Intro to Water Quality Modeling

Tim A. Wool
US EPA – Region 4
Atlanta, GA
wool.tim@epa.gov

Why Do We Model?

- Link a Stressor (Nutrients) to Response
  - Biomass
  - Dissolved Oxygen
  - pH
- Interpolate
  - What We Know to Don't Know
  - Response to Management Scenarios

Model Considerations

- What Questions?
- Model Selection
  - Model Familiarity
  - Training
  - Data Requirements

Model Selection

- Type of Waterbody
  - Rivers
    - Critical Condition
      - 7Q10 Flows
  - Lakes
    - Critical Conditions
      - Parameter Specific (seasonal, etc.)
  - Estuaries
    - Critical Conditions
      - Specific Tide
      - Freshwater Inflows
      - Seasonal

Model Selection

- Water Quality Standard
  - Never to Exceed a value
  - Never to Exceed a value x% of the Time
  - Daily Average of 5 mg/l No Less than 4 mg/l Ever
- Pollutant Source
  - Point Source Discharge
    - Steady Load
    - Permit Limits
  - Nonpoint Source
    - Unsteady Load
      - Function of Rainfall
    - Groundwater-Surface Water Interaction
    - Atmospheric Deposition

Model Selection

- Pollutant/Parameter
  - Conservative Process
  - Dissolved Oxygen
  - Nutrients – Chlorophyll
  - Bacteria
  - Temperature
  - Metals
  - Toxicants

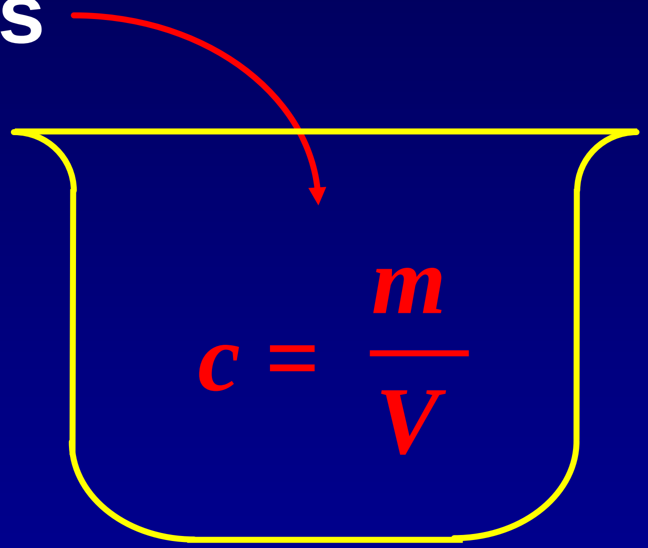
Model Selection

- Temporal Scale
  - Steady-State
  - Dynamic
- Spatial Scale
  - River Segment
  - Whole Watershed
- Available Data
  - No Data
  - Limited Data

Model Principles

Mass and Concentration

m = mass



$$c = \frac{m}{V}$$

V = volume

units: $\frac{M}{L^3}$

Assimilation Factor

$$c = \frac{1}{a} W$$

$$\xrightarrow{W} \quad \frac{1}{a} \quad \xrightarrow{c}$$

stimulus → system → response

physics, chemistry, biology

Modeling Modes

Simulation Mode: Given load (W) and assimilation factor (a), calculate

$$c = \frac{1}{a} W$$

Assimilative Capacity Design Model: Given desired concentration (c) and assimilation factor (a), calculate

$$W = a\,c$$

Environmental Modification Design Mode: Given desired concentration (c) and load (W), calculate

$$a = \frac{W}{c}$$

How Do We Determine "a" ?

"a"?

EMPIRICAL
Data-based
(Inductive)
Model

MECHANISTIC
Theory-based
(Deductive)
Model

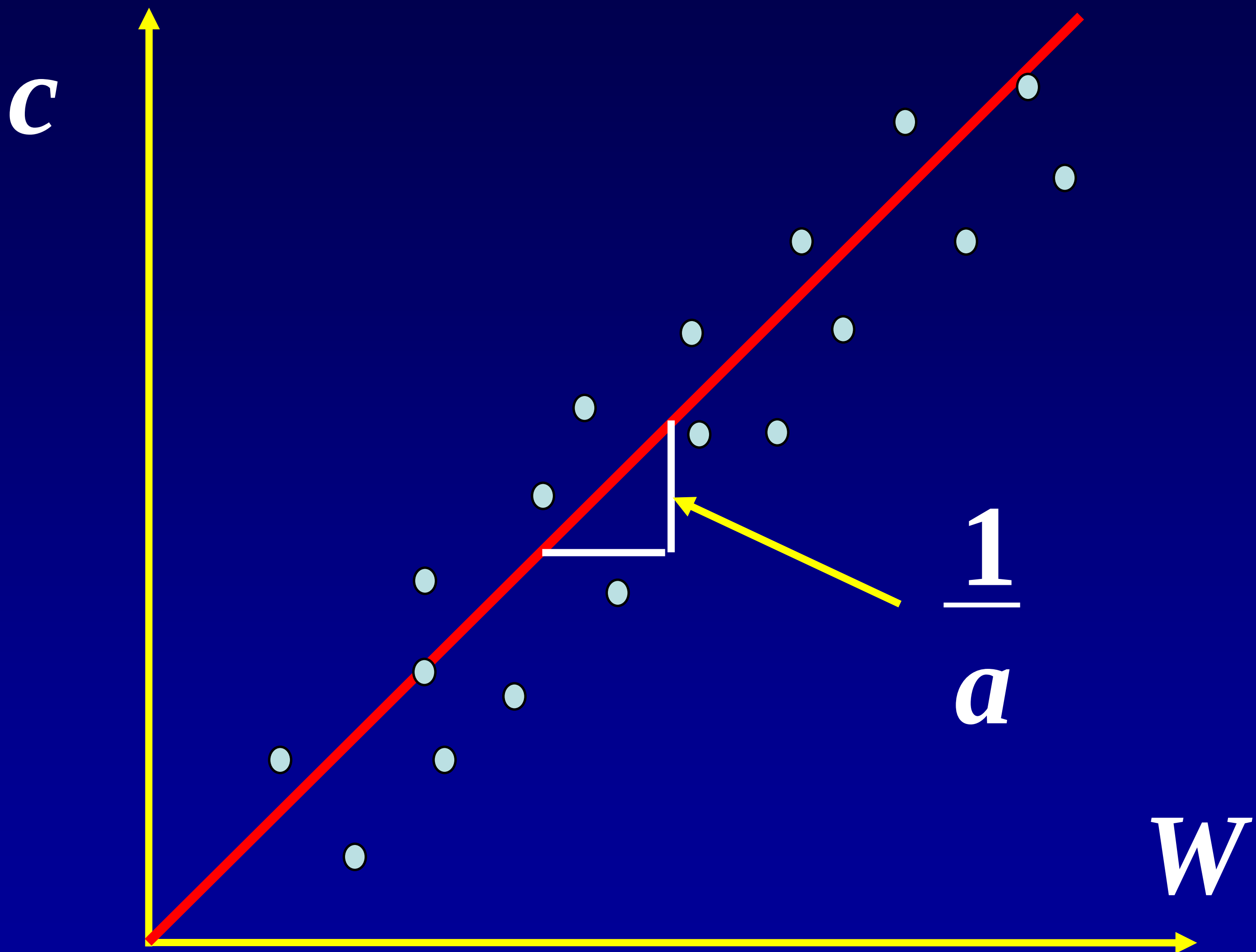
Steady-state & Transient Solutions

	Accumulation	Mass
Steady State		
sources = sinks	0	constant
Transient		
sources > sinks	+	increases
sources < sinks	-	decreases

Model Approaches

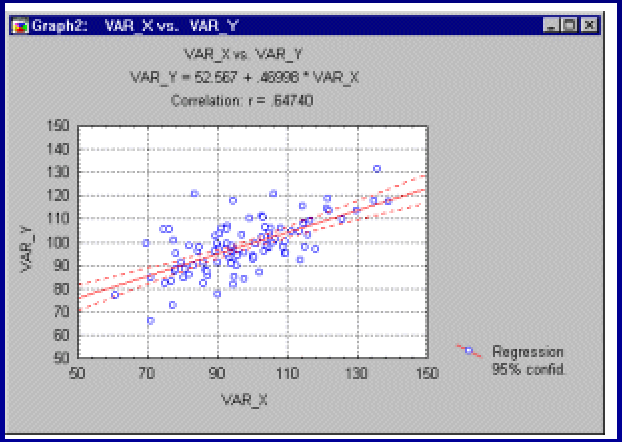
Statistical

Empirical Models



Multiple Regression

- Multiple linear regression attempts to model the relationship between two or more explanatory variables and a response variable by fitting a linear equation to observed data.



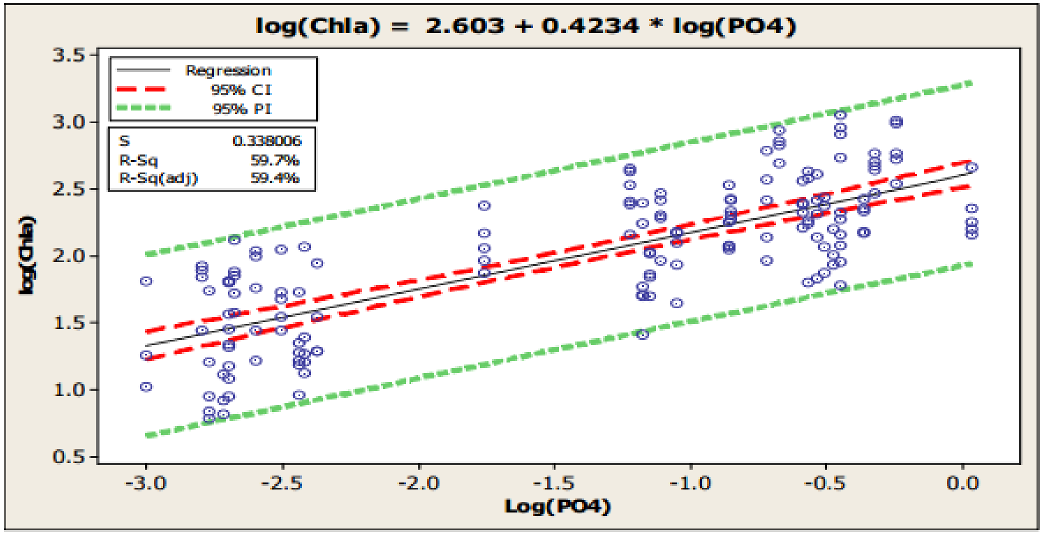


Figure 5-5: Periphyton and PO4-P Regression in the Jackson River

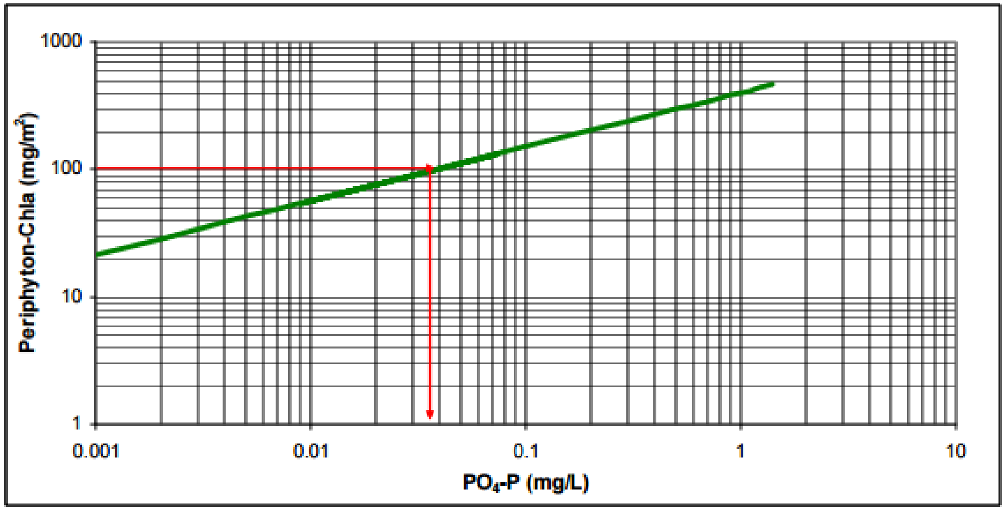
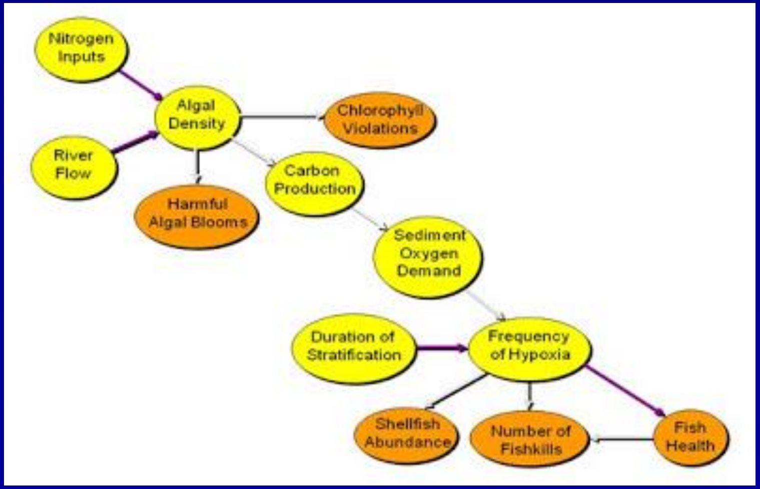


Figure 5-6: Periphyton-PO4-P Regression and TMDL Endpoint in the Jackson River

Bayesian Analysis

- Bayesian statistics is a subset of the field of statistics in which the evidence about the true state of the world is expressed in terms of degrees of belief or, more specifically, Bayesian probabilities. Such an interpretation is only one of a number of interpretations of probability and there are other statistical techniques that are not based on "degrees of belief".



Statistical -- Regression

Pro's

- Easily done
- Links stressors to response variables
- Uses site specific data for the waterbody

Con's

- May not account for all response variables
- Constrained by the data availability
- Confidence in the statistical fit
- Difficult to extrapolate to other conditions
- May not protect downstream

Model Approaches

Mechanistic

Mechanistic Models

- Mechanistic Models are based on:
  - Fundamental equations that produce physical/chemical/biological responses based on stressors (temporal and spatial)
  - Many of the fundamental relationship were developed using direct observation

Utility of Mechanistic Models

- Simplistic Representation of Reality
  - Cannot Simulate “Everything”
  - All Models are Wrong . . . .
- Interpolate
  - Known and Unknown
- Provides Linkage between
  - Loads and Response Variables
- Can Determine Important Processes
  - Nutrients/DO/Algae/Light
  - Management Strategies
- Determine Load Reductions to meet WQS
  - Never to Exceed
  - X% Exceedence
  - Duration, Frequency and Magnitude
- Evaluate Best Management Practices

Types of Mechanistic Models

- Landscape/Loading models
  - Runoff of water and dissolved materials on and through the land surface
  - Erosion of sediment and associated constituents from the land surface
- Receiving water models
  - Flow of water through streams and into lakes and estuaries
  - Transport, deposition, and transformation in receiving waters
  - Nutrient Expression (Chla, Periphyton, DO, SOD, etc.)
- Linked models
  - Combination of landscape and receiving water models

Using Mechanistic Models for TMDL

- Critical Conditions (Steady State)
  - Typically used for criteria development
- Nutrients
  - Usually not a critical condition
  - Seasonal Variation
  - Need to consider varying meteorological conditions
    - Low/Ave/High Flow years
    - Long-term Continuous Simulation
    - Should allow perturbations

Mechanistic Modeling

Pro's

- Linkage between stressors and response variables
  - Chlorophyll a (algae, benthic algae, macrophytes)
  - Light
  - Dissolved Oxygen
- Can Extrapolate
  - Environmental Conditions
  - Current vs. WQS Condition
  - Response in Time
  - Duration and Frequency

Con's

- Time consuming
- Costly
- Can be misapplied

Model Framework Considerations

- Public Domain
  - Share with Stakeholders
  - External Reviews
- Proven Record
  - Other Successful Applications
  - Publications
- Users Manual/Tutorials
- Training/Technical Support
- Peer Reviewed

●	Watershed
●	Receiving Water
◉	Ecology
○	Air
◉	Groundwater

BASINS

- BASINS -- EPA's Office of Water/ORD
  - A multipurpose environmental analysis system designed for use by regional, state, and local agencies in performing watershed and water quality-based studies
  - BASINS works with a geographic information system (GIS) framework and consists of:
    - National databases
    - Assessment tools
    - Watershed delineation tool
    - Classification utilities
    - Characterization reports
    - Watershed loading and transport models (HSPF, SWAT, SWMM, PLOAD)
    - Water quality models (WASP, AQUATOX)
    - Data Download (NHDPlus, USGS NWIS, STORET, NLCD, NALDAS)

HSPF

●	Watershed
◉	Receiving Water
○	Ecology
○	Air
◉	Groundwater

- Most Widely Used
- Detailed watershed simulation model
- Watershed hydrology
- Runoff/sediment/pollutant generation and transport
- One-dimensional stream hydrology and transport
- Pesticide fate and transport simulation

LSPC

●	Watershed
◉	Receiving Water
○	Ecology
○	Air
◉	Groundwater

- The Loading Simulation Program in C++ (LSPC) is a watershed modeling system that includes streamlined Hydrologic Simulation Program FORTRAN (HSPF) algorithms for simulating hydrology, sediment, and general water quality on land as well as a simplified stream transport model. It is a EPA-accepted TMDL modeling application, developed by Tetra Tech, Inc., partially under contract with EPA. A key advantage of LSPC is that it has no inherent limitations in terms of modeling size or model operations and has been applied to large, complex watersheds. In addition, the Microsoft Visual C++ programming architecture allows for seamless integration with modern-day, widely available software such as Microsoft Access and Excel.

●	Watershed
◉	Receiving Water
◉	Ecology
○	Air
◉	Groundwater

SWAT

- SWAT is a river basin, or watershed, scale model developed
  - SWAT was developed to predict the impact of land management practices on water, sediment, and agricultural chemical yields in large complex watersheds with varying soils, land use, and management conditions over long periods of time.
  - The model is physically based and computationally efficient; it uses readily available inputs and allows users to study long-term impacts.
  - SWAT is a continuous time model (i.e., a long-term yield model). The model is not designed to simulate detailed, single-event flood routing.

SWMM

●	Watershed
◉	Receiving Water
○	Ecology
○	Air
◉	Groundwater

- SWMM is a dynamic rainfall-runoff simulation model developed by EPA.
  - It is applied primarily to urban areas and for single-event or long-term (continuous) simulation using various timesteps
  - It was developed for the analysis of surface runoff and flow routing through complex urban sewer systems.
  - Flow routing is performed for surface and sub-surface conveyance and groundwater systems, including the options of nonlinear reservoir channel routing and fully dynamic hydraulic flow routing. In the fully dynamic hydraulic flow routing option, SWMM simulates backwater, surcharging, pressure flow, and looped connections.
  - SWMM has a variety of options for quality simulation, including traditional buildup and washoff formulation as well as rating curves and regression techniques.
  - Universal Soil Loss Equation (USLE) is included to simulate soil erosion.
  - SWMM incorporates first order decay and particle settling mechanism in pollutant transport simulations and includes an option of simple scour-deposition routine.
  - Storage, treatment, and other BMPs can also be simulated.

Bathtub

- Simulates steady-state flow and transport conditions in lakes and reservoirs
  - Simulates eutrophication related conditions within the water body
  - Eutrophication can be defined as the nutritional enrichment of water bodies leading to an excessive production of organic materials by algae and/or aquatic plants.
- Performs steady-state water and nutrient balances for spatially segmented hydraulic networks
  - Accounts for advective and diffusive transport, and nutrient sedimentation
  - Predicts water quality conditions including total phosphorus, total nitrogen, chlorophyll-a, transparency, and hypolimnetic oxygen depletion
  - These are all related to eutrophic condition

Time	Dimension	Diel	DO	Nutrients	Algae	Benthic Algae	Macro Algae	Light	pH/Alk	Temp	Sediment Diagenesis	Sediment Transport	Toxicants	Metals	Mercury	Bacteria
SS	1-D			TP	●											

CE-QUAL-ICM

- CE-QUAL-ICM is a flexible, multi-dimensional water quality model developed by the ERDC Environmental Laboratory and suited for application in lakes, rivers, estuaries and coastal waters.
- ICM represents multiple biogeochemical cycles, including the aquatic carbon cycle, nitrogen cycle, phosphorus cycle and oxygen cycle.
- ICM also simulates physical factors, including salinity, temperature and suspended solids. The structure allows variables to be activated or inactivated and facilitates the addition of specific features required by individual projects.

Time	Dimension	Diel	DO	Nutrients	Algae	Benthic Algae	Macro Algae	Light	pH/Alk	Temp	Sediment Diagenesis	Sediment Transport	Toxicants	Metals	Mercury	Bacteria
TV	1/2/3-D	●	●	N/P/Si	●	●	●	●	●	●	●	●				

CE-QUAL-W2

- CE-QUAL-W2 is a two-dimensional, longitudinal/vertical, hydrodynamic and water quality model. Because the model assumes lateral homogeneity, it is best suited for relatively long and narrow waterbodies exhibiting longitudinal and vertical water quality gradients. The model has been applied to rivers, lakes, reservoirs, and estuaries.
- Model capabilities:
  - Hydrodynamic. The model predicts water surface elevations, velocities, and temperatures. Temperature is included in the hydrodynamic calculations because of its effect on water density
  - Water quality. The water quality algorithms incorporate 21 constituents in addition to temperature including nutrient/phytoplankton/dissolved oxygen (DO) interactions during anoxic conditions. Any combination of constituents can be simulated. The effects of salinity or total dissolved solids/salinity on density and thus hydrodynamics are included only if they are simulated in the water quality module.

Time	Dimension	Diel	DO	Nutrients	Algae	Benthic Algae	Macro Algae	Light	pH/Alk	Temp	Sediment Diagenesis	Sediment Transport	Toxicants	Metals	Mercury	Bacteria
TV	1/2/3-D	●	●	N/P/Si	●	●				●		●				

EFDC

- EFDC is a 2-D/3-D orthogonal curvilinear grid hydrodynamic model.
- EFDC can solve for the circulation and transport of material in complex environments including, estuaries, coastal embayments, lakes and offshore.
- EFDC Model Includes Internally Linked
  - Hydrodynamics
  - Water Quality
  - Sediment Transport and Toxic Transport & Fate
- EFDC-Hydro Can Be Linked to WASP and CE-QUAL-ICM

Time	Dimension	Diel	DO	Nutrients	Algae	Benthic Algae	Macro Algae	Light	pH/Alk	Temp	Sediment Diagenesis	Sediment Transport	Toxicants	Metals	Mercury	Bacteria
TV	1/2/3-D	●	●	N/P/Si	●			●		●		●	●			

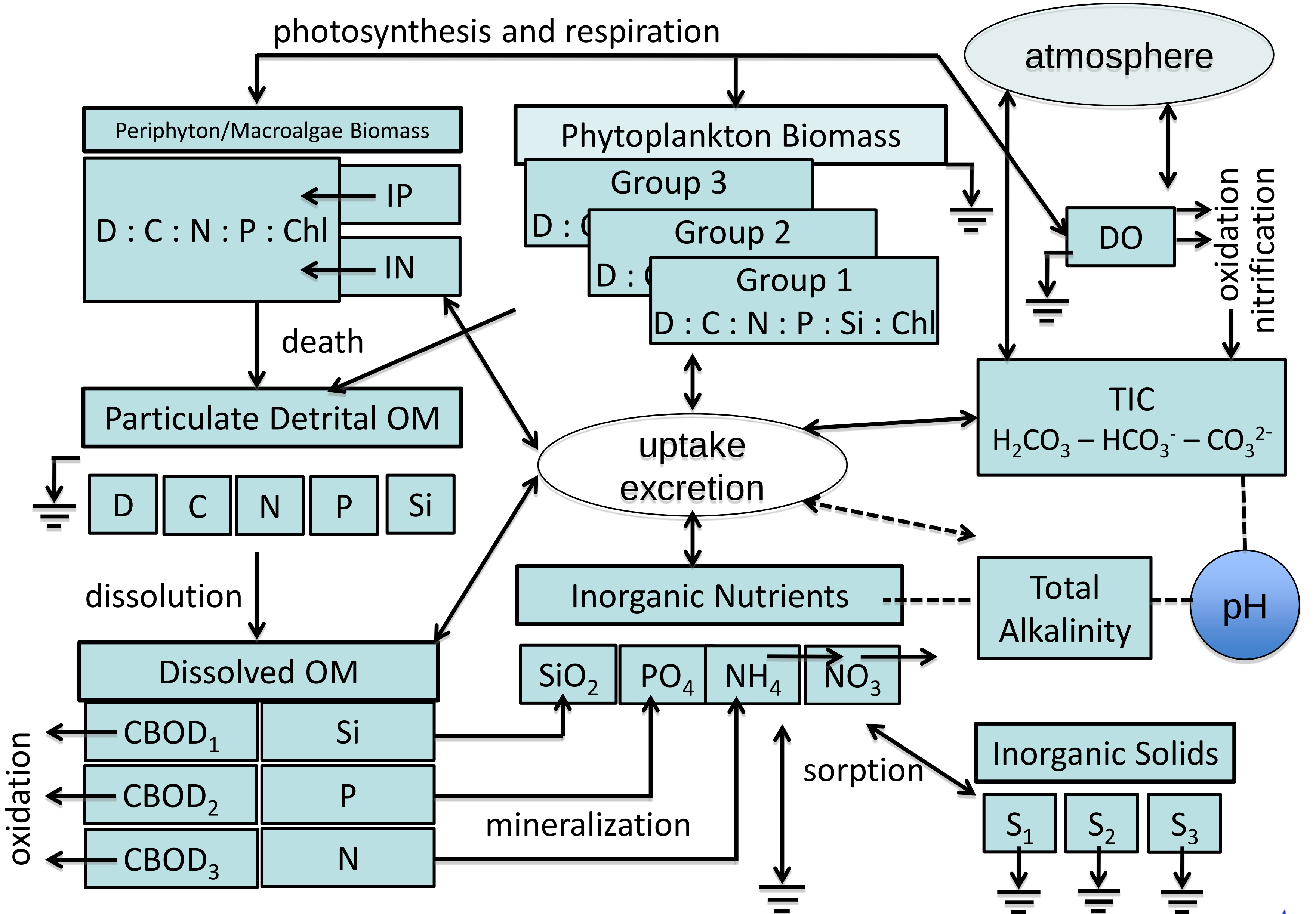
QUAL2K/Kw

- The QUAL2K model simulates nutrient dynamics, algal production, and dissolved oxygen with the impact of benthic and carbonaceous demand in streams.
- QUAL2K is similar to QUAL2E but QUAL2K is enhanced with two species of CBOD and internal sediment processes.
  - In addition, QUAL2K models pH and alkalinity.
  - The pathogen die-off is modeled as a function of temperature, light intensity, and settling.

WASP

- WASP is a generalized modeling framework based on the finite-volume concept for quantifying fate and transport of water quality variables in surface waters.
- Multiple Modules:
  - Advanced Eutrophication (Nutrients, DO, Algae, Benthic Algae, Macro Algae, CBODs, pH/Alk, Temperature, Bacteria)
  - Organic Chemical/Nano Materials (chemicals & solids)
  - Metal Speciation
  - Mercury

Time	Dimension	Diel	DO	Nutrients	Algae	Benthic Algae	Macro Algae	Light	pH/Alk	Temp	Sediment Diagenesis	Sediment Transport	Toxicants	Metals	Mercury	Bacteria
TV	1/2/3-D	●	●	N/P/Si	●	●	●	●	●	●	●	●	●	●	●	●


photosynthesis and respiration
atmosphere
Periphyton/Macroalgae Biomass
D : C : N : P : Chl
IP
IN
Phytoplankton Biomass
Group 3
Group 2
Group 1
D : C : N : P : Si : Chl
DO
oxidation
nitrification
death
Particulate Detrital OM
D
C
N
P
Si
uptake
excretion
TIC
H2CO3 – HCO3- – CO32-
dissolution
Inorganic Nutrients
Total Alkalinity
pH
Dissolved OM
SiO2
PO4
NH4
NO3
CBOD1
CBOD2
CBOD3
Si
P
N
oxidation
sorption
mineralization
Inorganic Solids
S1
S2
S3

TMDL/WQ Endpoints

- Biomass/Concentration (Algae, Periphyton, Macrophytes)
- Dissolved Oxygen
- pH
- Light
- Community Shifts

Questions ?