WATER QUALITY MODELING

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CE-QUAL-W2 Workshop

August 16 - 18, 2022

US Army Corps of Engineers

Environmental Systems Modeling Team

ERDC ENGINEER RESEARCH & DEVELOPMENT CENTER

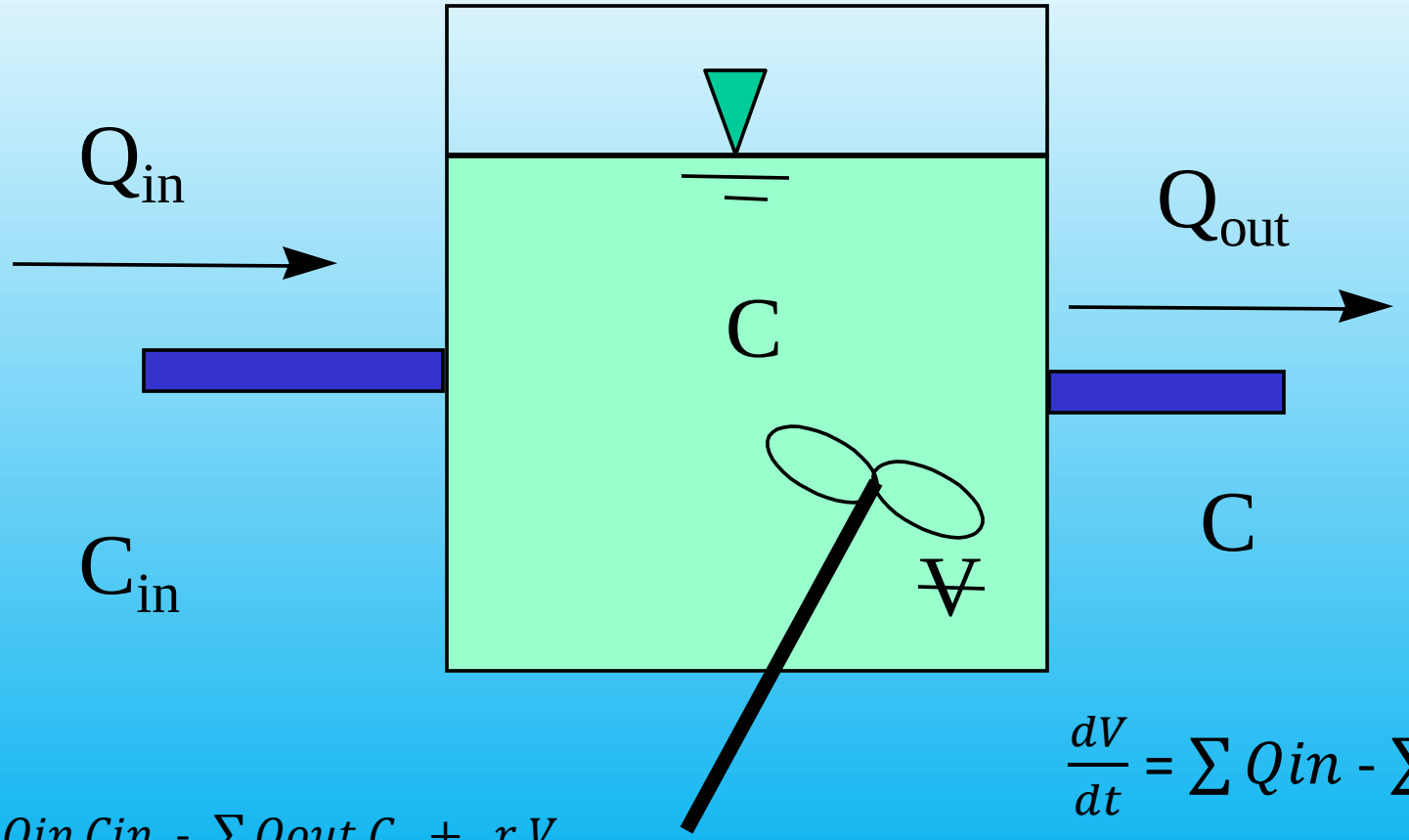
Outline

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

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.

Conceptual Water Quality Model



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

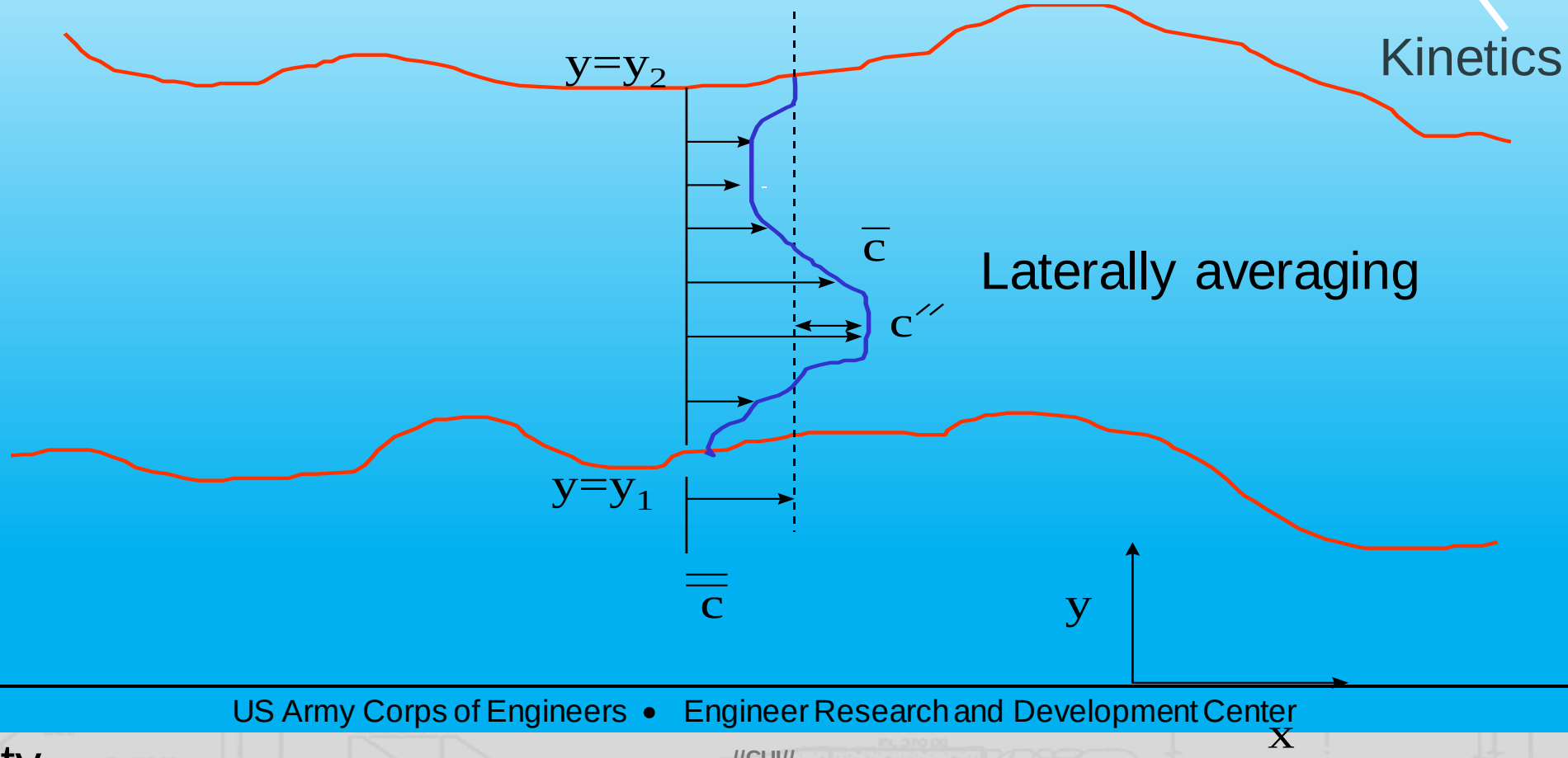
change in mass over time | total inflow of mass | total outflow of mass | kinetic transformations

$$\frac{dV}{dt} = \sum Qin - \sum Qout$$

CE-QUAL-W2 Water Quality

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

Kinetics



Laterally averaging

Mass Balance

- Mass of all substances in model is conserved, not created nor destroyed.
- Mass can be transformed from one from 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

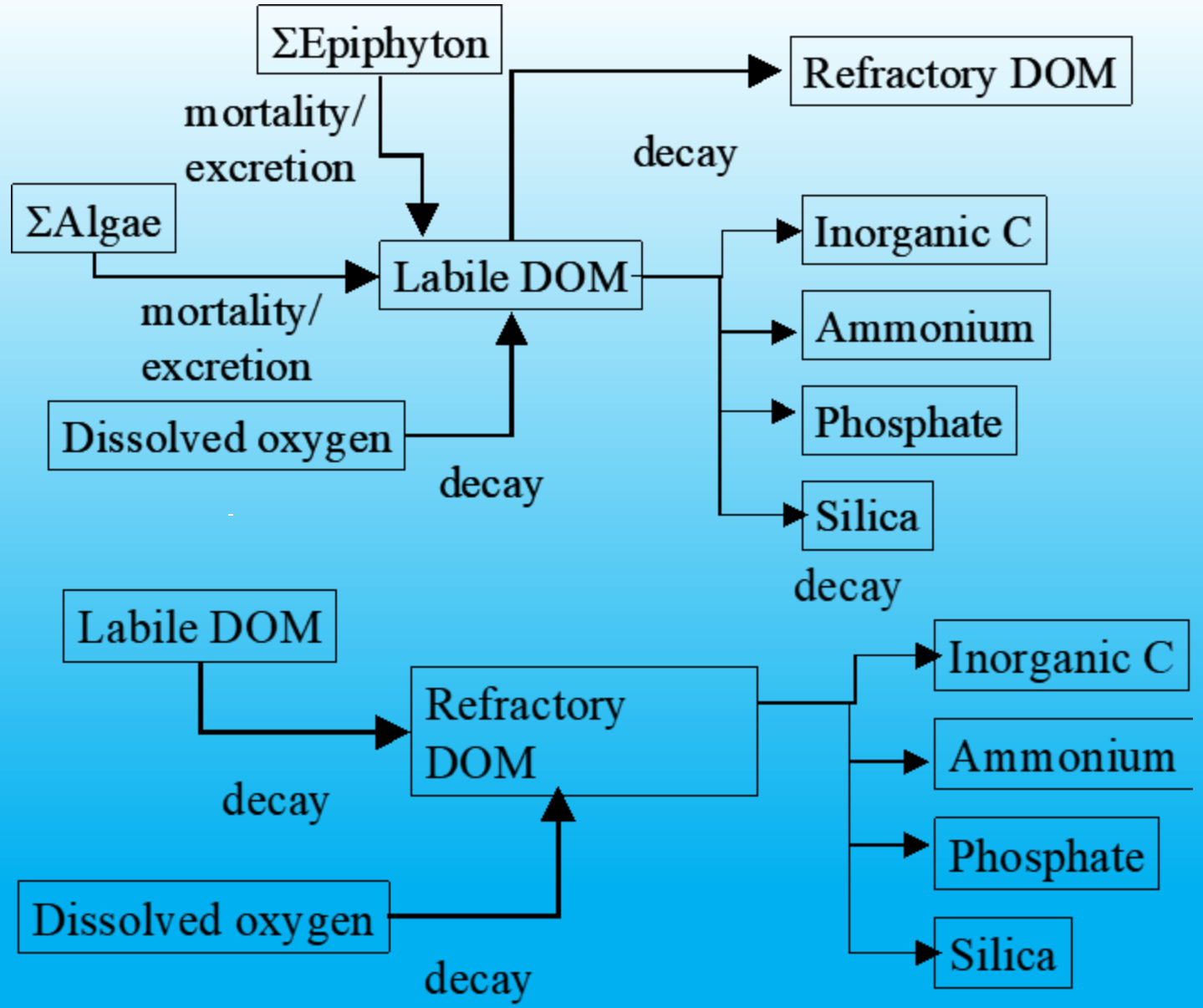
Conservation

- 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.

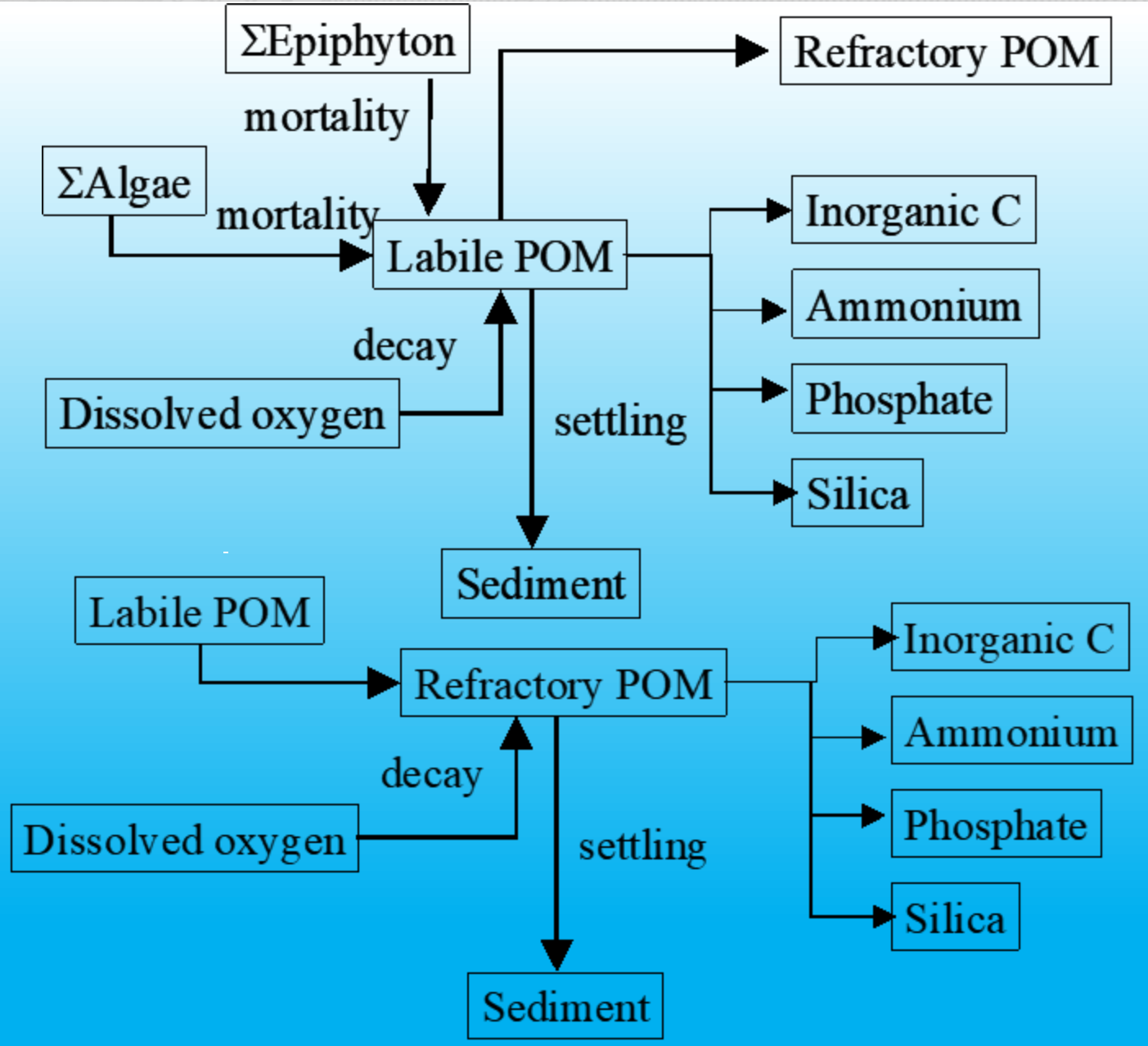
CE-QUAL-W2 Water Quality

- 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

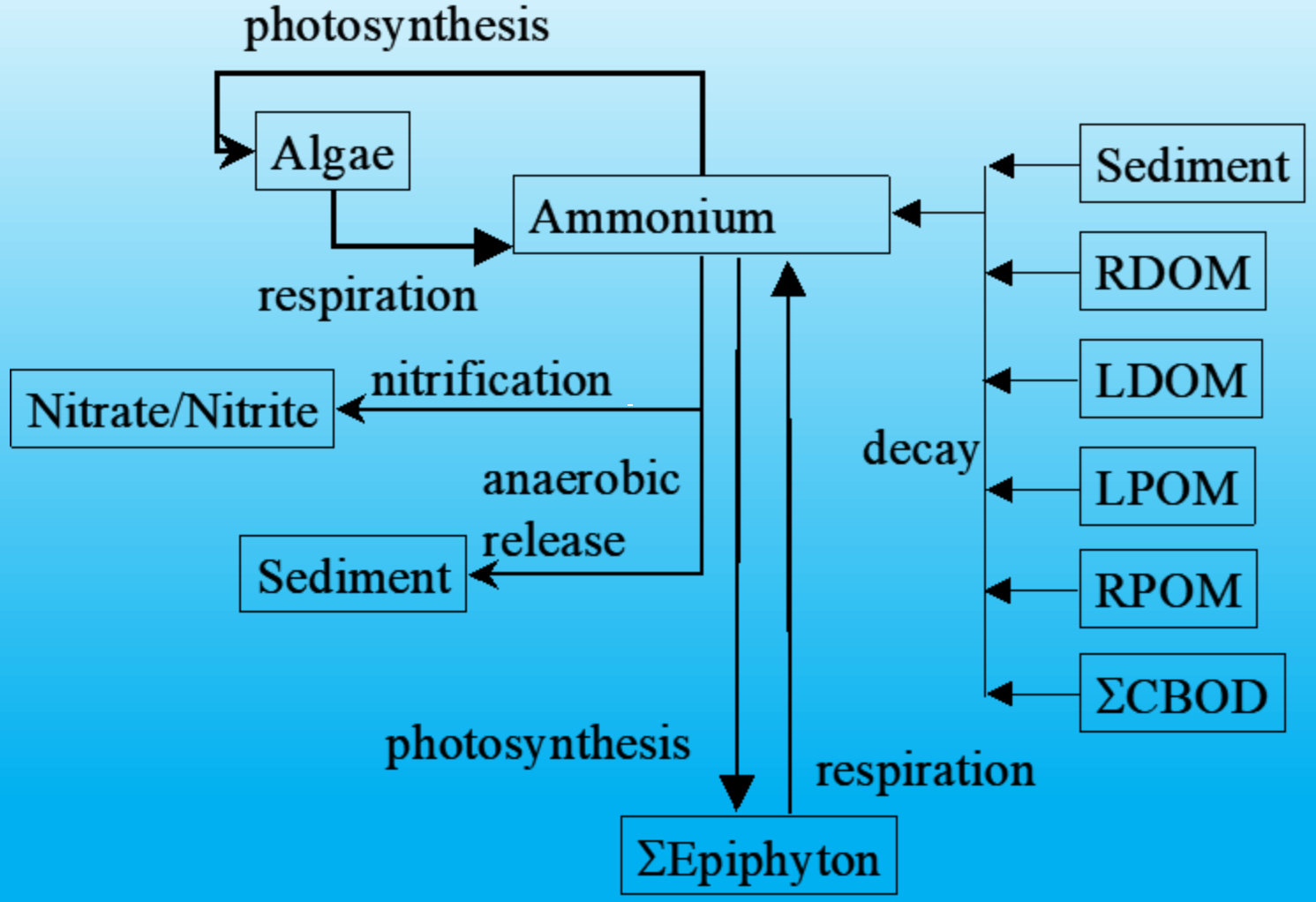
CE-QUAL-W2 DOM



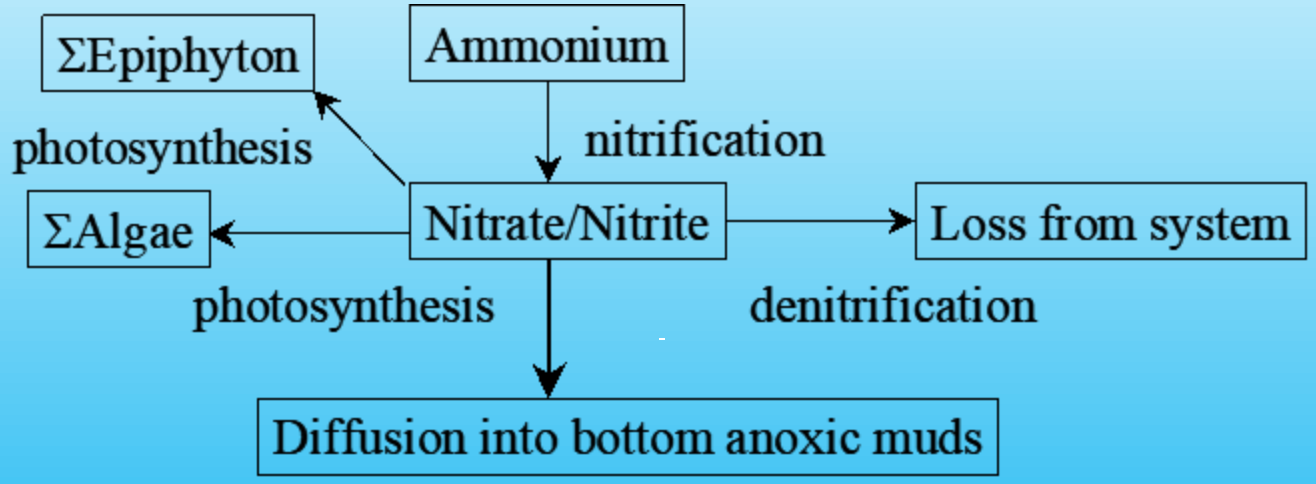
CE-QUAL-W2 POM



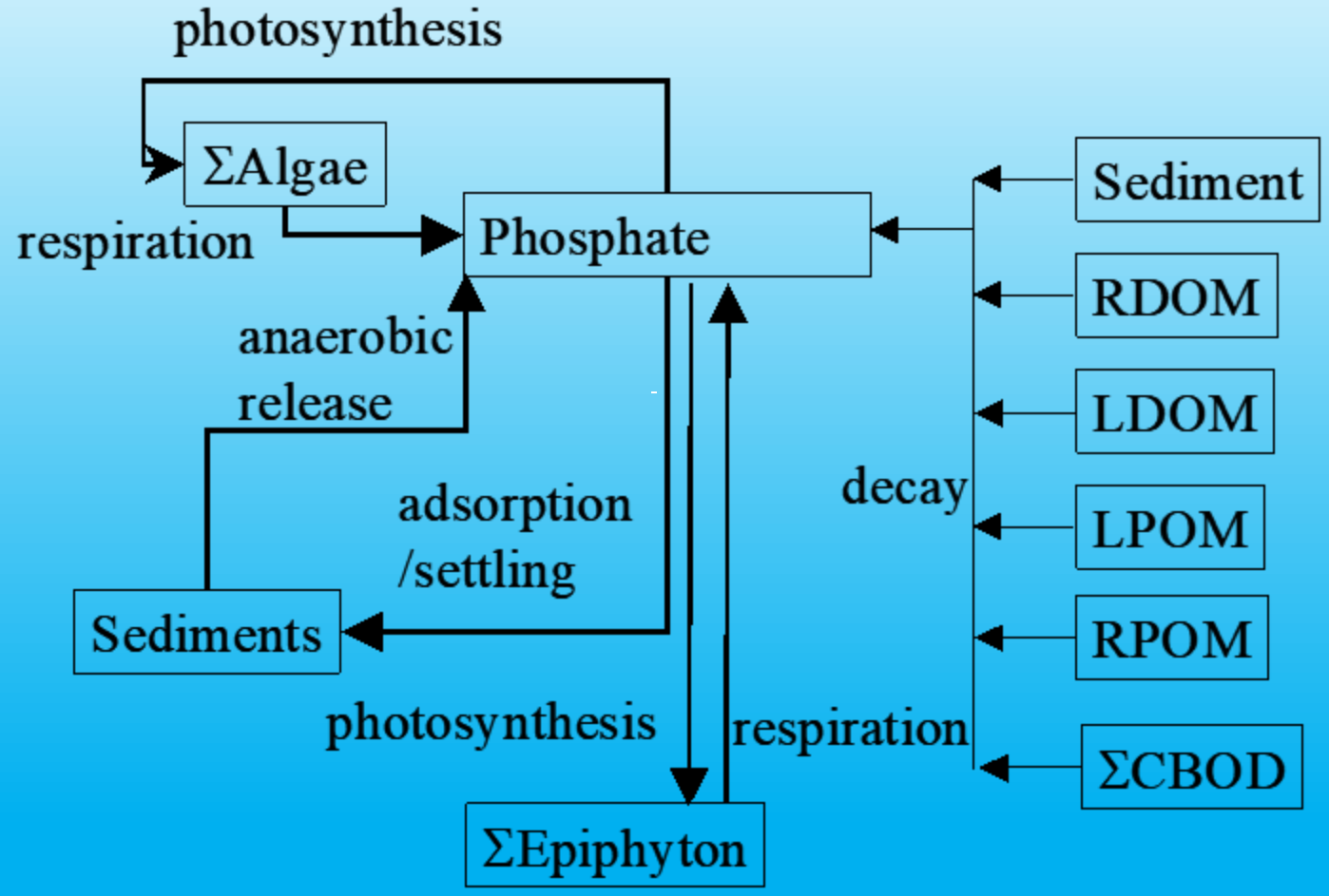
CE-QUAL-W2 Ammonium



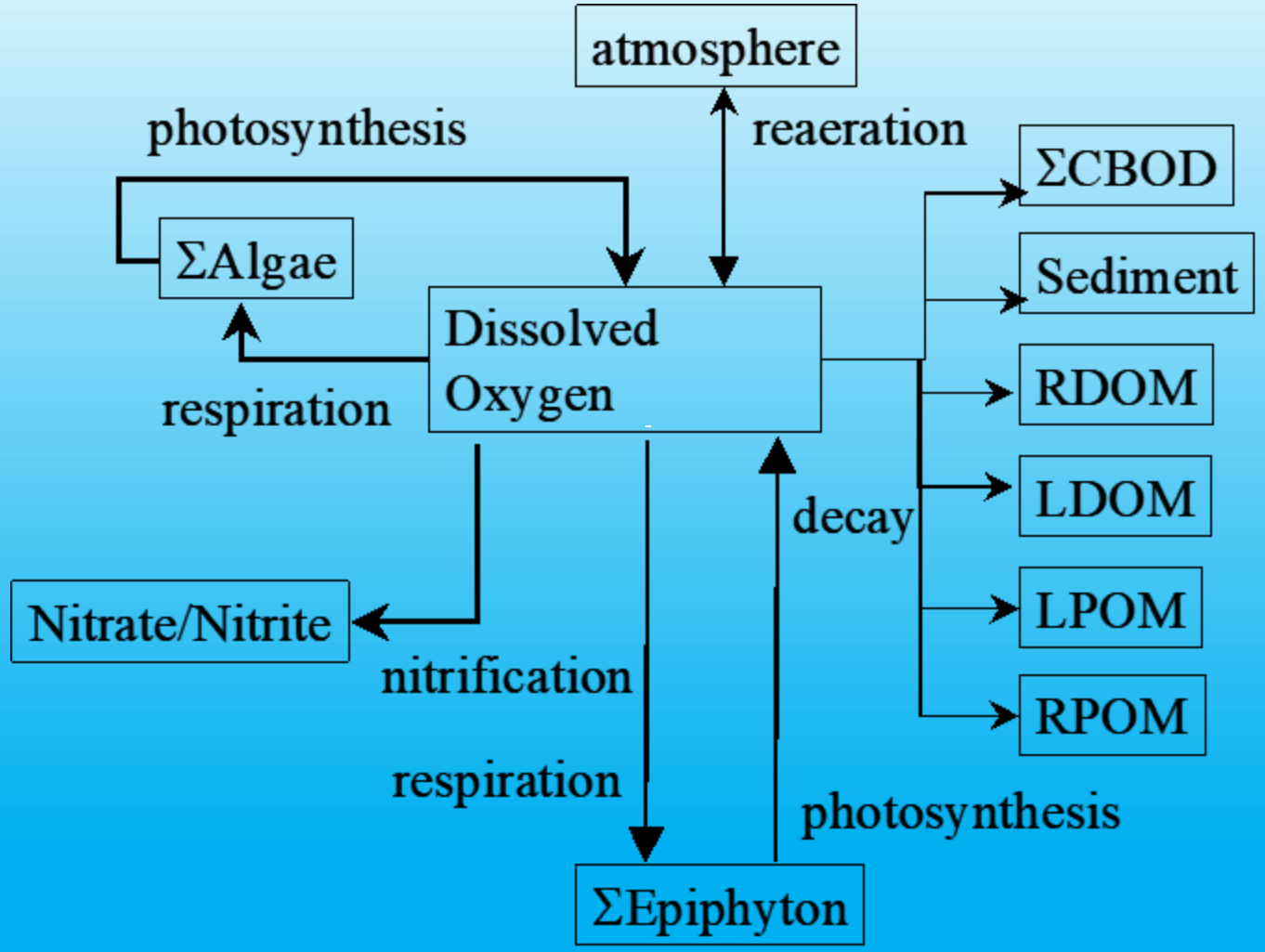
CE-QUAL-W2 Nitrate/Nitrite



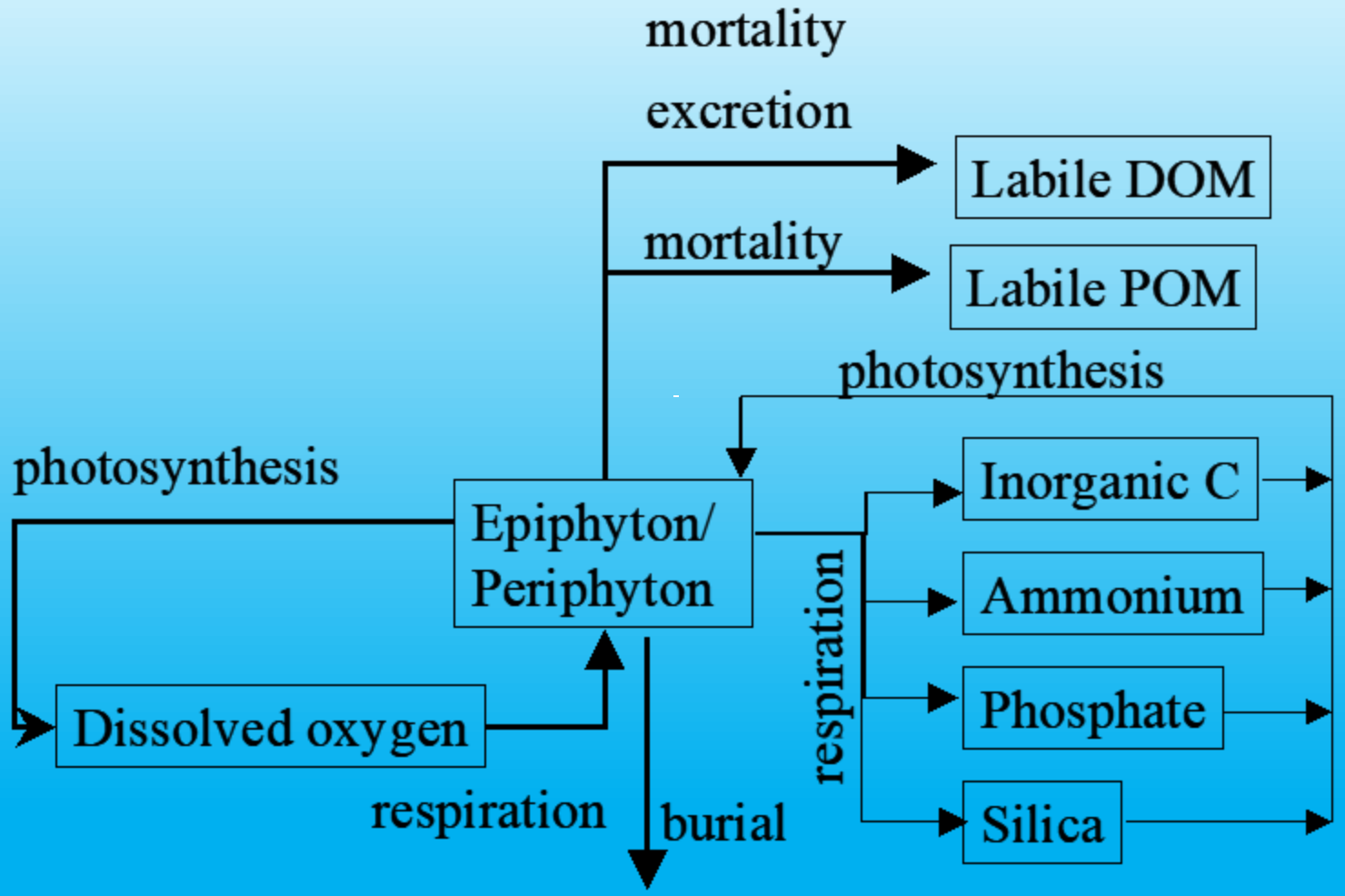
CE-QUAL-W2 Phosphate



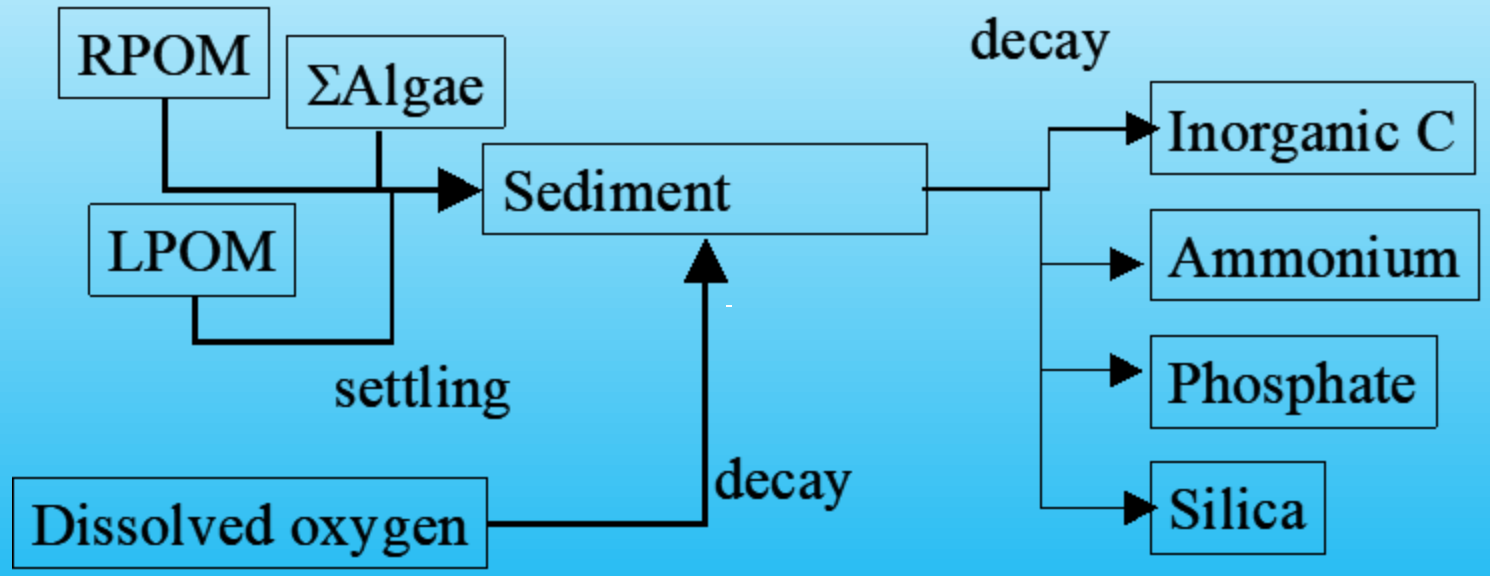
CE-QUAL-W2 DO


atmosphere
photosynthesis
reaeration
ΣCBOD
ΣAlgae
Sediment
Dissolved
Oxygen
RDOM
respiration
LDOM
decay
Nitrate/Nitrite
LPOM
nitrification
RPOM
respiration
photosynthesis
ΣEpiphyton

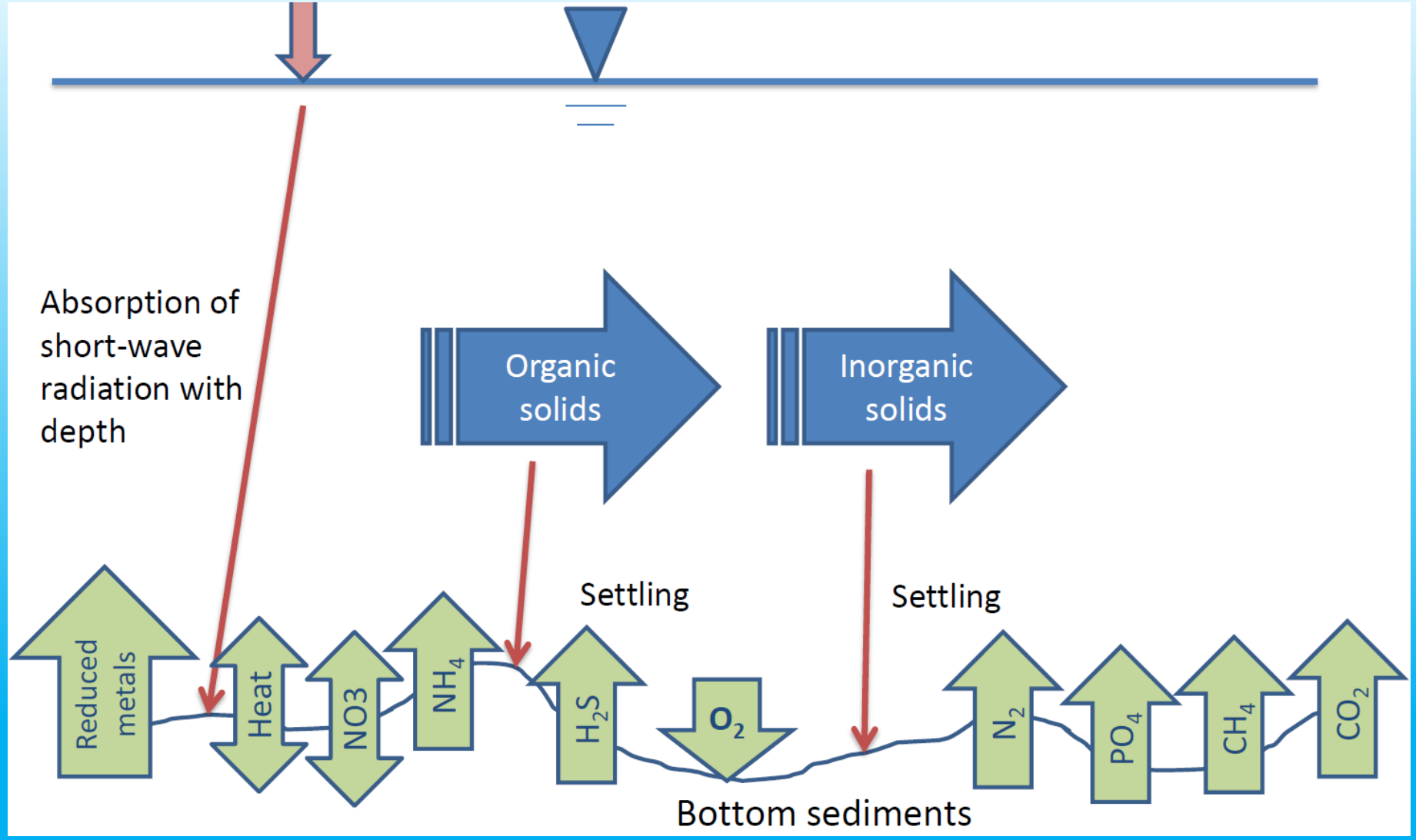
CE-QUAL-W2 Algae



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: $\delta_C \Phi_{\det ritus} + \delta_C \Phi_{a\lg ae}$

Total organic carbon: $\delta_C \Phi_{\det ritus} + \delta_C \Phi_{a\lg ae} + \delta_C \Phi_{LDOM} + \delta_C \Phi_{RDOM}$

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

Particulate organic nitrogen: $\delta_N \Phi_{\det ritus} + \delta_N \Phi_{a\lg ae}$

Total organic nitrogen: $\delta_N \Phi_{LDOM} + \delta_N \Phi_{RDOM} + \delta_N \Phi_{\det ritus} + \delta_N \Phi_{a\lg ae}$

Total nitrogen: $\delta_N \Phi_{LDOM} + \delta_N \Phi_{RDOM} + \delta_N \Phi_{\det ritus} + \delta_N \Phi_{a\lg ae} + \Phi_{NH4} + \Phi_{NO3}$

Total Kheldahl Nitrogen (TKN): $\delta_N \Phi_{LDOM} + \delta_N \Phi_{RDOM} + \delta_N \Phi_{\det ritus} + \delta_N \Phi_{a\lg ae} + \Phi_{NH4}$

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

Particulate organic phosphorus: $\delta_P \Phi_{\det ritus} + \delta_P \Phi_{a\lg ae}$

Total organic phosphorus: $\delta_P \Phi_{LDOM} + \delta_P \Phi_{RDOM} + \delta_P \Phi_{\det ritus} + \delta_P \Phi_{a\lg ae}$

Total phosphorus: $\delta_P \Phi_{LDOM} + \delta_P \Phi_{RDOM} + \delta_P \Phi_{\det ritus} + \delta_P \Phi_{a\lg ae} + \Phi_{PO4} + \delta_{PISS} \Phi_{ISS}$

Carbonaceous BOD, CBOD: $\delta_{OM} \Phi_{RDOM} + \delta_{OM} \Phi_{LDOM} + \delta_{OM} \Phi_{a\lg ae} + \delta_{OM} \Phi_{\det ritus}$

Nitrogenous BOD, NBOD:

$\delta_N \delta_{NH4} \Phi_{RDOM} + \delta_N \delta_{NH4} \Phi_{LDOM} + \delta_N \delta_{NH4} \Phi_{a\lg ae} + \delta_N \delta_{NH4} \Phi_{\det ritus} + \delta_{NH4} \Phi_{NH4}$

Questions?