WATER QUALITY MODELING

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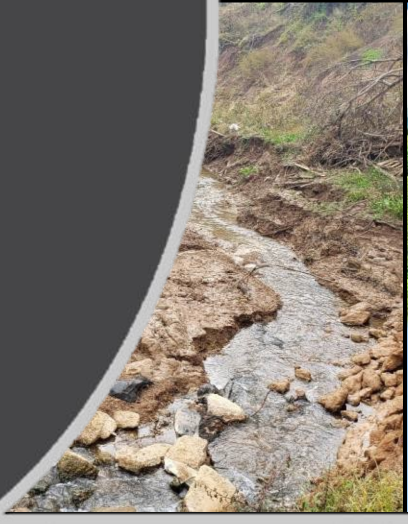

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Outline

1. Important Terms
2. Water Quality Definition
3. Conceptual Model
4. Assumptions
   - Mass Balance
   - Conservative
   - Complete Process Representation
5. Boundary Conditions
6. Initial Conditions
7. Water quality capabilities
   - State variables
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   - WQ processes

Important Terms

- State Variables: Fundamental variables in a model that describe the state of the system at any given time. These variables are intrinsic to the system and are typically governed by differential equations representing the physical, chemical, or biological processes. In other words, they are incorporated into the advection-diffusion and transformation processes.
  - Examples: Concentrations of various substances (e.g., nutrients like nitrogen and phosphorus, dissolved oxygen, temperature, microbial populations).
- Derived Variables: Calculated from the state variables and other known quantities within the system. They provide additional insights or outputs that are not directly modeled by the state equations but are important for interpreting the system's behavior.
  - Examples: Saturation levels of dissolved oxygen (derived from temperature and oxygen concentration), water quality indices (calculated from various state variables), and total suspended solids (which might be derived from measurements of turbidity and flow rates), and Total Dissolved Gas (TDG, derived by summing dissolved oxygen and nitrogen)

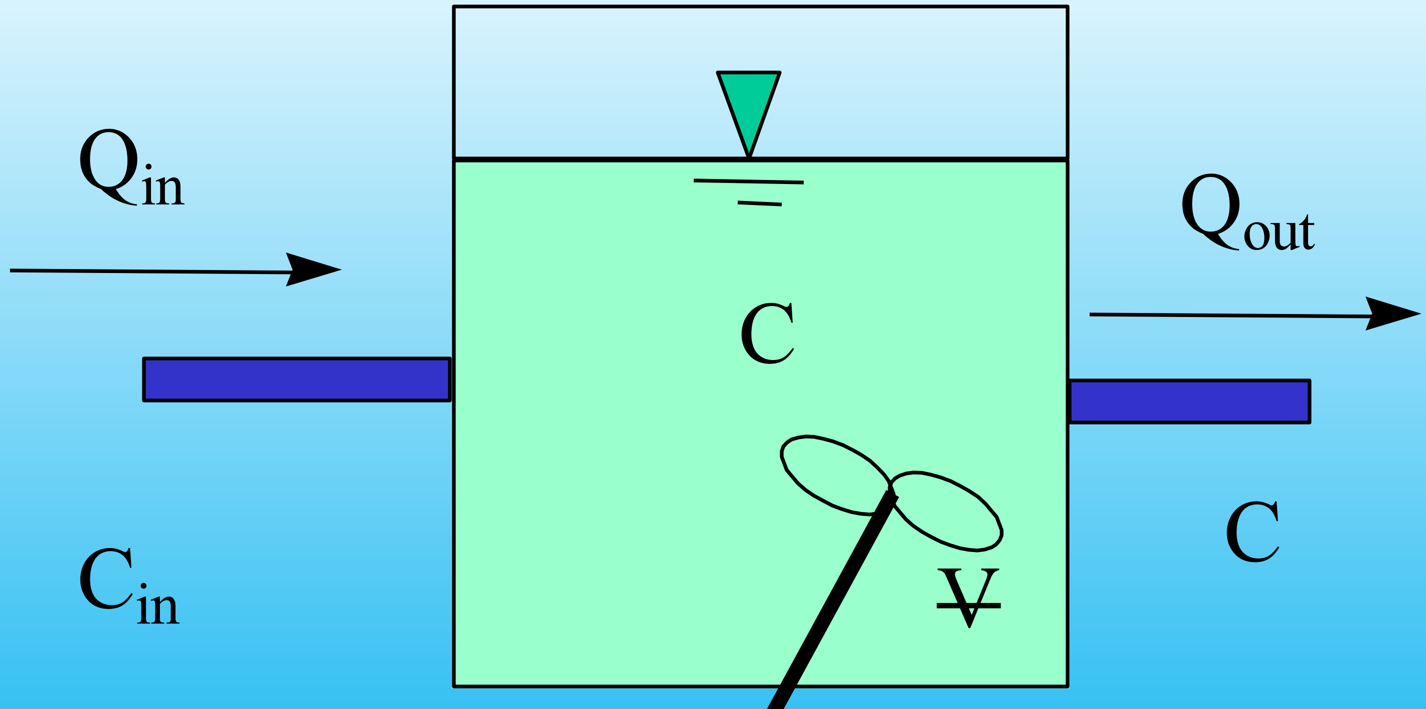
Important Terms, Continued

- Conservative Constituents: Do not undergo any chemical, biological, or physical transformation as they move through the system. Their concentration changes only due to dilution, mixing, or advection.
    - Examples: Chloride, sodium, and other non-reactive tracers or substances. These substances can be used to track water movement and mixing patterns without altering their properties.
- Non-Conservative Constituents: Undergo chemical, biological, or physical transformations as they move through the system. Their concentration changes due to processes such as chemical reactions, biological uptake or release, and physical transformations.
    - Examples: Nutrients like nitrate and phosphate (subject to biological uptake and transformation), organic matter (subject to decomposition), and pollutants like heavy metals (which can adsorb to sediments or precipitate).

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 <u>conservative</u> dissolved substances.
- Chemical components include dissolved substances whose levels are impacted by physical, chemical , and biological processes (<u>non-conservative</u>).
- 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



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

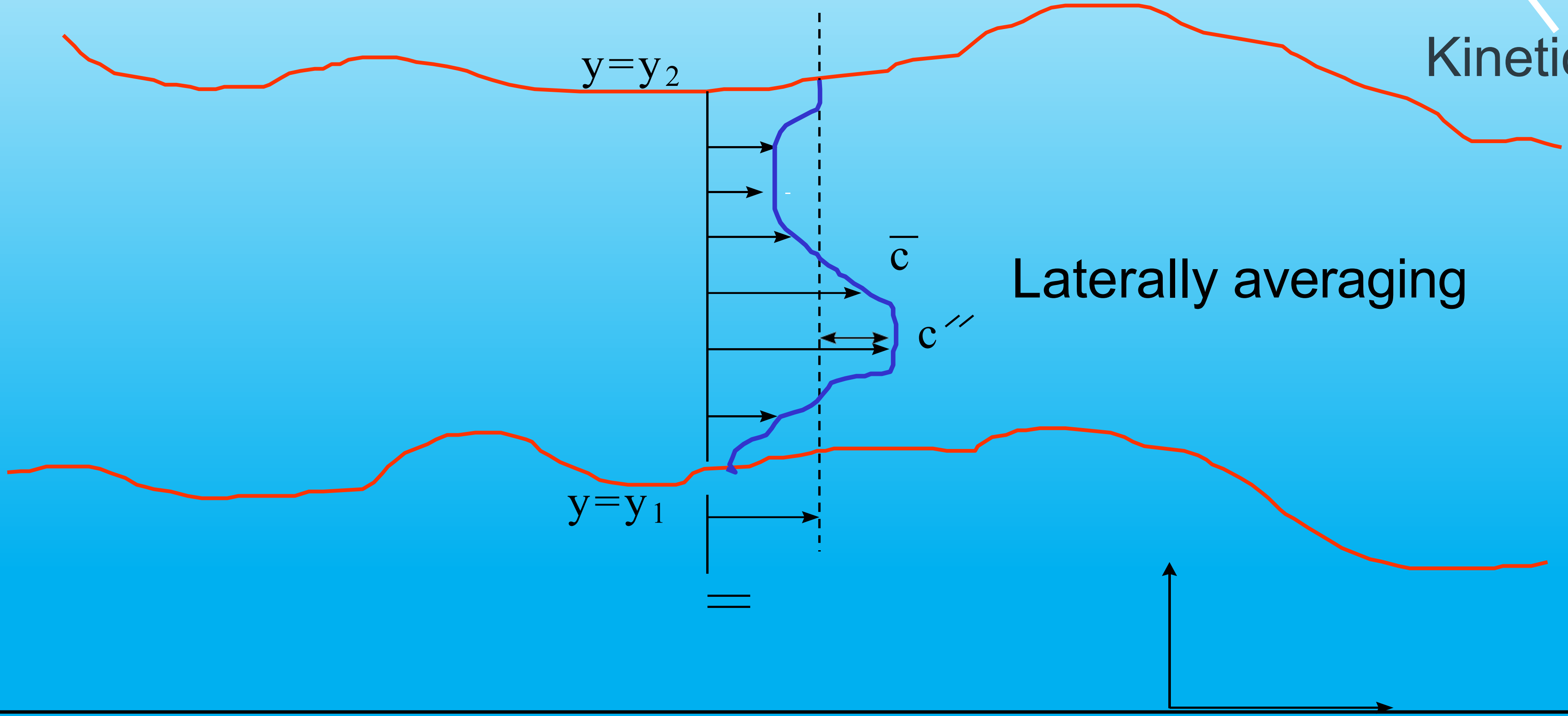
$$\frac{dCV}{dt} = \sigma\ Qin\ Cin\ -\ \sigma\ Qout\ C\ +\ r\ V$$

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



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 NH_4 to NO_2/NO_3 to N_2)
- Mass can enter and leave model by specified processes and means.
- Important that our representation of process is thorough and complete as possible

Conservation of Mass and Energy

- 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.

Boundary Conditions

- Upstream/Downstream Boundaries: Conditions at the edges of the modeled domain, where water enters or leaves the system.
- Point Sources: Direct discharges into the water body from specific locations, such as wastewater treatment plants, industrial outfalls, and stormwater drains.
  - Tributary Inflows: Inputs from rivers, streams, and other watercourses entering the modeled water body.
- Non-Point Sources: Diffuse sources of pollution such as agricultural runoff, urban runoff, and atmospheric deposition.
  - May be simulated as tributary inflows
  - Often obtained from SWAT and other hydrology models
- Meteorology: Atmospheric conditions and phenomena that influence the water body, such as precipitation, temperature, wind speed, and solar radiation, which impact processes like evaporation, mixing, and thermal stratification.

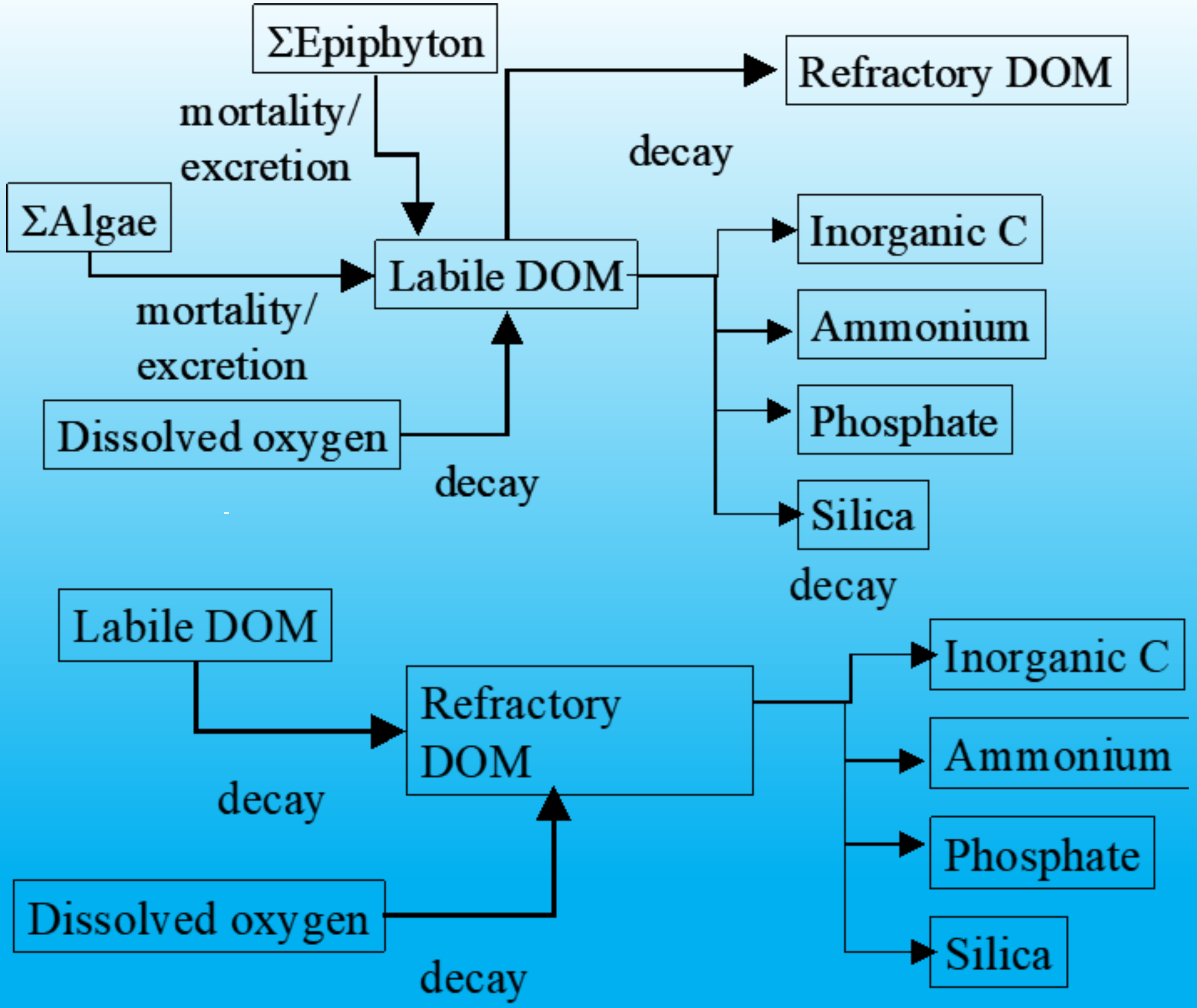
Initial Conditions

- Initial conditions describe the state of the water body at the start of the simulation. They provide a baseline from which the model begins to simulate changes over time.
- These are often obtained from the observed time series data that provide the boundary conditions throughout the model simulation.
- Examples:
  - Initial water surface elevation
  - Initial reservoir inflow and outflow
  - Initial vertical water temperature profiles
  - Initial longitudinal temperature gradient
    - Average temperature of each cross-section
  - Initial algae concentrations

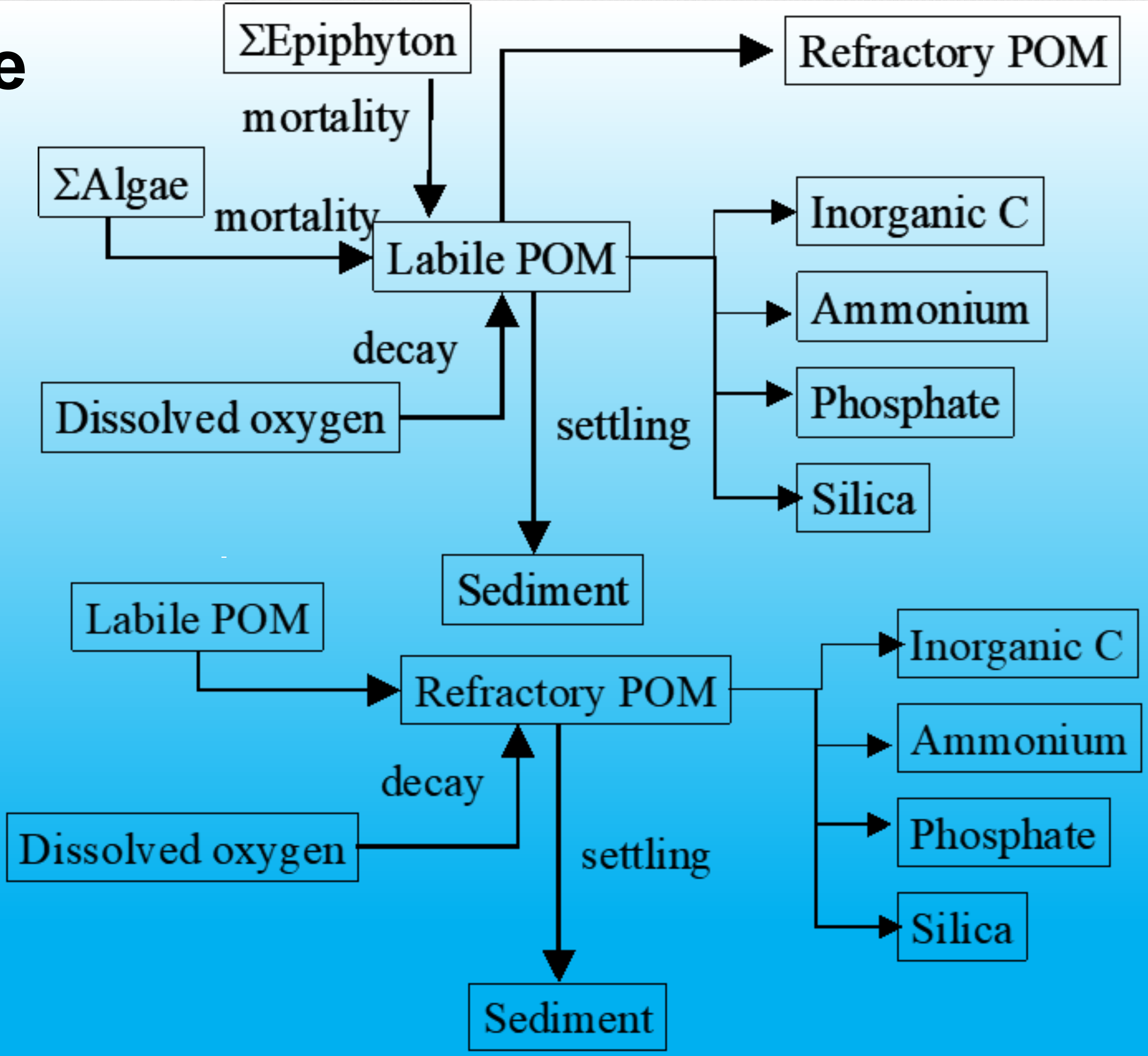
CE-QUAL-W2 Water Quality

- 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

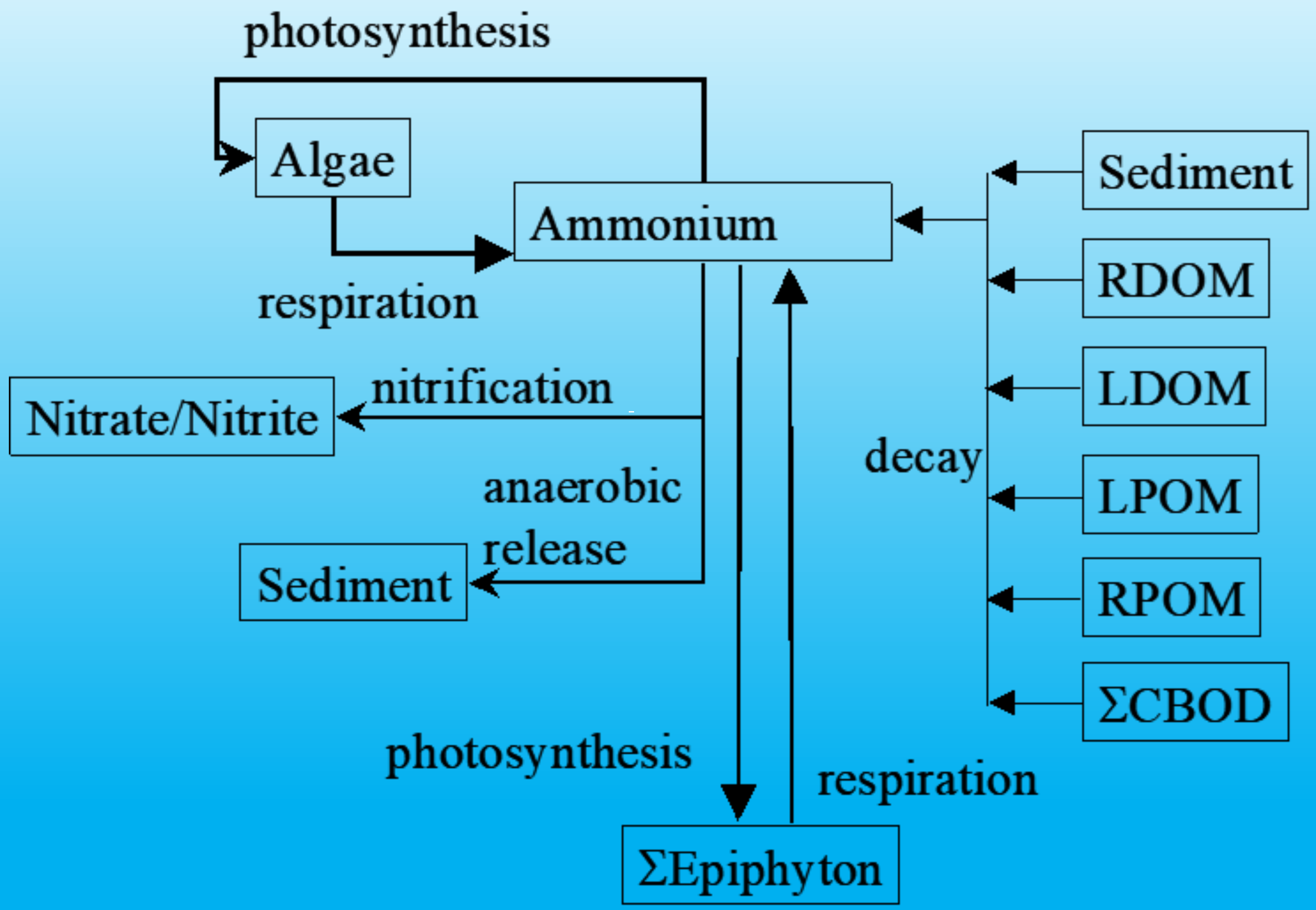
CE-QUAL-W2 Dissolved Organic Matter (DOM)



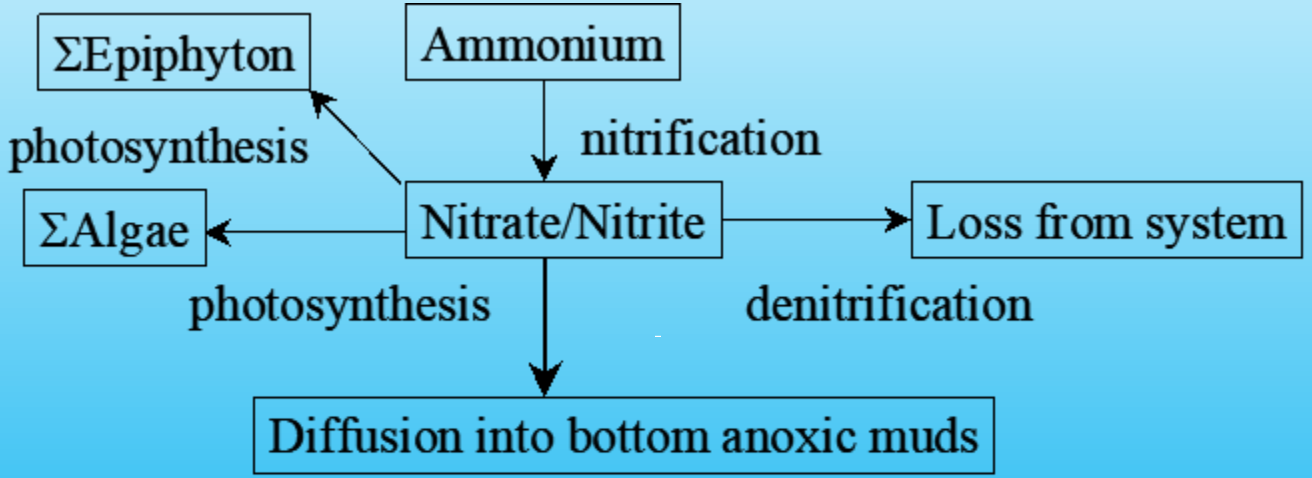
CE-QUAL-W2 Particulate Organic Matter (POM)



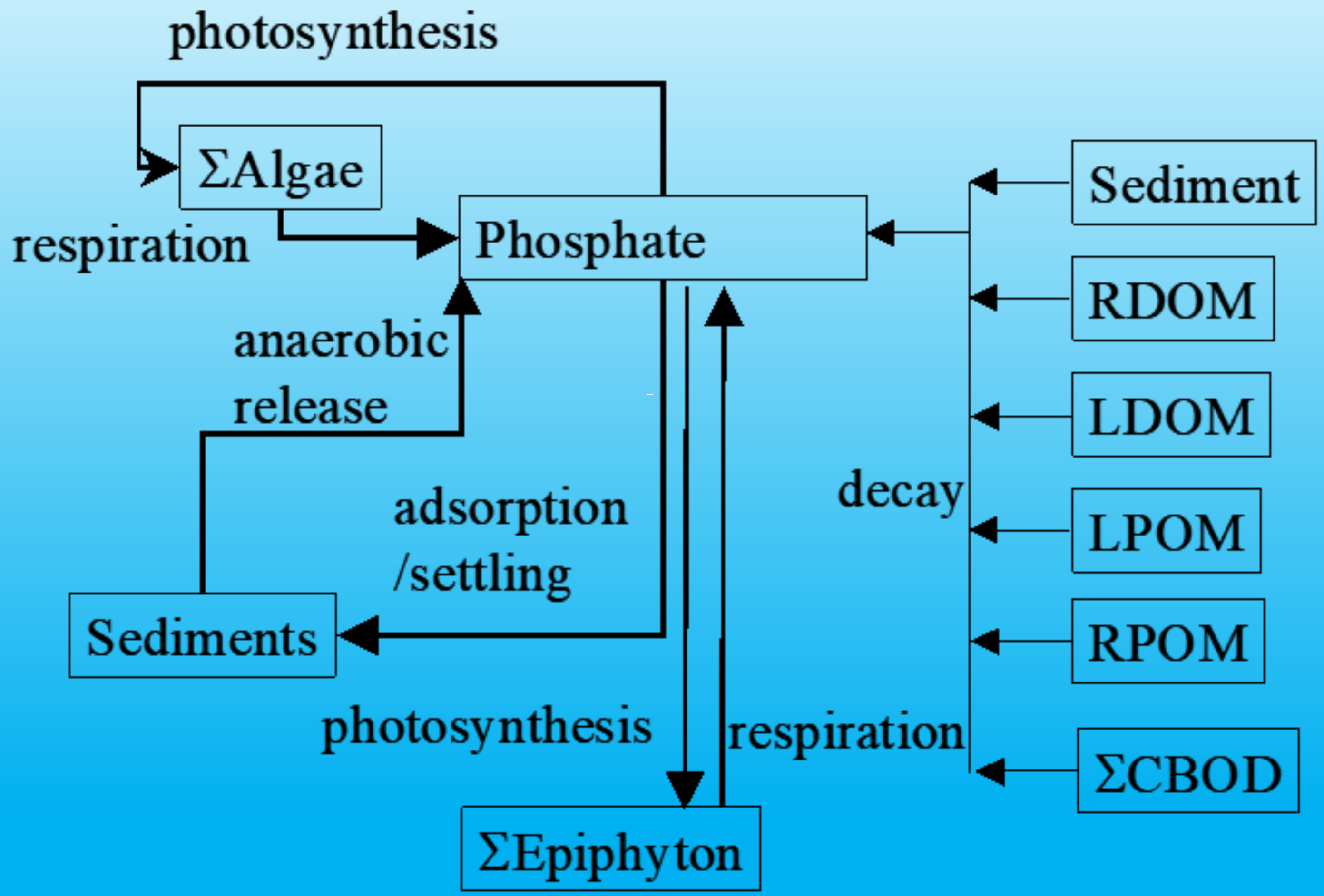
CE-QUAL-W2 Ammonium



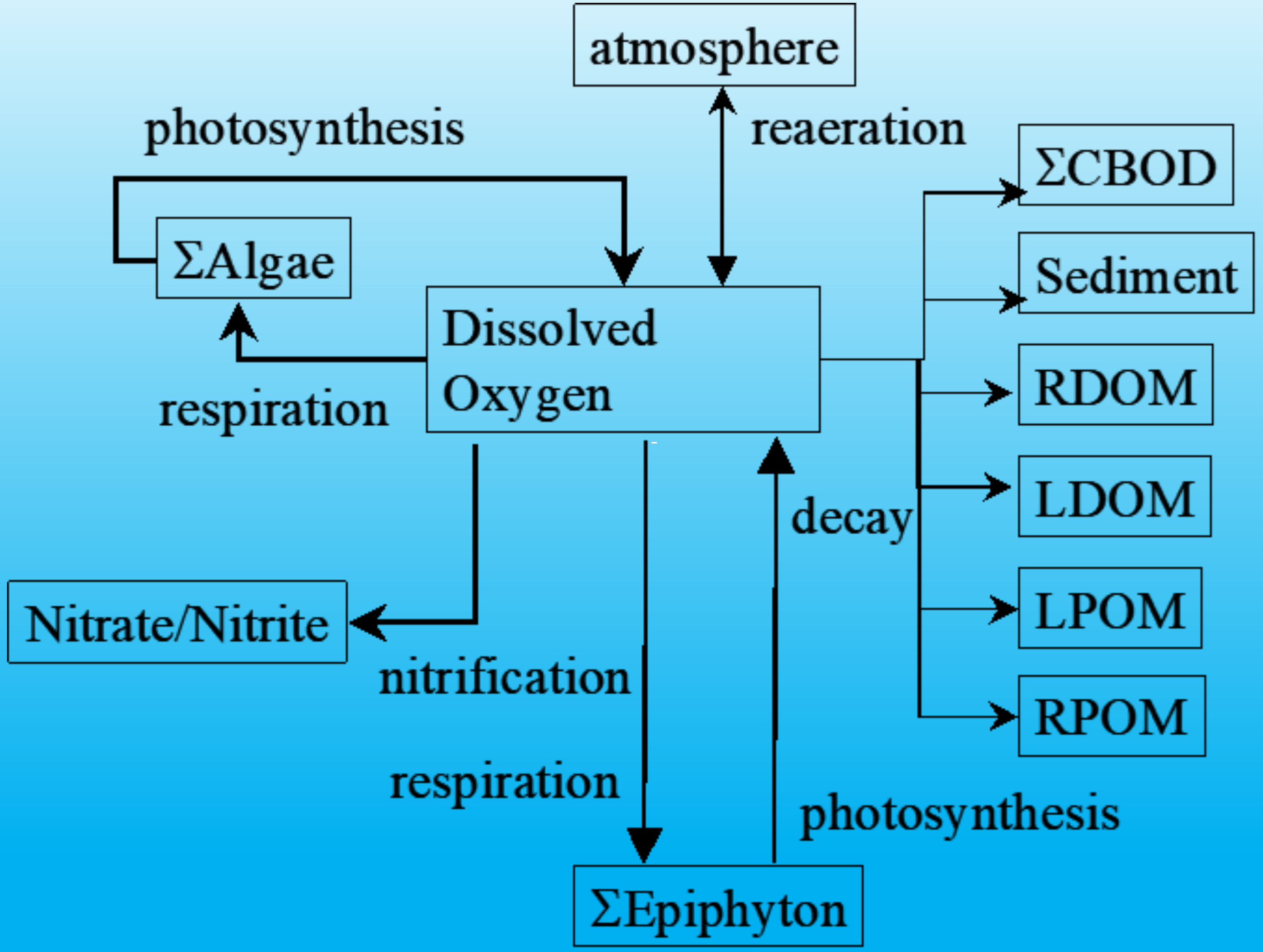
CE-QUAL-W2 Nitrate/Nitrite



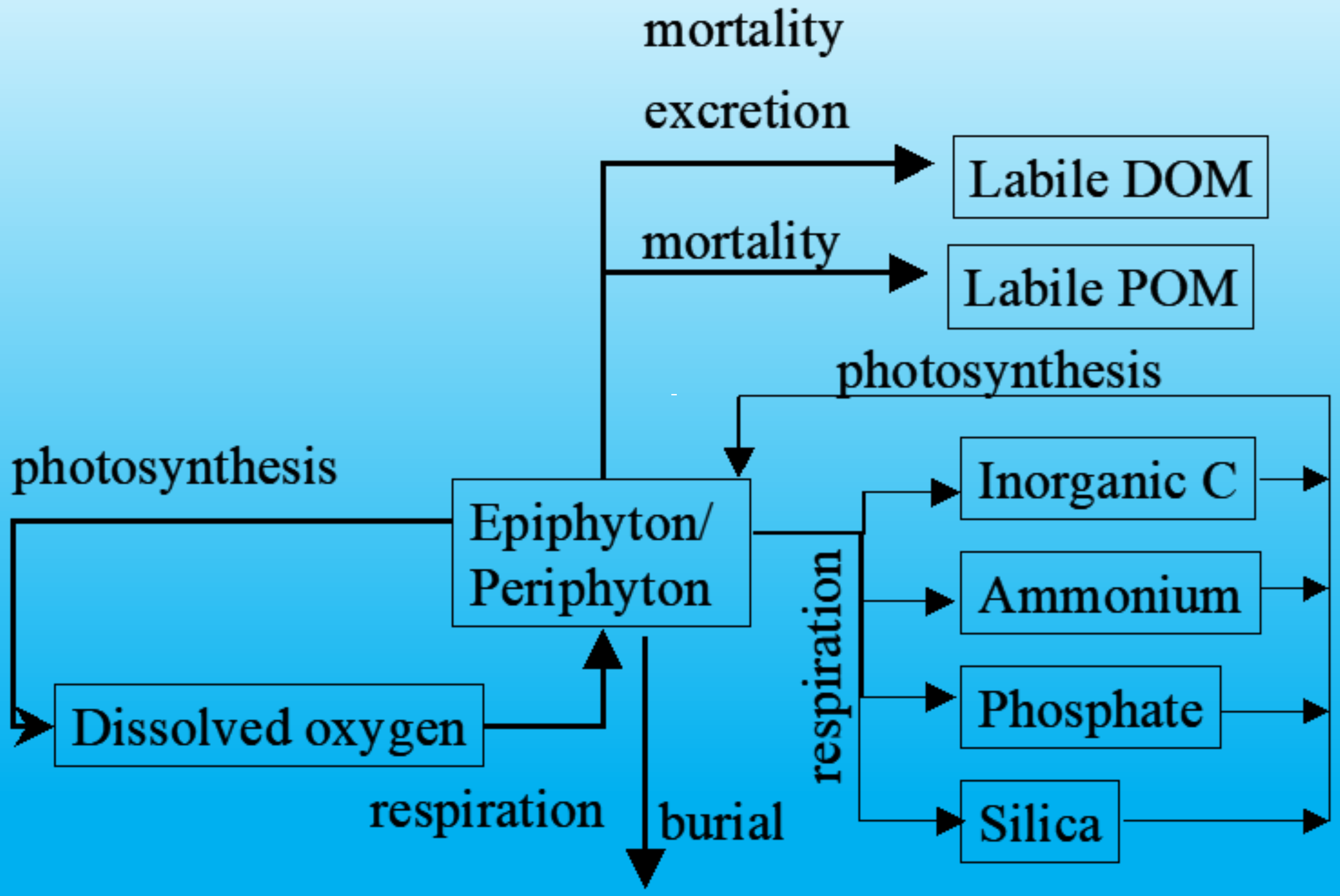
CE-QUAL-W2 Phosphate



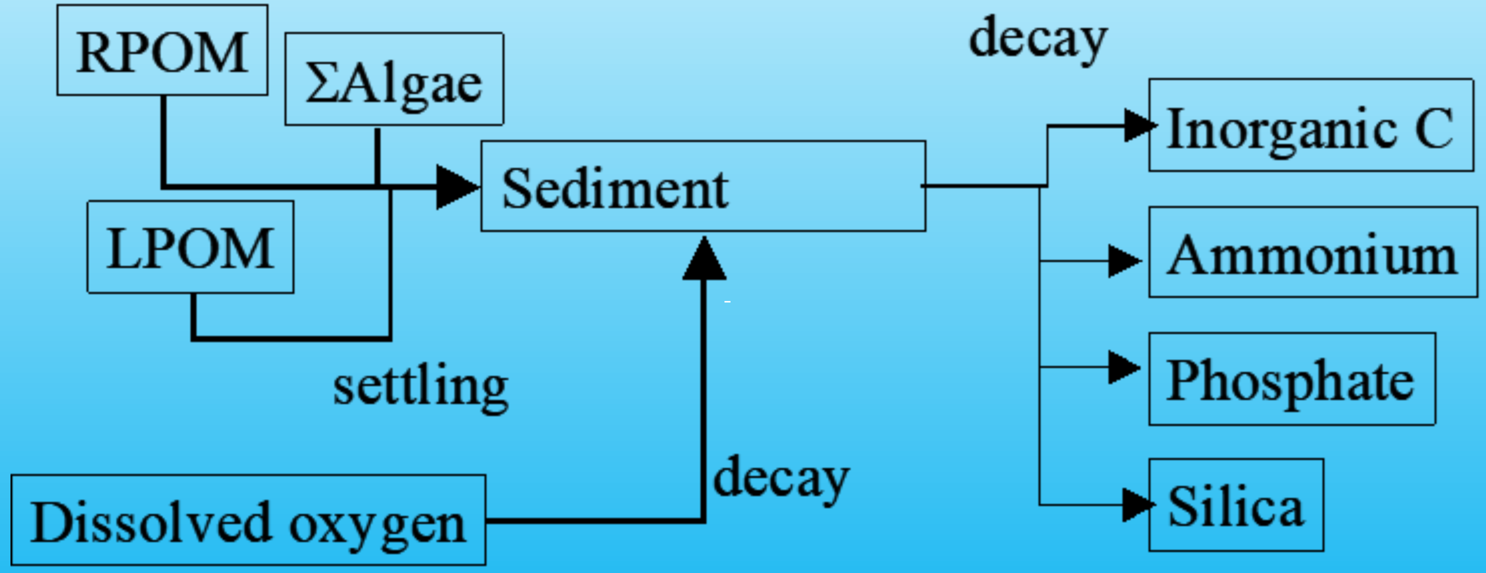
CE-QUAL-W2 Dissolved Oxygen (DO)



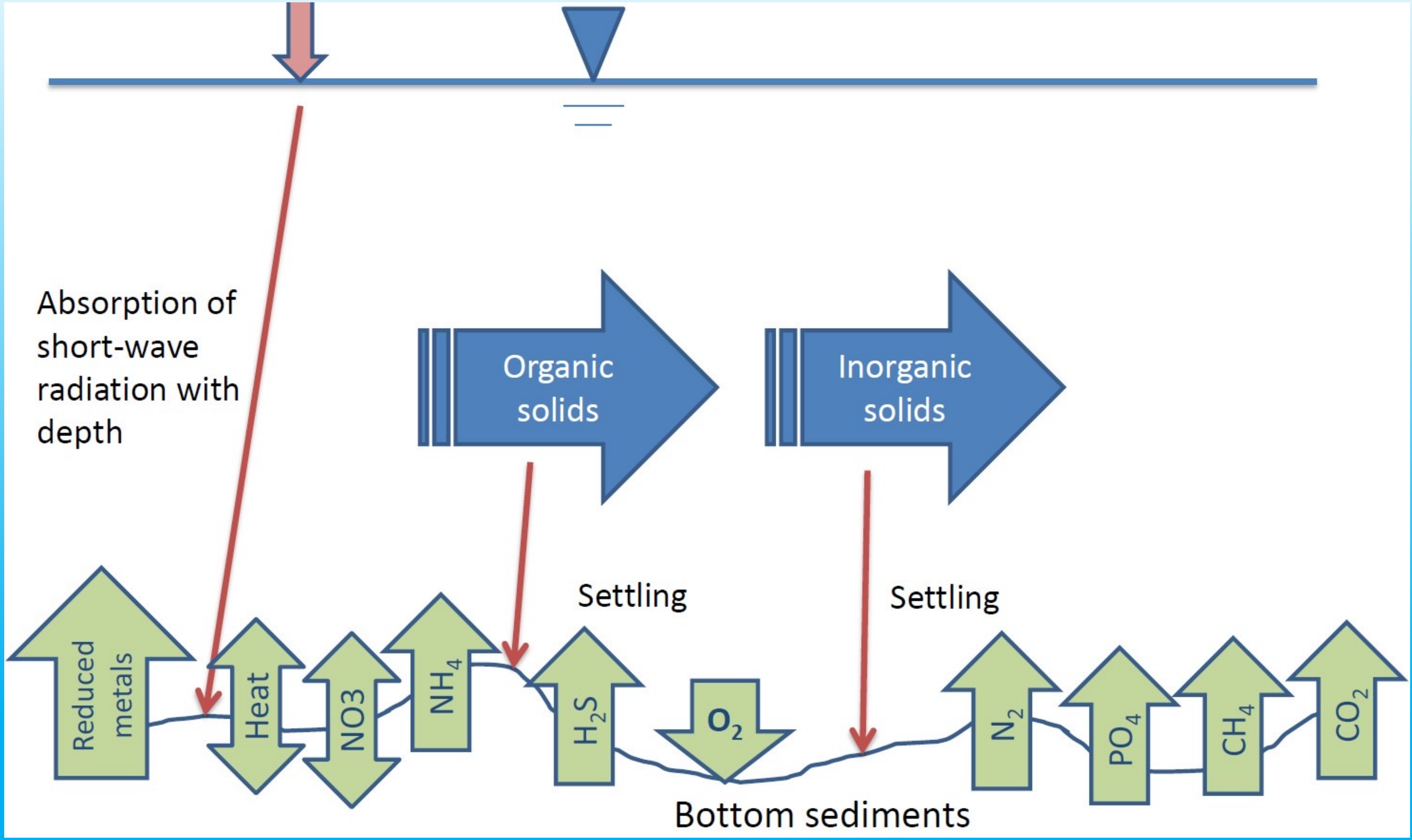
CE-QUAL-W2 Algae



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:

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

Data Limitations

- Availability and Quality of Data:
  - Insufficient Data: Lack of historical or real-time data for model calibration and validation.
  - Data Quality: Inaccuracies and inconsistencies in data collection methods, leading to unreliable inputs.
  - Spatial and Temporal Resolution: Inadequate resolution of data to capture local variations and short-term dynamics.
- Missing Data: Gaps in data records can impede the development of accurate models.

Model Complexity and Assumptions

- Simplified Representations:
  - Models often simplify complex physical, chemical, and biological processes, which can lead to oversimplification and loss of important details.
  - Assumptions and approximations may not always reflect real-world conditions accurately.
- Parameter Estimation:
  - Difficulty in accurately estimating model parameters due to variability and uncertainty in natural systems.
  - Sensitivity of models to parameter values can lead to significant variations in output.

Questions?