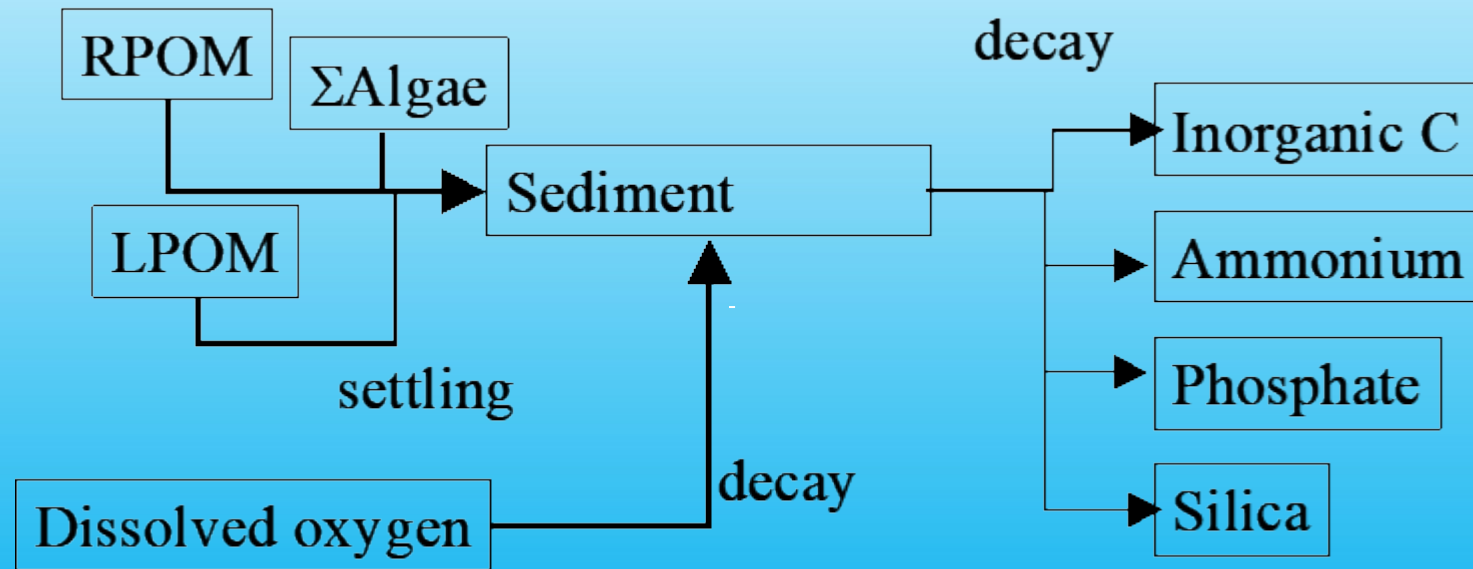# CE-QUAL-W2 Nitrate/Nitrite

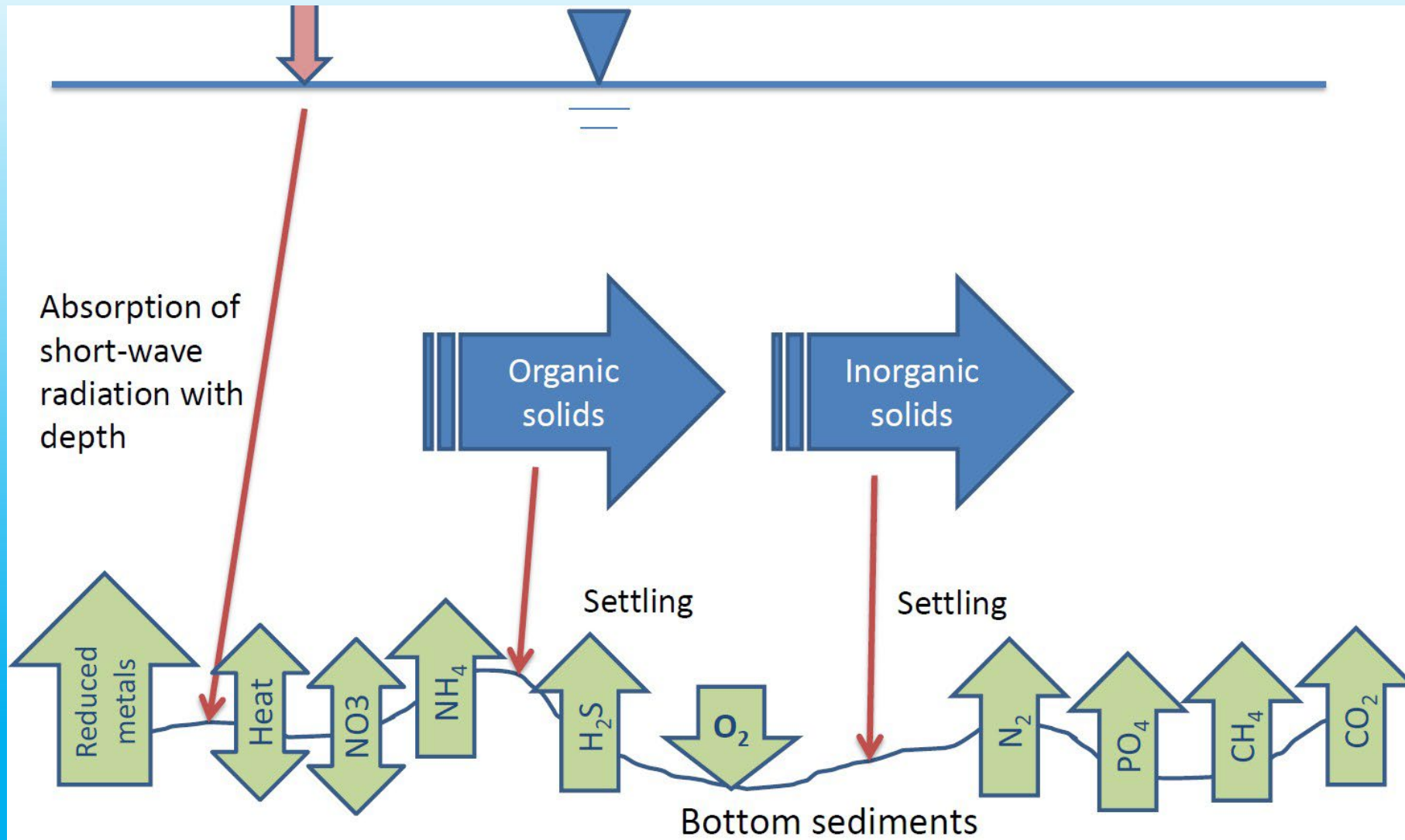# CE-QUAL-W2 Phosphate

CE-QUAL-W2 DO

CE-QUAL-W2 Algae

CE-QUAL-W2 Bed Sediment – First Order Approach

CE-QUAL-W2 Bed Sediment – Sediment Diagenesis Model

Conversions between CE-QUAL-W2 State Variables and Commonly Used Field Data

Dissolved organic carbon: $\delta_C \Phi_{LDOM} + \delta_C \Phi_{RDOM}$

Particulate organic carbon: $\delta_C \Phi_{detritus} + \delta_C \Phi_{algae}$

Total organic carbon: $\delta_C \Phi_{detritus} + \delta_C \Phi_{algae} + \delta_C \Phi_{LDOM} + \delta_C \Phi_{RDOM}$

Dissolved organic nitrogen: $\delta_N \Phi_{LDOM} + \delta_N \Phi_{RDOM}$

Particulate organic nitrogen: $\delta_N \Phi_{detritus} + \delta_N \Phi_{algae}$

Total organic nitrogen: $\delta_N \Phi_{LDOM} + \delta_N \Phi_{RDOM} + \delta_N \Phi_{detritus} + \delta_N \Phi_{algae}$

Total nitrogen: $\delta_N \Phi_{LDOM} + \delta_N \Phi_{RDOM} + \delta_N \Phi_{detritus} + \delta_N \Phi_{algae} + \Phi_{NH4} + \Phi_{NO3}$

Total Kheldahl Nitrogen (TKN): $\delta_N \Phi_{LDOM} + \delta_N \Phi_{RDOM} + \delta_N \Phi_{detritus} + \delta_N \Phi_{algae} + \Phi_{NH4}$

Dissolved organic phosphorus: $\delta_P \Phi_{LDOM} + \delta_P \Phi_{RDOM}$

Particulate organic phosphorus: $\delta_P \Phi_{detritus} + \delta_P \Phi_{algae}$

Total organic phosphorus: $\delta_P \Phi_{LDOM} + \delta_P \Phi_{RDOM} + \delta_P \Phi_{detritus} + \delta_P \Phi_{algae}$

Total phosphorus: $\delta_P \Phi_{LDOM} + \delta_P \Phi_{RDOM} + \delta_P \Phi_{detritus} + \delta_P \Phi_{algae} + \Phi_{PO4} + \delta_{PISS} \Phi_{ISS}$

Carbonaceous BOD, CBOD: $\delta_{OM} \Phi_{RDOM} + \delta_{OM} \Phi_{LDOM} + \delta_{OM} \Phi_{algae} + \delta_{OM} \Phi_{detritus}$

Nitrogenous BOD, NBOD:

$\delta_N \delta_{NH4} \Phi_{RDOM} + \delta_N \delta_{NH4} \Phi_{LDOM} + \delta_N \delta_{NH4} \Phi_{algae} + \delta_N \delta_{NH4} \Phi_{detritus} + \delta_{NH4} \Phi_{NH4}$

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Questions?

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