Modeling 101 for TMDLs

Overview of modeling fundamentals and application

National 303(d) Training Workshop

June 2, 2025

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EPA's Water Modeling Workgroup

Informal Water Modeling Workgroup (WMW) Started in 2014

Officially chartered in 2017 by ORD, OW, Lead Region Water Director

Webinars

- 2015-Present, 40 webinars
- >10,000 Attendees, >30,000 YouTube views
- https://www.epa.gov/waterdata/surface-water-quality-modeling-training

Annual Training Workshops

- Co-hosted with ACWA and EPA
- Hands-on model trainings, plus a project manager-related track

Disclaimer

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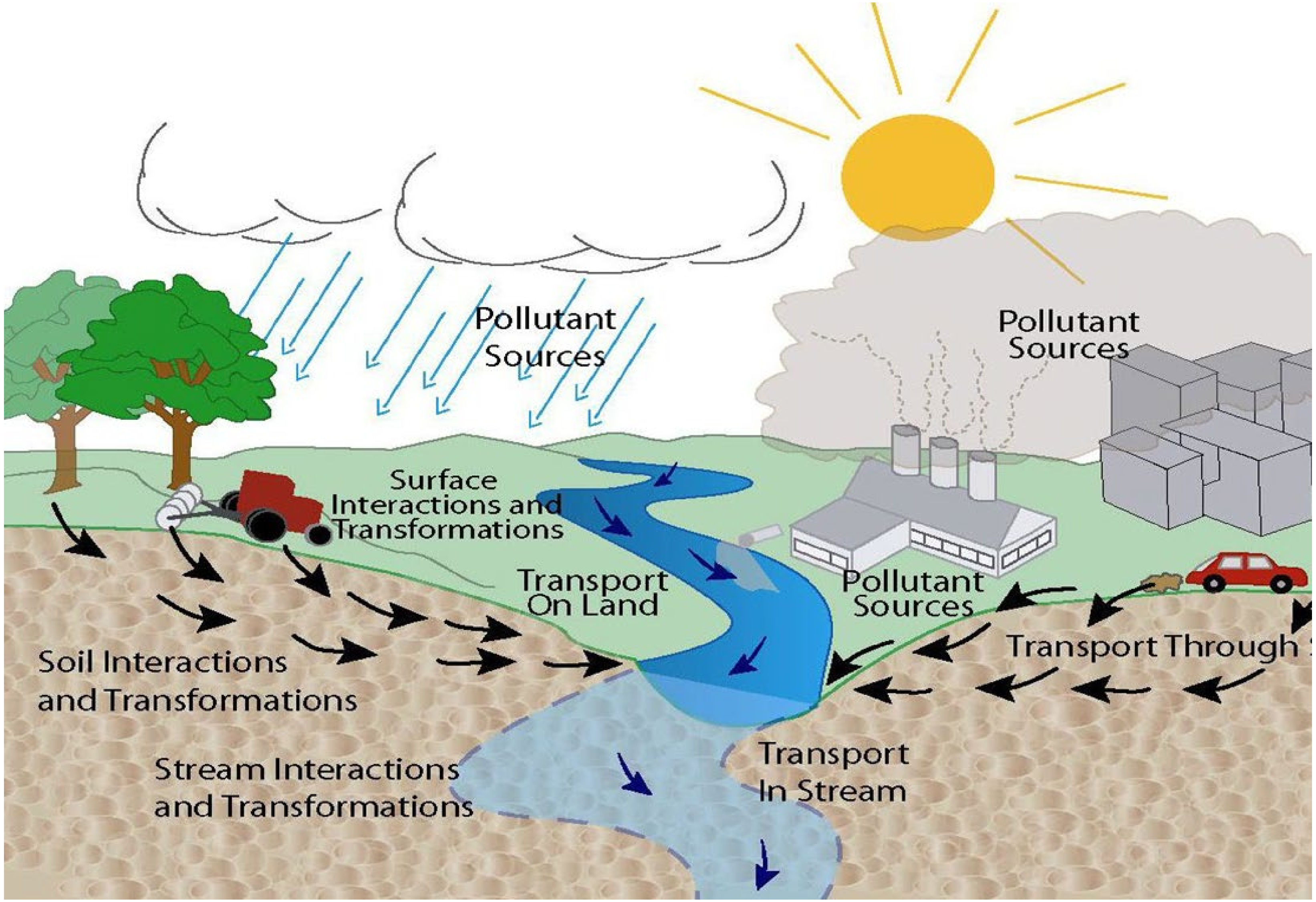
Objective

- Modeling topics
  - General modeling terminology
  - Model selection
  - Types of models
  - Crash-course in commonly used models
  - Model calibration
  - Scenario & TMDL development
  - Helpful modeling utilities
- Intended for managers & staff with limited modeling experience

Setting the Stage

What is a water quality model?

A simplified mathematical representation of pollutant fate, transport and degradation within a watershed and/or water body



Utility of models

Can be important for a variety of CWA programs

- Total maximum daily loads (TMDLs)
- Waste load allocations (WLAs)
- Numeric nutrient criteria (NNCs)
- Development of Best Management Practices (BMPs)

Limitations of models

Remember no model is perfect

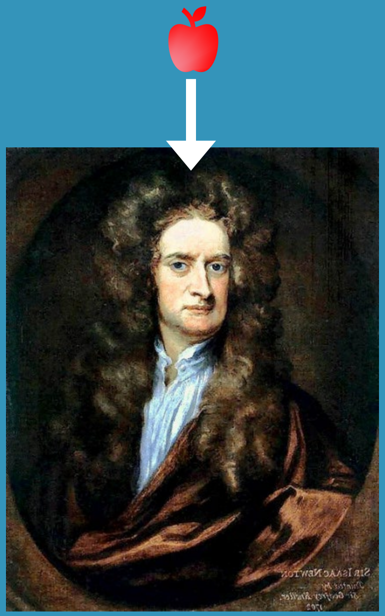
They are only as ‘good’ as their input data, assumptions, & calibration data

They are not the decision

They are a tool that can be used to make an informed decision

They must be ‘proven’ useful

It’s NOT a Black Box



Conservation of Mass

Conservation of Momentum

Conservation of Energy

Known Water Quality Processes

Checked Against Measurements

Model Selection

Model development process

Phase I
Science & Policy

Model Planning

- Problem formulation and endpoint determination
- Quality Assurance Project Plan (QAPP)
- Modeling tool selection

Phase II
Science

Model Build

- Data gathering (historic, field monitoring)
- Supplemental data collection
- Model input preparation and configuration

Phase III
Science

Model Calibration and Performance Evaluation

- Calibration (modeled vs. measured)
- Peer review
- Sensitivity/uncertainty analysis

Phase IV
Science & Policy

Model Acceptance and Application

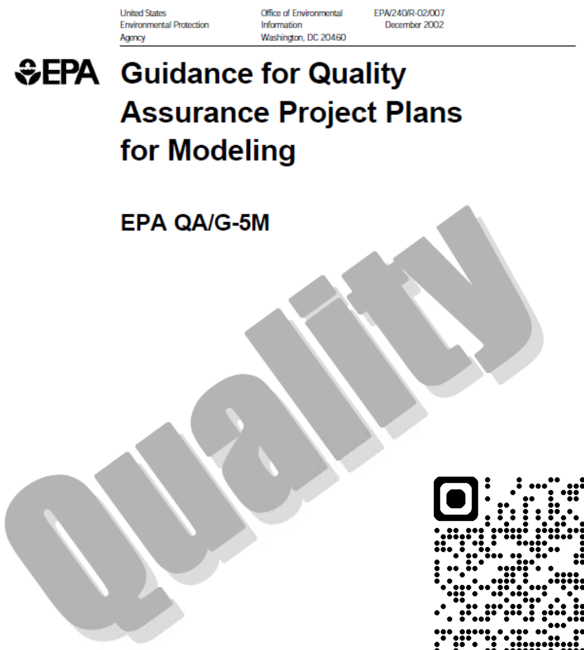
- Determination of suitability for proposed application
- Analysis of model alternatives – Compliance scenarios

Stakeholder engagement

- Model without stakeholder buy-in has limited utility
- Modeling workgroup
  - Requires representatives with high technical proficiency for meaningful feedback
- Engage/inform decision makers

Model QAPP

- Blueprint for the modeling project
  - Ensures that data and models will meet the project's overall objectives and goals
- Similar to other QAPPs, but tailored to modeling projects
- Required for EPA contracts
- Model QAPP elements
  1. Project management
  2. Measurement and data acquisition
  3. Assessment and oversight
  4. Output validation and usability

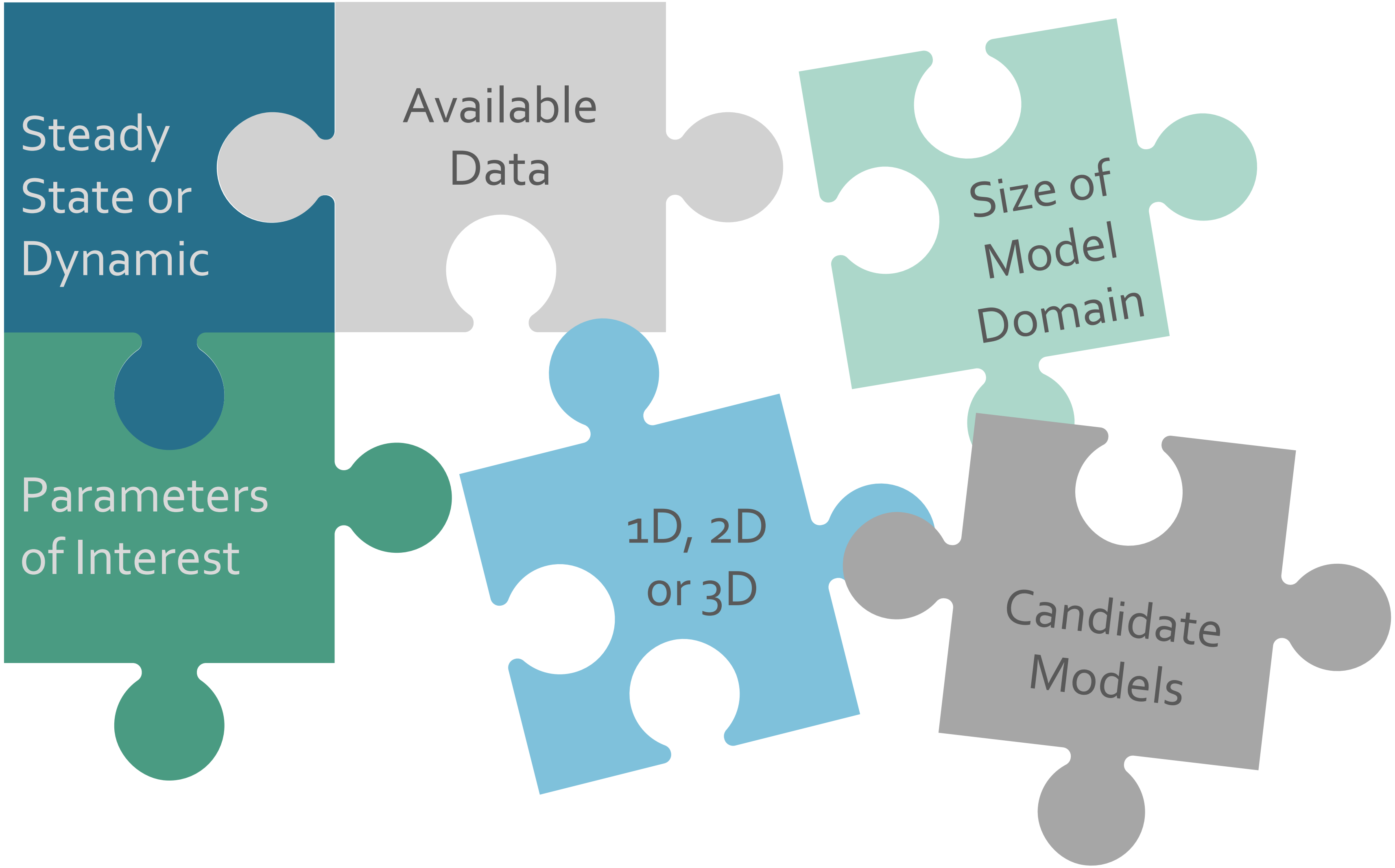

United States Environmental Protection Agency | Office of Environmental Information Washington, DC 20460 | EPA/240/R-02/007 December 2002

EPA Guidance for Quality Assurance Project Plans for Modeling

EPA QA/G-5M

QAPP

Who, what, how, and when we are going to build a model



Importance of model selection

- Your project / decision has specific requirements
- No single model can solve every problem
- A misapplied model may lead to sub-optimal decision
- Essential to understand basic concepts / processes behind models to help select the best tool for the job

Model Selection:

Problem Formulation

What are your project objectives & management decision?

What are the model endpoints & parameter(s) of concern?

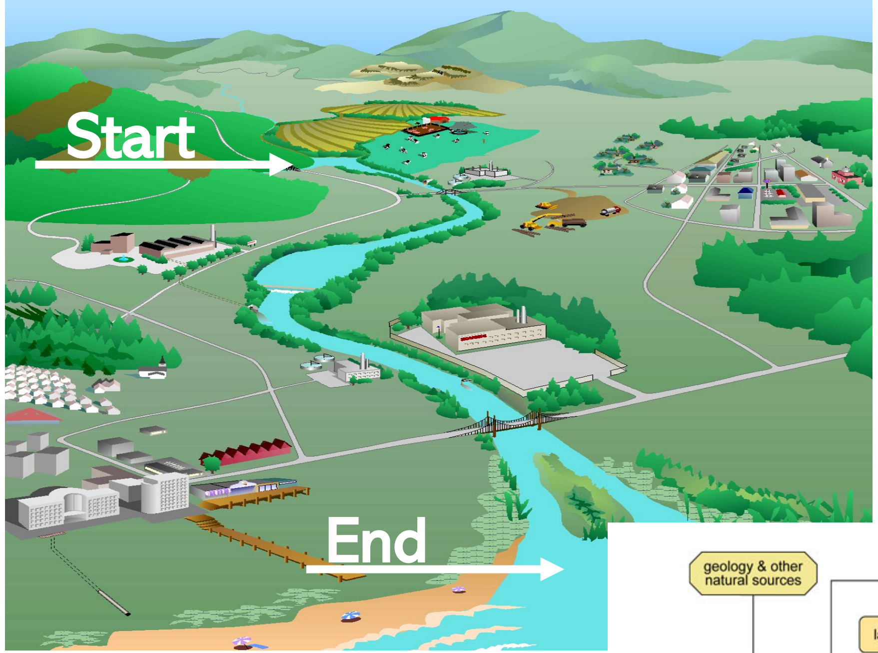
What processes are important to your system & parameter of concern?

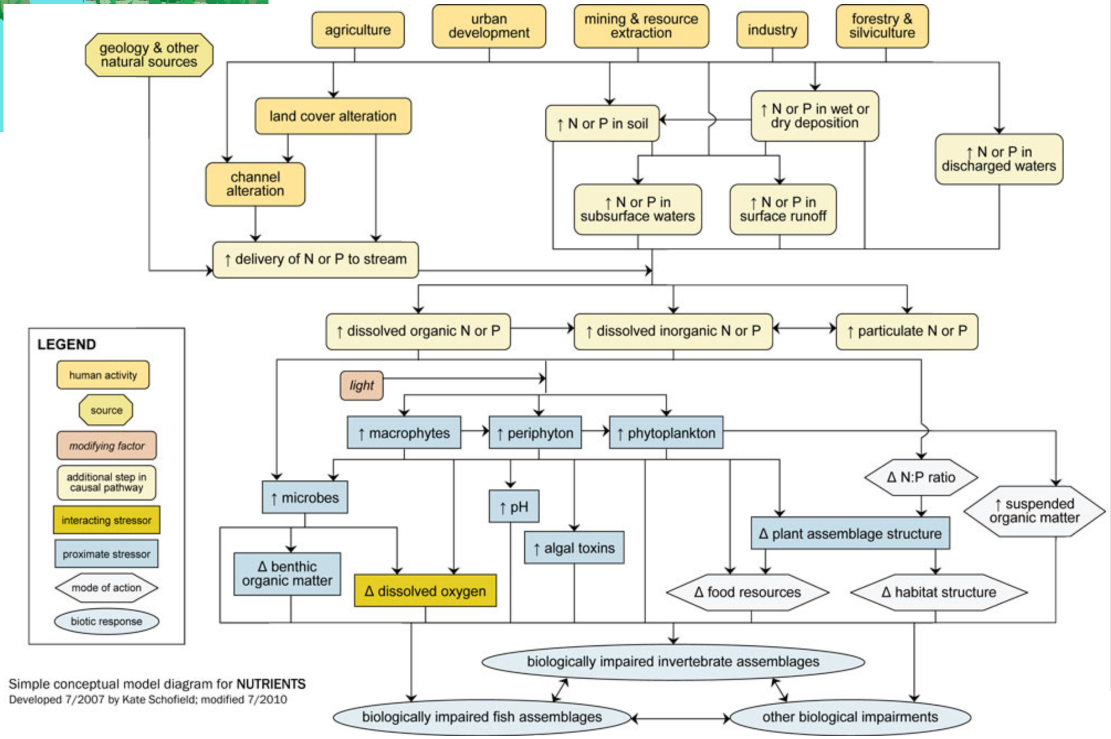
What is the acceptable level of uncertainty?

What are the appropriate spatial & temporal scales?

What are the resources available?

Conceptual Model…a good place to start





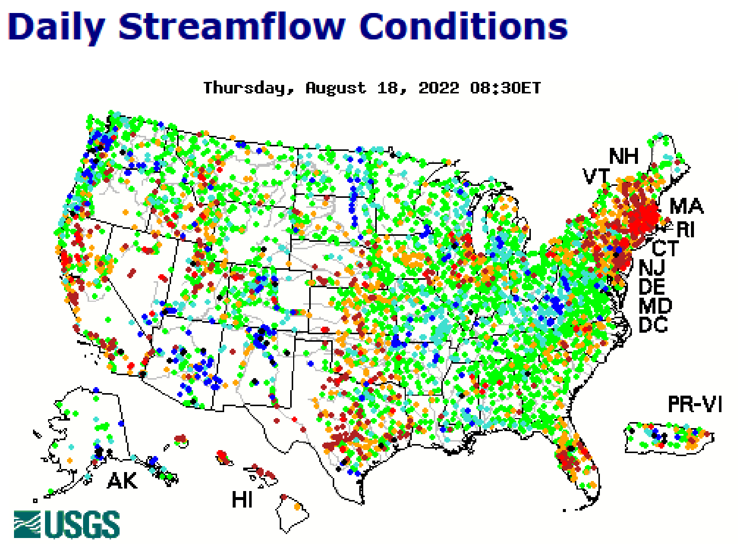
https://www.epa.gov/sites/default/files/2015-12/nut-cd_sim_1000.jpg

Model Selection:

Waterbody Type

Is the model appropriate for the waterbody type & critical condition?

- Waterbody type
  - Rivers
  - Lakes
  - Estuaries
- Critical condition
  - 7Q10
  - Seasonal (e.g., growing season)
  - Specific tidal condition



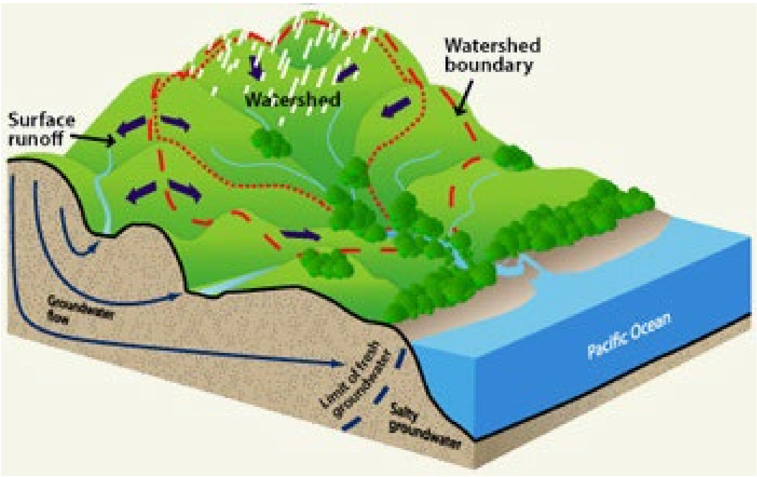
Fausch et al. 2002

Model Selection:

Pollutant Source

Can the selected model simulate the nature and source of pollutant?

- Pollutant form
  - Pulsed vs. chronic
  - Are totals sufficient or is partitioning required?
- Point source
  - Time-variable or constant load
  - Permit limit
- Nonpoint source
  - Time-variable or constant load
  - Function of rainfall
  - Groundwater-surface water interaction
  - Atmospheric deposition



Model Selection:

Endpoints

- What is the endpoint for your parameter of concern?
  - Can the model simulate it?
- What stressors or processes are needed to simulate the parameter of concern?
  - Can the model simulate those stressors or processes?
  - Is a linked modeling approach required?
- If endpoint based on a water quality standard, can the model simulate the frequency, magnitude & duration?
  - Never to exceed a value or a value 5% of the time
  - Daily average of 5 mg/L & never less than 4 mg/L
  - Diel change / fluctuation

Additional considerations

Temporal	Steady-state Dynamic (time-variable) Daily / monthly / annual output
Spatial	Single river segment Whole watershed Dimensions – 1D/2D/3D
Practical constraints	Data availability Financial cost Model familiarity and training/support
Transparency	Public domain freeware Open source code Proprietary black box
Regulatory and legal implications	EPA approved model Defensibility of model output Cost of load reductions or BMPs
Risks of incorrect decision	Acceptable amount of uncertainty Major risks to humans or aquatic life

Model Selection Golden Rule

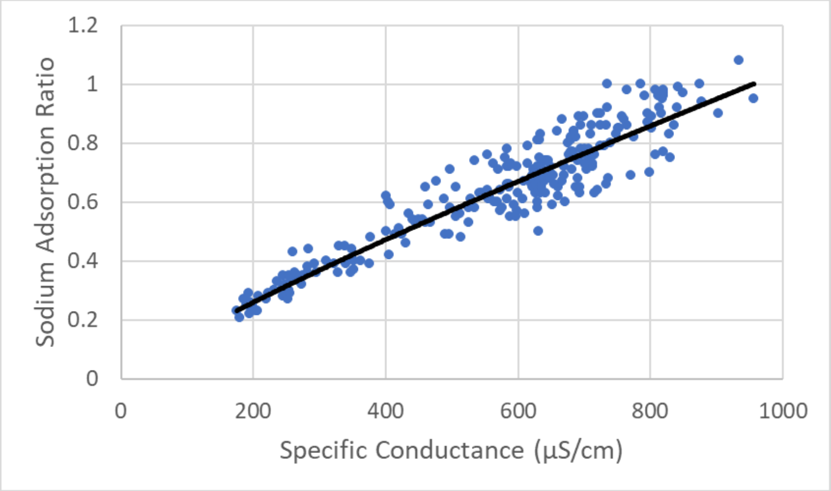
Choose a model that is only as complex as necessary to address the problem/objective

Basic Types of Models

Statistical vs. mechanistic models

Statistical (Empirical)

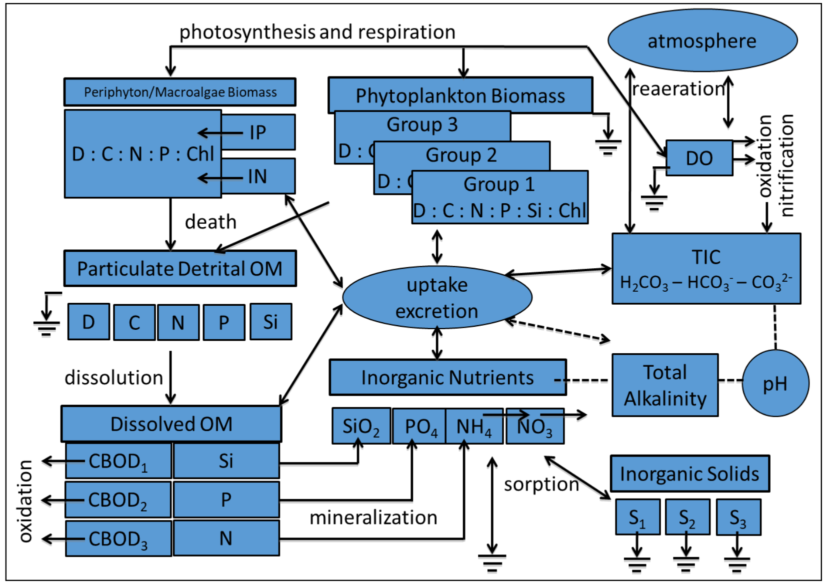
Observed relationship among experimental data



Ex: best-fit model (linear regression)

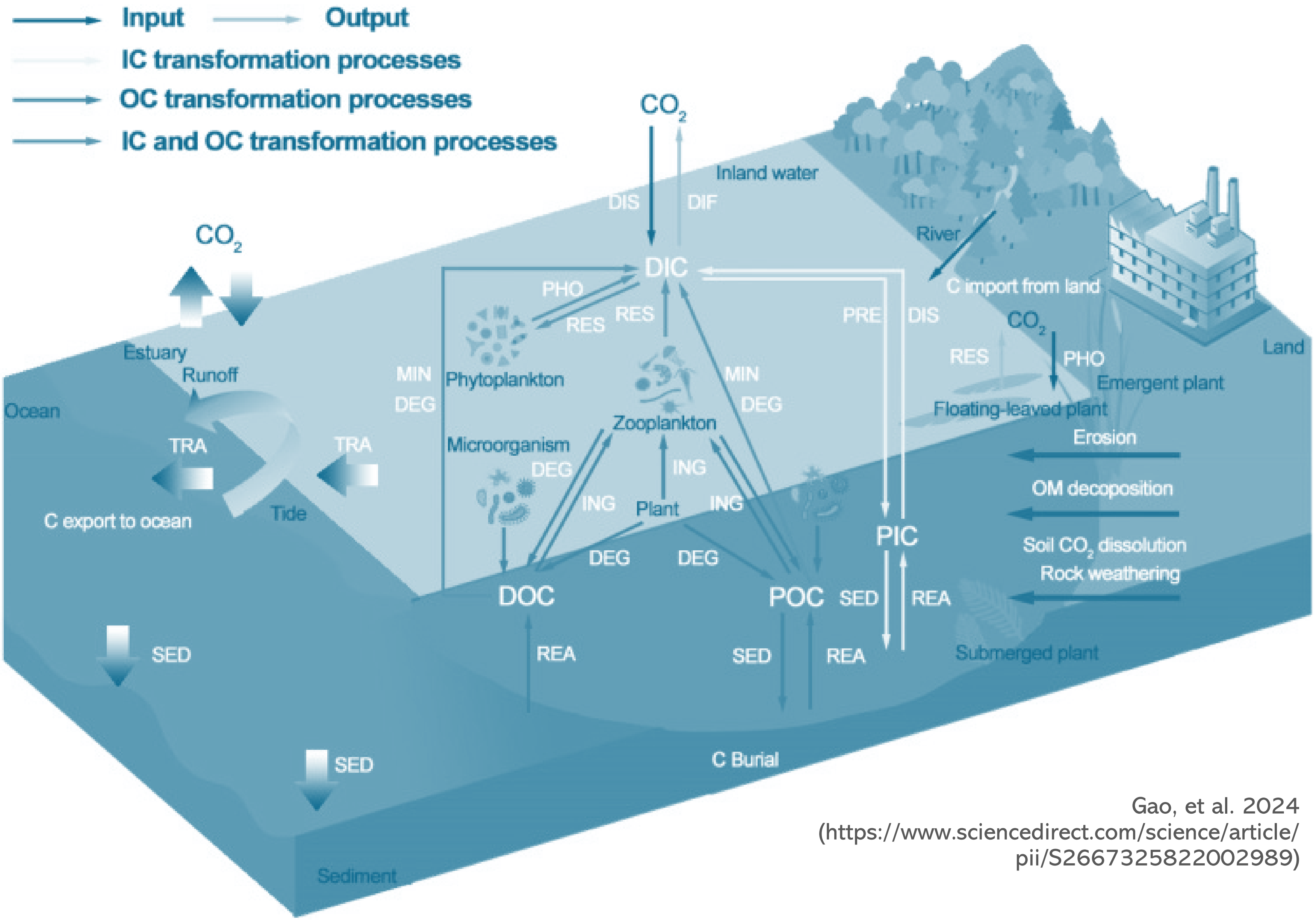
Mechanistic (Process-based)

Based on fundamental processes/ equations relating model variables



Ex: WASP / LSPC / HSPF

Mechanistic or Process-based Models



Gao, et al. 2024 (https://www.sciencedirect.com/science/article/pii/S2667325822002989)

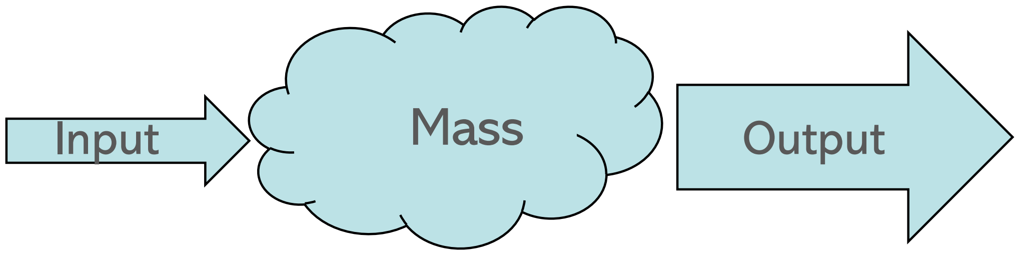
Steady State Model

- Input = output; mass is constant
- Simple mechanistic approach
- Single definable condition (flow, temp, light, nutrients);
  Can consider diel variation (photic period)
- Can be useful for DO and acute stressors
- Difficult to define single critical condition for complex problems

Dynamic model (time variable)

Input > or < output

Mass can vary



Can simulate responses under varying environmental, meteorological, loading conditions

- Seasonal variation
- Variable flows; wet vs. dry year conditions
- Storm flow vs. 7Q10 critical condition
- Environmental perturbation

Can evaluate frequency, magnitude & duration of response variables or chronic stressors

- Daily average DO shall not be less than 5.0 mg/L and never less than 4.0 mg/L

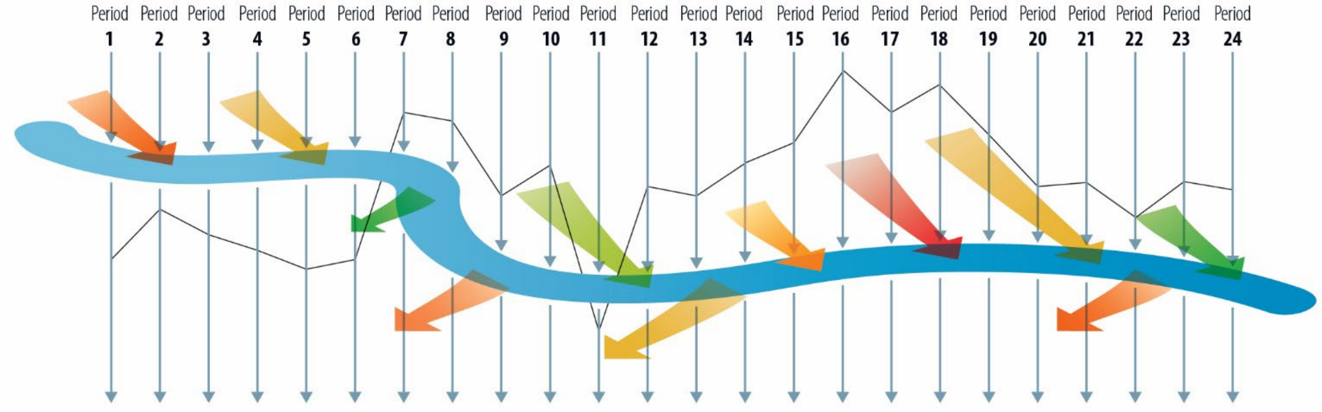
Steady state vs. dynamic model

- Steady-state model
  - Snapshot in time
  - Constant inputs and outputs

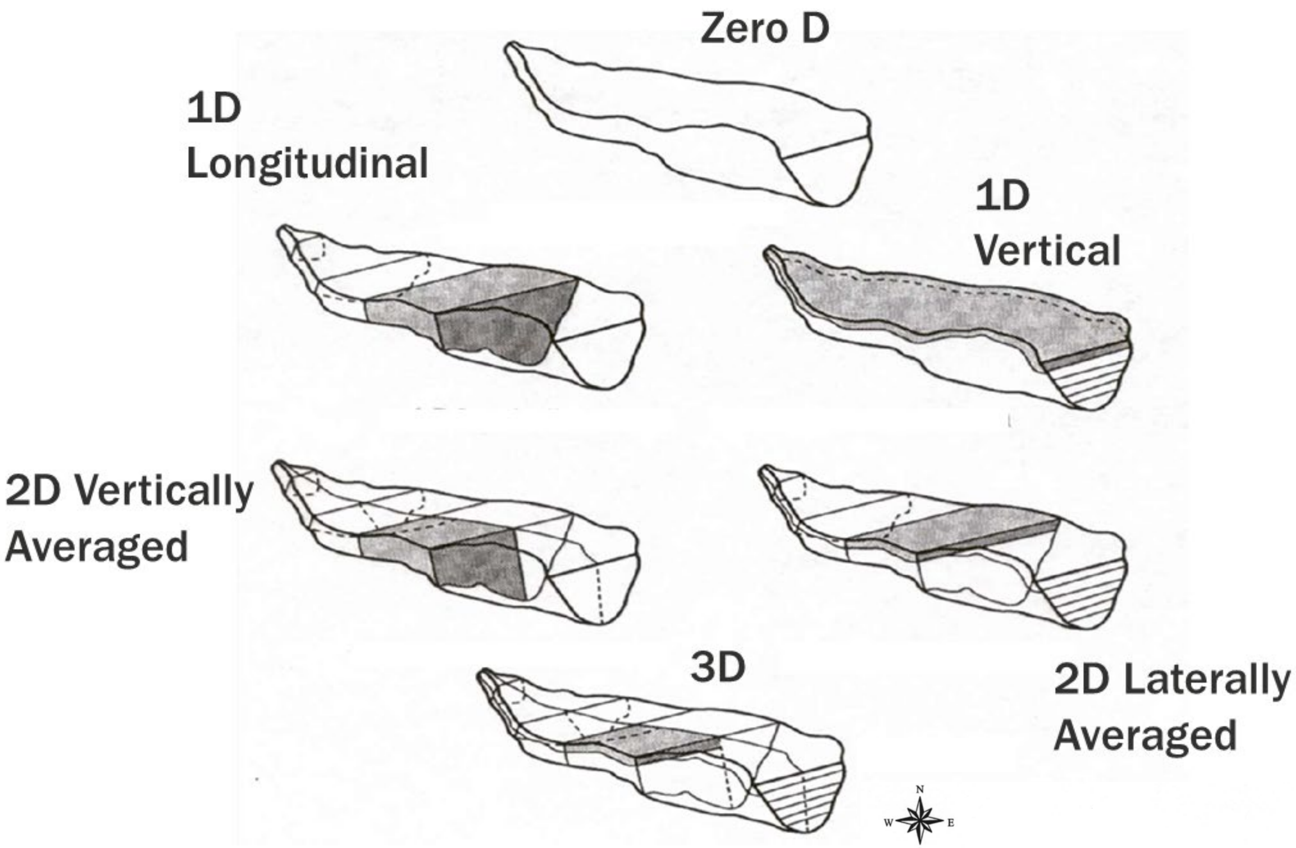
- Simple Mass Balance Models
- QUAL2K

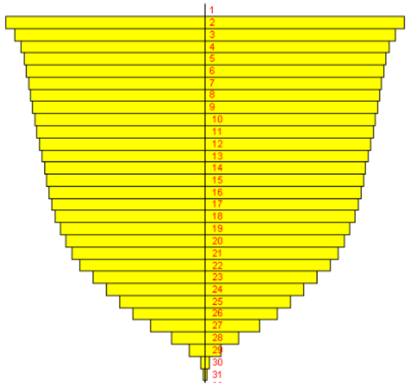
- Dynamic model
  - Time varying
  - Variable inputs and outputs

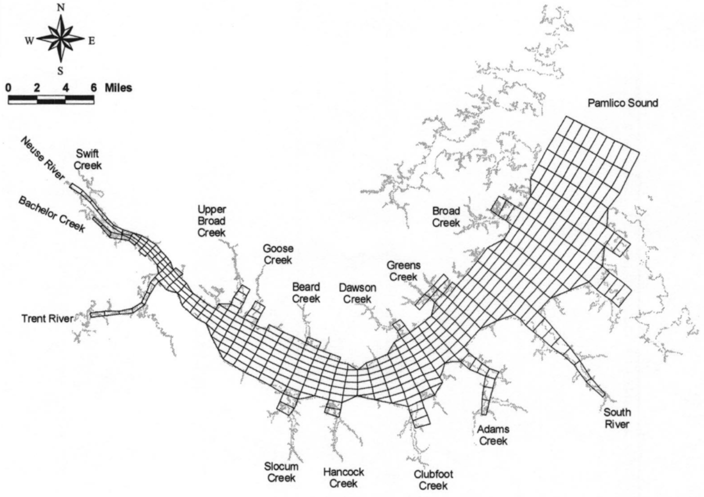
- HSPF
- QUAL2Kw
- CE-QUAL-W2
- EFDC/WASP



Model Dimensions





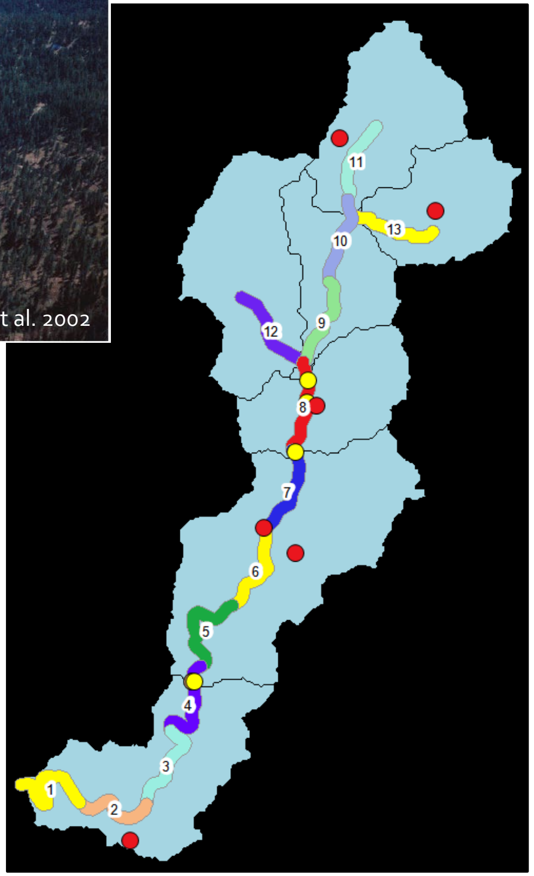


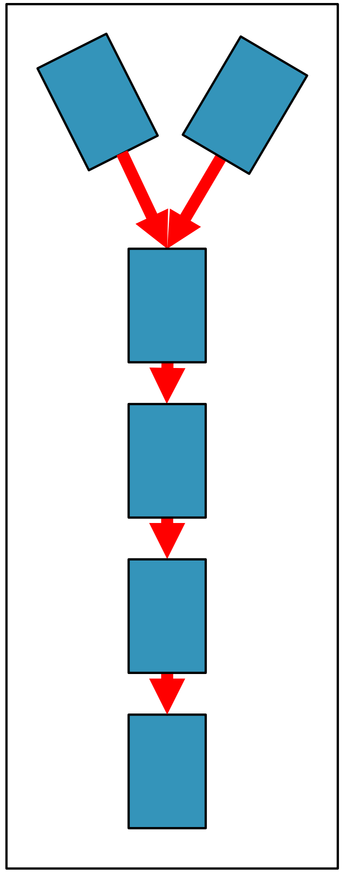
Wells 2013

Overview of Modeling Components

Models only approximate natural variability


Fausch et al. 2002

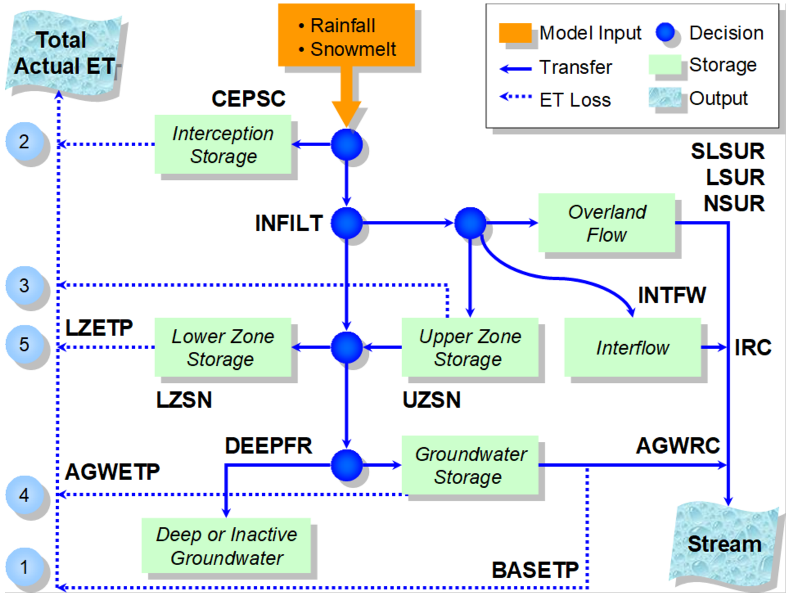




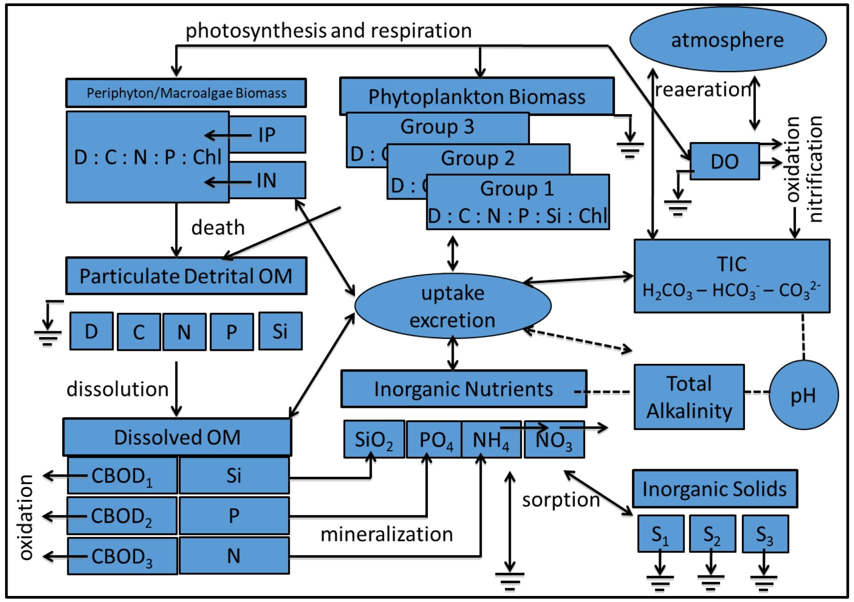
They are simplistic representations of reality

Water quantity vs. water quality model

Watershed / Water quantity



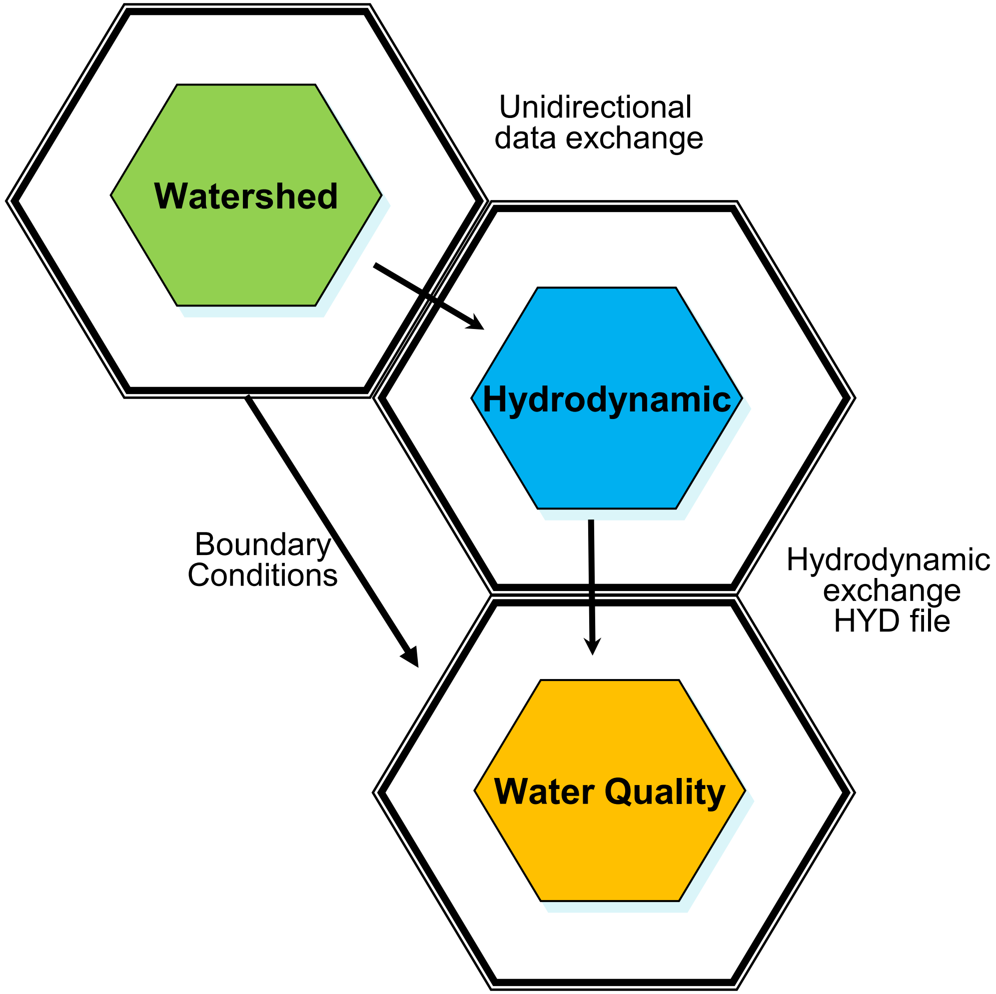
Water quality



Modeling Frameworks:

Linked Models

- Watershed – land-based loads and point source contributions
- Water quality – instream water quality
- Hydrodynamic – physical processes
  - Estuaries, lakes, open water



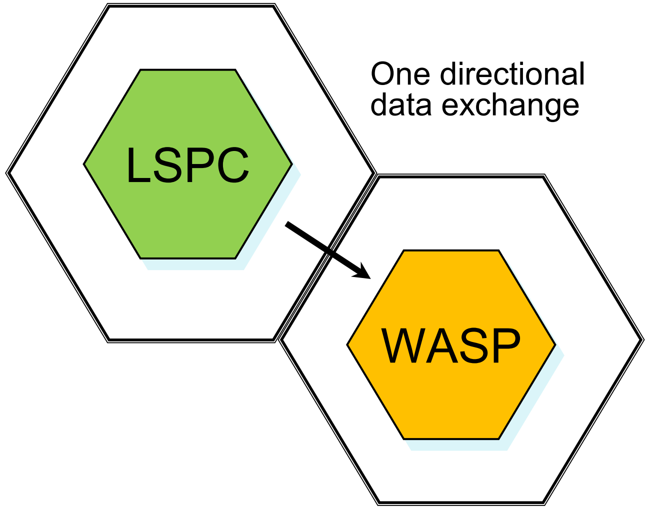
Model Configuration:

Riverine

Two-model system to represent WQ in riverine systems

- Watershed model simulates watershed loading
  - Integrates land attribute & meteorological data
  - Ex: LSPC / HSPF / SWMM / SWAT

- Water quality model simulates instream response
  - Integrates point source & nonpoint (watershed) sources
  - Ex: WASP / QUAL2K



Model Configuration:

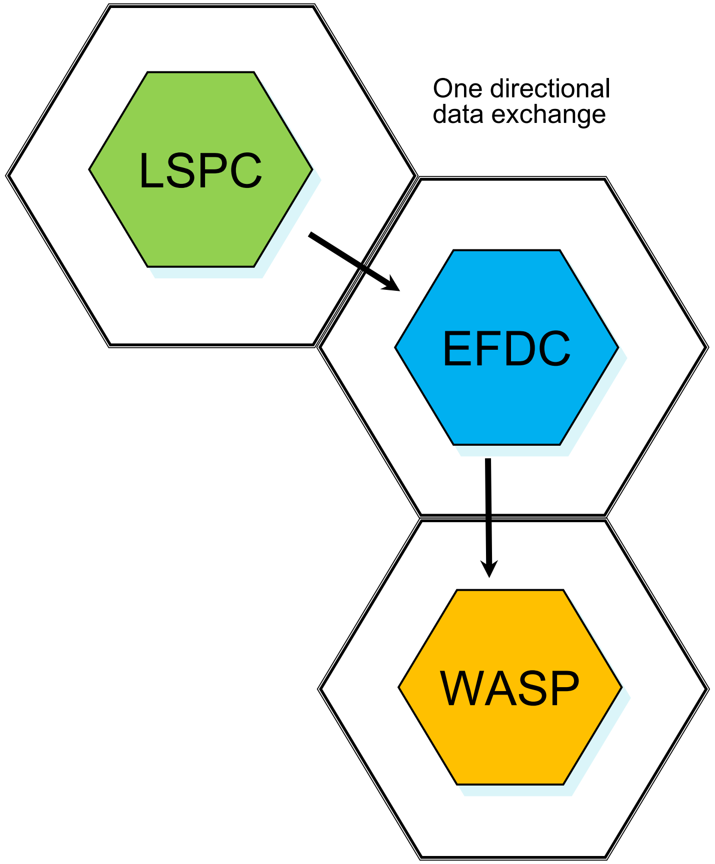
Lakes and Estuaries

Three-model system to represent water quality in lakes & estuaries

- LSPC simulates watershed loadings
- EFDC simulates hydrodynamics
- WASP simulates water quality response

Steady-state models rarely used

- Typically require dynamic models

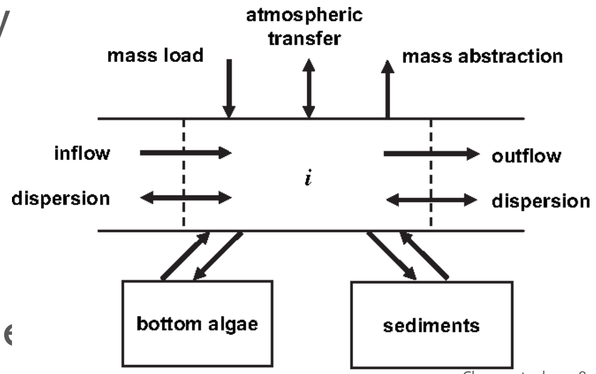


Capabilities of Common Water Quality Models

QUAL2K and QUAL2Kw

1-dimensional river model

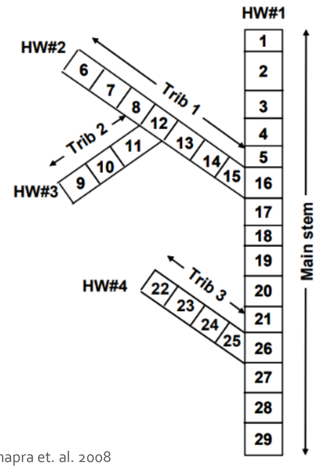
- 1D - stream channel uniformly mixed vertically & laterally
- QUAL2K steady state version– provides “snapshot” for a single period
- QUAL2Kw dynamic version (“w” stands for State of Washington)
- Flow is steady state → water quality varies over diel cycle
- Excel interface



Chapra et. al. 2008

Simulates

- Nutrients (subspecies)
- Physical: Temperature, DO, pH & alkalinity
- Biological: Phytoplankton, benthic algae, bacteria
- Sediment diagenesis routine for organic matter decomposition



Chapra et. al. 2008

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

CE-QUAL-W2

W2 is a 2-d (longitudinal/vertical, hydrodynamic & water quality model

- Applied to branching rivers, estuaries, lakes & reservoirs

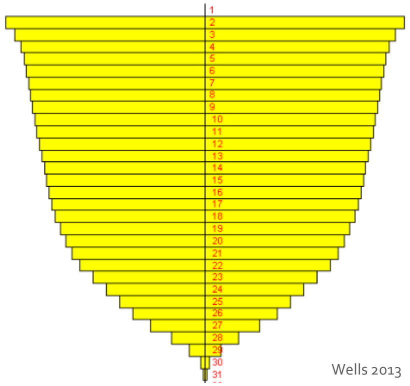
Best suited for long/narrow waterbodies, particularly reservoirs

- Exhibit longitudinal and vertical WQ gradients
- Assumes lateral homogeneity (i.e., averaged)

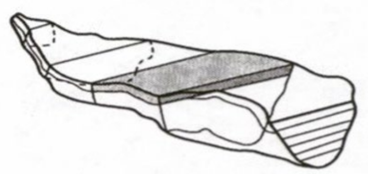
Simulates:

- Hydrodynamics: water surface elevation, velocity (longitudinal / vertical) & temperature
- Physical: temperature, DO, salinity, TDS, TSS
- Biological: algae, benthic algae, phytoplankton & fish habitat volumes
- Nutrients (subspecies) & CBOD

Water quality model is modular, allowing model to be tailored to project needs



Wells 2013



Wells 2013

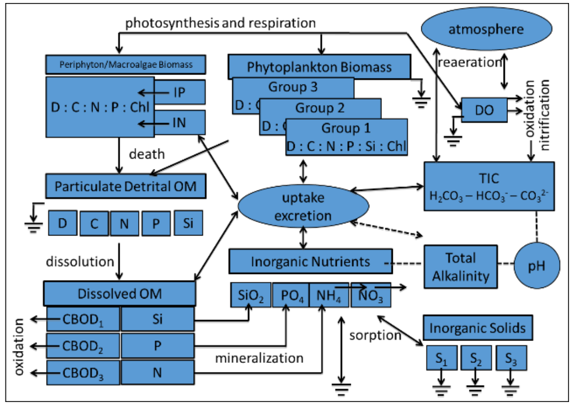
Time	Dimension	Diel	DO	Nutrients	Algae	Benthic Algae	Macro Algae	Light	pH/Alk	Temp	Sediment Diagenesis	Sediment Transport	Toxicants	Metals	Mercury	Bacteria
Time Variable	1/2-D	●	●	N/P/Si	●	●	●	●	●	●	●	●				●

WASP

1,2,3-dimensional WQ model

- **Requires separate hydrodynamic model** for 2 or 3-d (e.g. EFDC)

Suitable for lakes, ponded weirs, rivers, streams, estuaries and reservoirs



Wool et al. 2020

Simulates

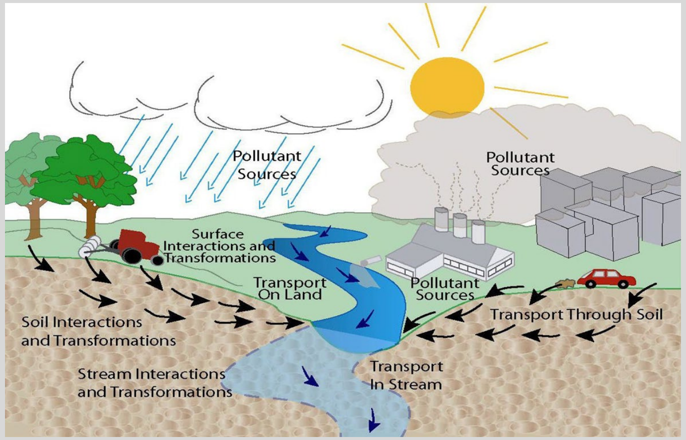
- Eutrophication: Nutrients (subspecies), DO, algae, benthic algae, macro algae, CBOD, pH/Alkinility, temperature, bacteria, & sediment oxygen demand
- Toxicants: Organic chemical/Nano materials (chemicals & solids), metal speciation & Hg/MeHg

Modular framework allows constituents to be activated/deactivated to customize project

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

Approach	Time Variable	Steady State	1-D	2-D	3-D	Diel Variation	Dissolved Oxygen	Algae	Multiple Algae	Benthic Algae	Macro Algae	Predictive Light	pH / Alkalinity	Temp	Sediment Diagenesis	Sediment Transport	Nutrients	Toxicants	Fish / Inverts
AQUATOX	●		●	●		●	●	●	●	●	●	●		●	●	●	N/P	●	●
BATHTUB		●	●					●									TP		
CE-QUAL-ICM	●		●	●	●	●	●	●	●	●	●	●	●	●	●	●	N/P/Si		
CE-QUAL-W2	●		●	●		●	●	●	●	●	●			●	●	●	N/P/Si		
EFDC	●		●	●	●	●	●	●	●			●		●	●	●	N/P/Si	●	
EPD-RIV1	●		●			●	●	●						●			N/P/Si		
QUAL2K/Kw		●	●			●	●	●	●	●			●	●	●		N/P/Si		
WASP or EFDC/WASP	●		●	●	●	●	●	●	●	●	●	●	●	●	●	●	N/P/Si	●	

Waterbody Models – Capabilities



Capabilities of Common Watershed Models

Common Watershed Models

- SWAT
  - Suitable for agricultural landscapes, BMPs, and management practices
  - Limited representation of urban landscapes
  - HAWQS – national web-based model based on SWAT – large scale data source
- HSPF and LSPC
  - Suitable for landscapes with mixed land-use (agricultural, urban / suburban, forested)
  - HSPF has limited detention basin capabilities
- SWMM
  - Suitable for urban landscapes w/ complex piping, pumping, & storage networks
  - Limited representation of non-urban landscapes

All are time-variable, output daily / sub-daily values, & require moderate to high effort to set-up

Watershed model summary

Modules	AGNPS / AnnAGNPS	BASINS	DRAINMOD	EPIC	GLEAMS	GWLF	HSPF	LSPC	SWAT	SPARROW	WARMF	SWMM
Hydrology												
Surface	●	●		●	●					●	●	
Surface & Ground Water		●	●			●	●	●	●			●
Water Quality												
Use defined							●	●				●
Sediment	●	●		●	●	●	●	●	●	●	●	●
Nutrients	●	●	●	●	●	●	●	●	●	●	●	●
Toxic/Pesticide	●	●		●	●		●	●	●	●	●	●
Metals		●					●	●	●		●	●
BMP Types												
Detention Basins	●	●						●	●			●
Infiltration practices									●			●
Vegetative Practices	●	●				●		●	●			
Wetlands			●	●							●	

Traits of a workhorse model

Versatile

- Predict multiple parameters
- Applicable to diverse problems
- Modular (add / remove parameters easily)
- Intuitive to use

Open-source, non-proprietary

- Avoids expensive service contracts

Widely-used & well-documented

- Track record of defensible results

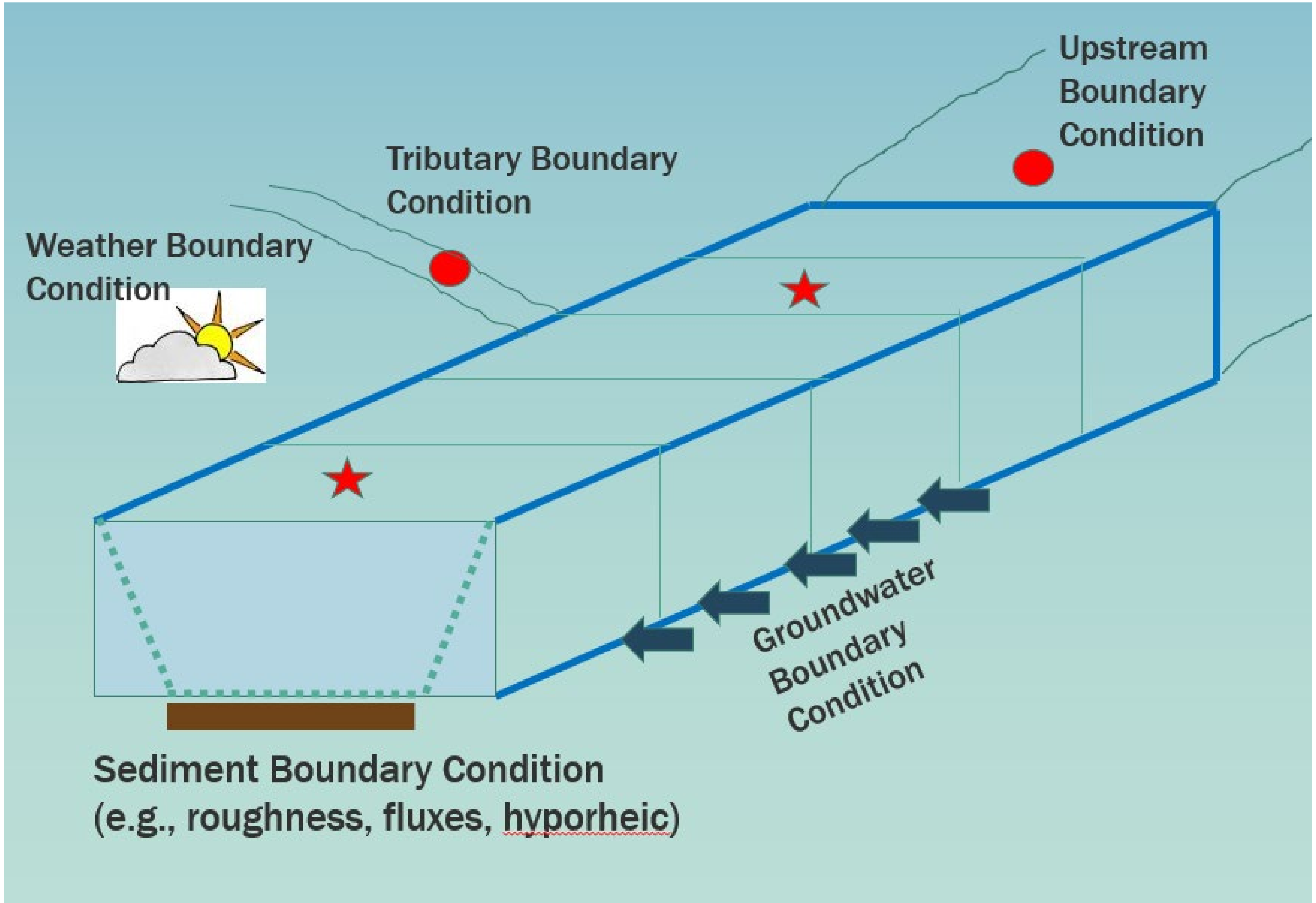
Large user community

Example workhorse models

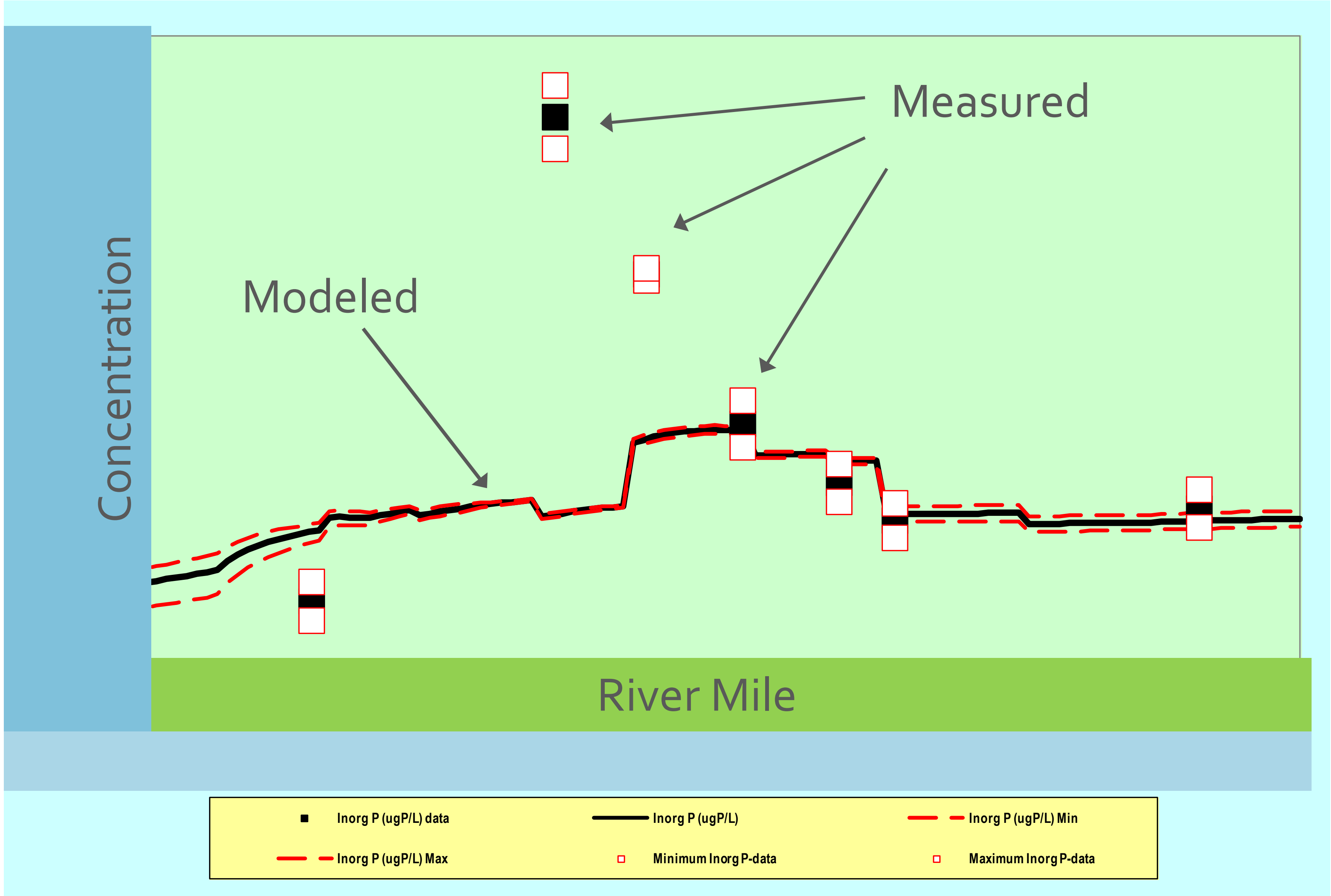
- QUAL2K
- CE-QUAL-W2
- WASP
- SWAT
- SWMM
- HSPF / LSPC

Building blocks

1D river model example

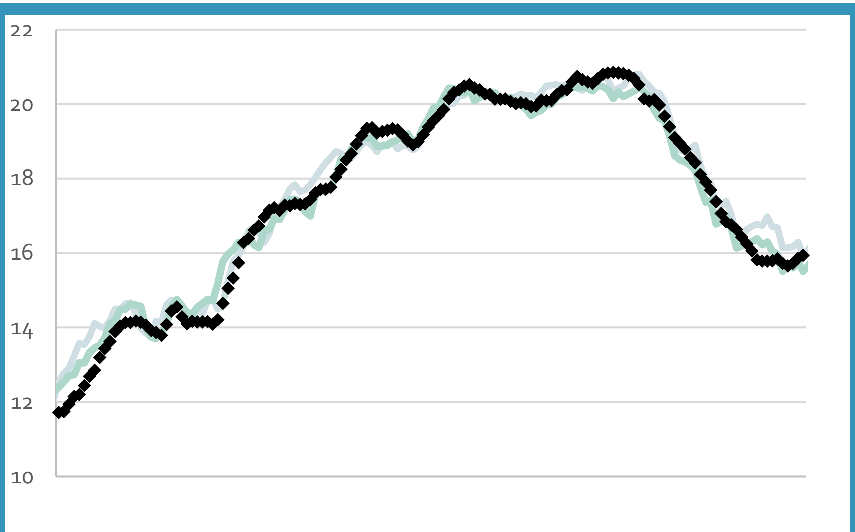


Inorganic Phosphorus in Big Moose Creek (7/31/2017)



Model Development Challenges

- System complexity
- Data Limitations of All Kinds
  - Gaps
  - Unmeasured boundary inputs
  - Measurement error
- Simplifying assumptions in model
- Large literature ranges for rate constants
- Data entry mistakes



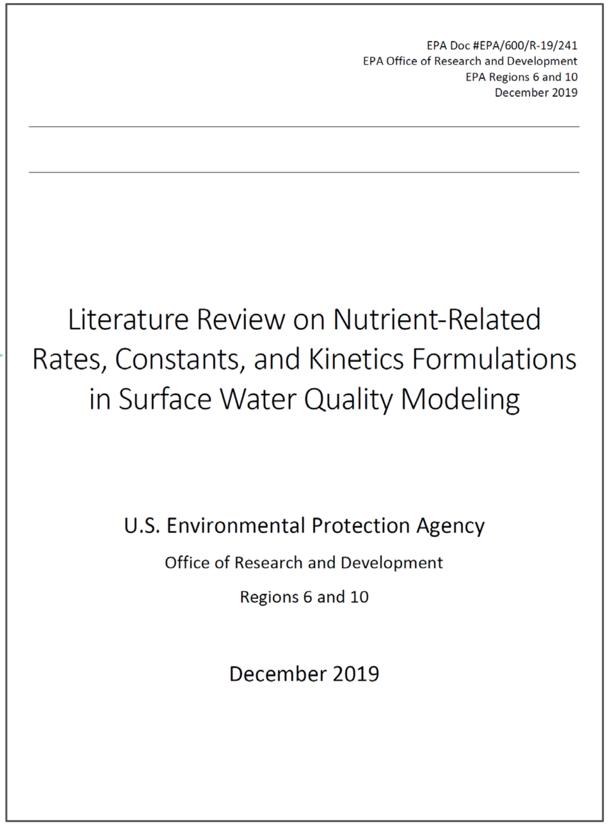
Model Calibration

What is model calibration?

Process of improving a model by adjusting or estimating factors for which data are not available

Iterative process

- Model assumptions are documented and reasonable
- Kinetic constants within acceptable range
- Data gaps filled with reasonable assumptions/methods
- Constrained by monitoring data availability &



EPA Doc #EPA/600/R-19/241
EPA Office of Research and Development
EPA Regions 6 and 10
December 2019

Literature Review on Nutrient-Related Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling

U.S. Environmental Protection Agency
Office of Research and Development
Regions 6 and 10

December 2019

Model Performance

Two methods for assessing model performance

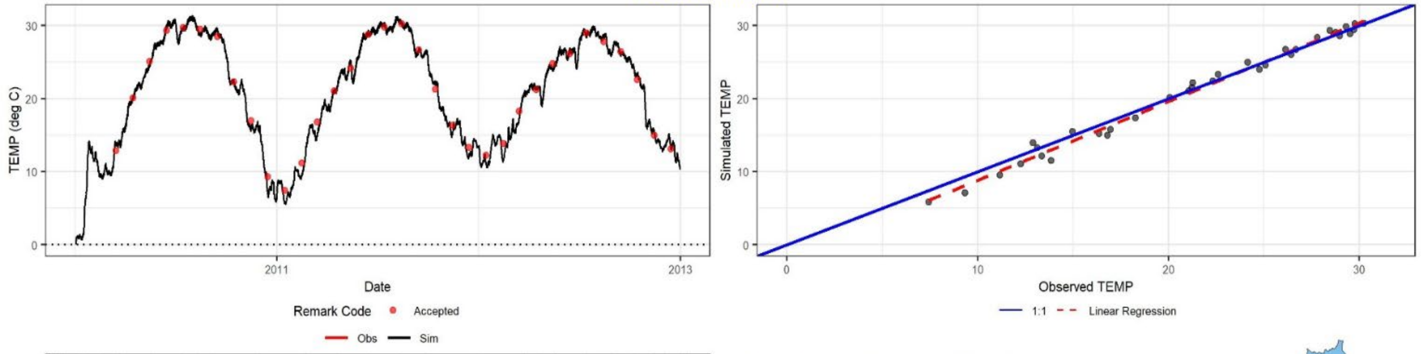
Quantitative

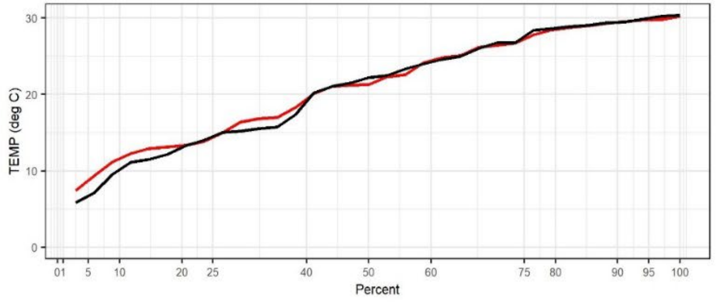
- Summary statistics
- Goodness of Fit statistics

Qualitative

- Time series plots
- Animations
- Frequency / probability

Lake Sarah
Parameter: TEMP





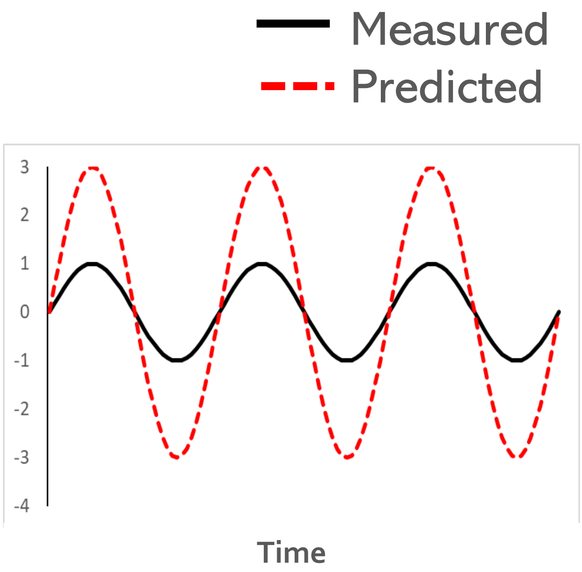
Dataset	Average	10%	20%	50%	80%	90%
OBS	21.210	12.46	13.65	21.80	28.58	29.45
SIM	20.912	11.22	13.71	22.31	28.70	29.43

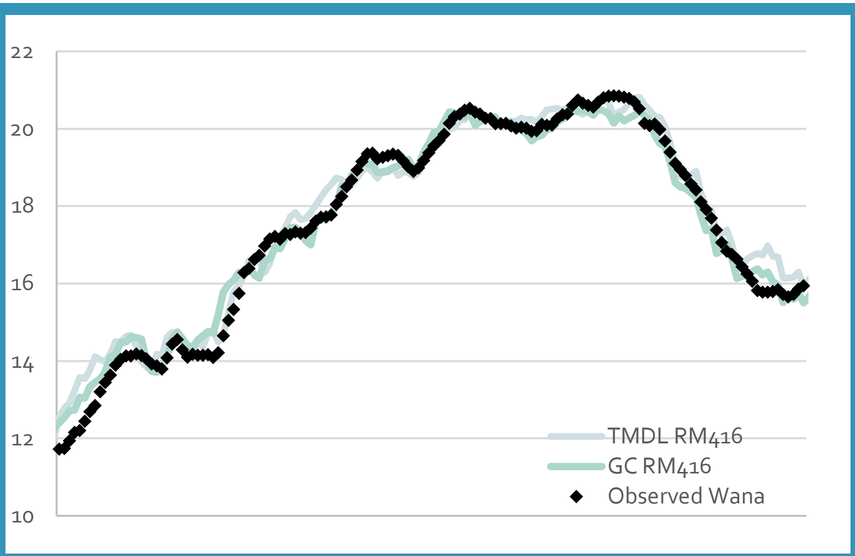
GoF Metric	Value
Num Obs	34.0000
R2	0.9889
NSE	0.9791
RMSE	0.9803
NRMSE %	4.3000
d	0.9952

(Calib Station: LS-01; WASP Seg: 1)

Model Performance

- Model bias (Accuracy)
  - How much do predicted values differ from measured central tendency?
- Model variance (Precision)
  - How much do the predicted values vary relative to measured ranges?
- Model correlation (Temporal dynamics)
  - How well do temporal dynamics of predicted values capture dynamics of measured values?





Calibration Process

General Calibration Sequence

Flow

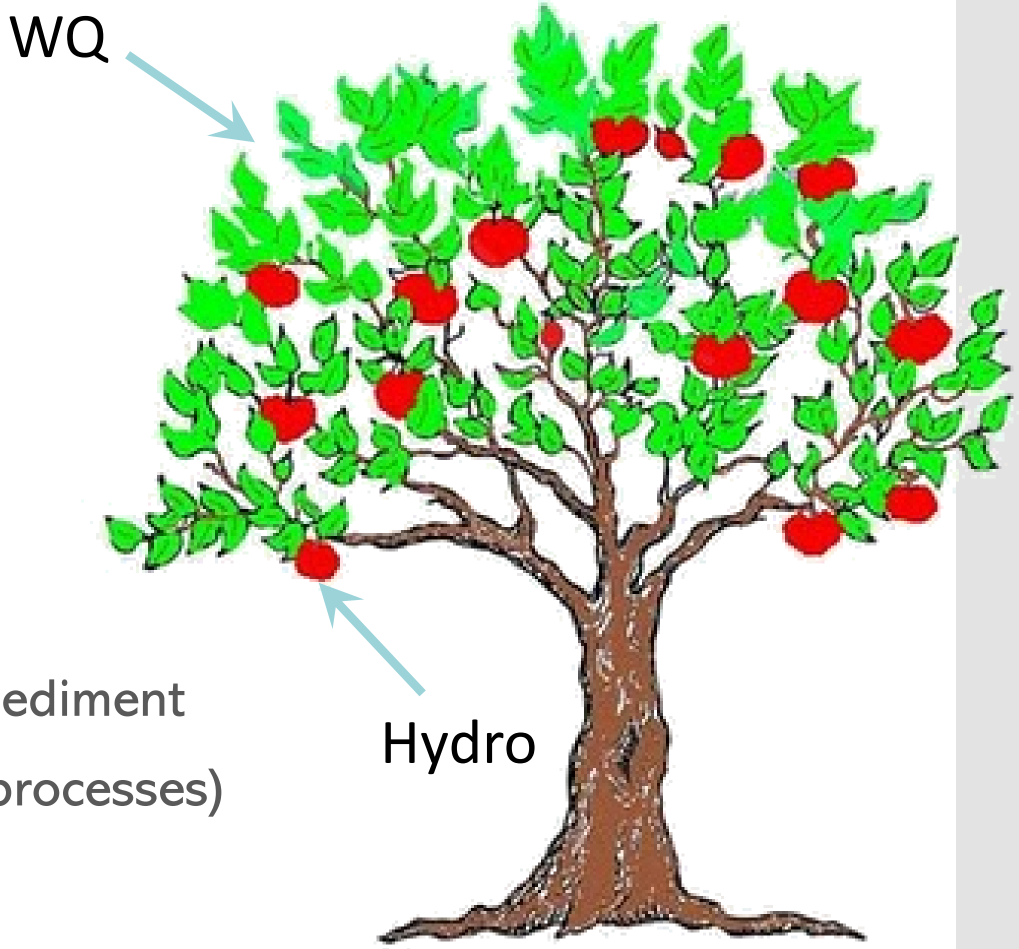
- Hydrology
- Hydrodynamics

Sediment

- Transport
- Erosion/Deposition

Water quality

- Transport associated with sediment
- Transformation (reactions, processes)



Hydro Calibration Sequence

Flow (hydrology/hydrodynamics)

- Water balance – annual, seasonal, monthly, daily, hourly
- Hydrograph components – rise, peak, recession timing
  - Storm flows / surface runoff
  - Base flow / groundwater flow
- Hydrodynamics
  - Water Surface Elevations
  - Current velocities
  - Stratification and mixing
    - Temperature/salinity

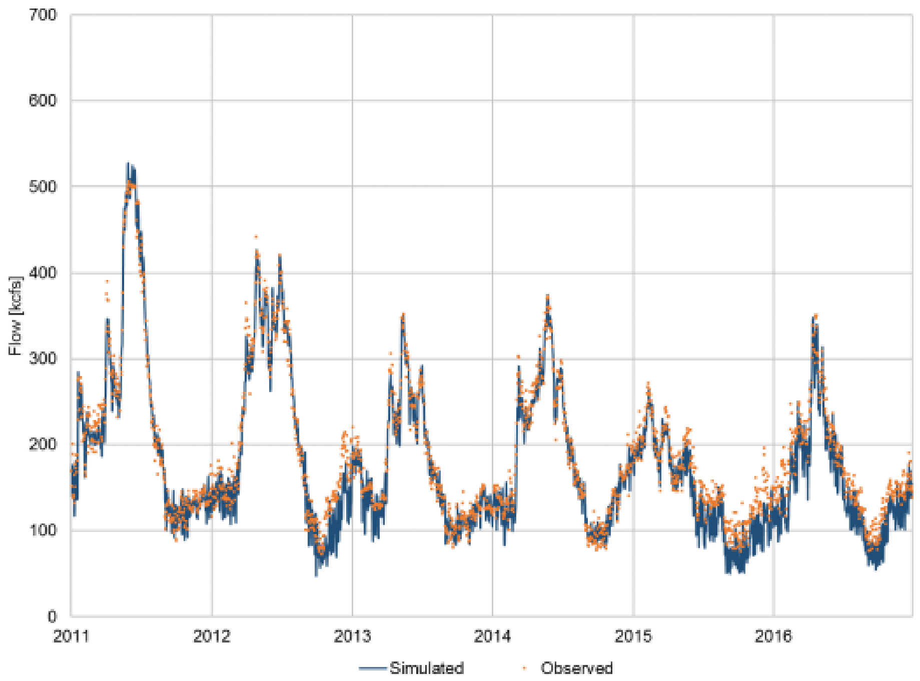
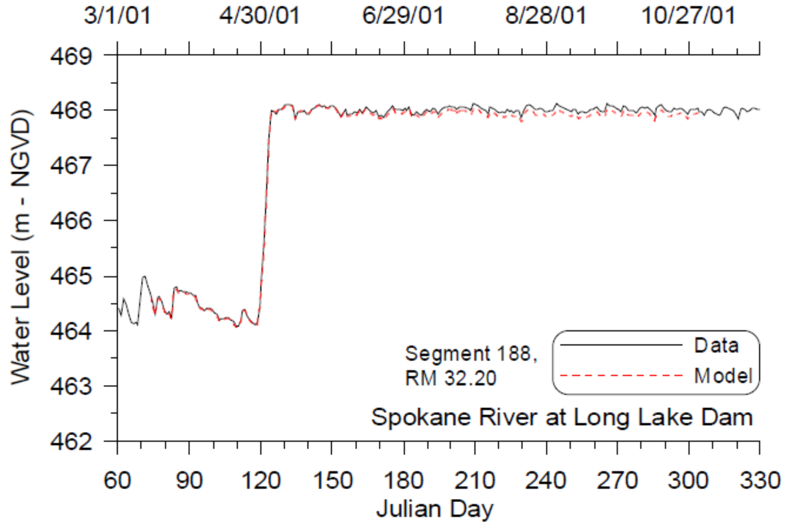


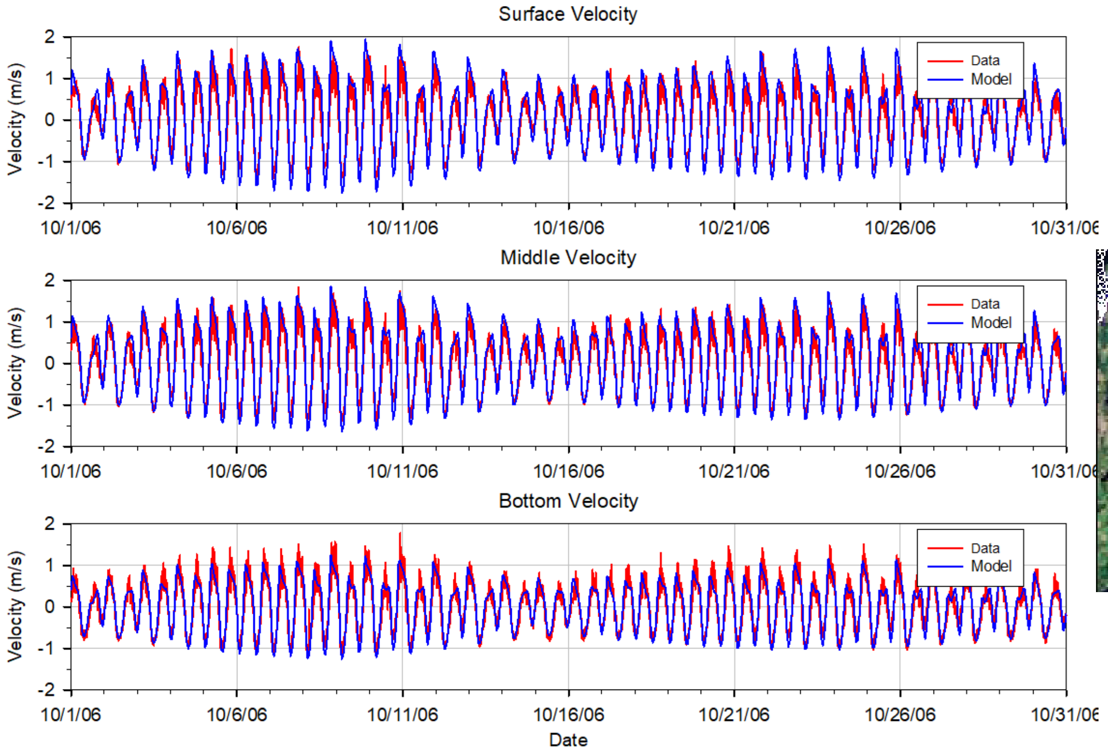
Figure B.1-6 Simulated versus observed flow at BON, period 2011 – 2016

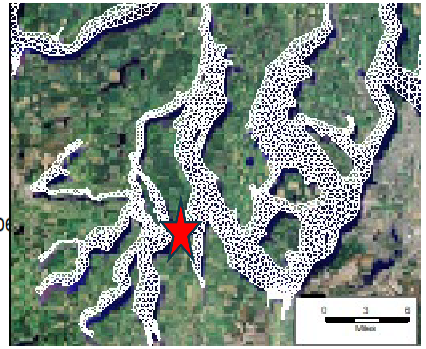
Hydrodynamic Calibration

Reservoir – Water Surface Elevation



Estuary – Current Velocities





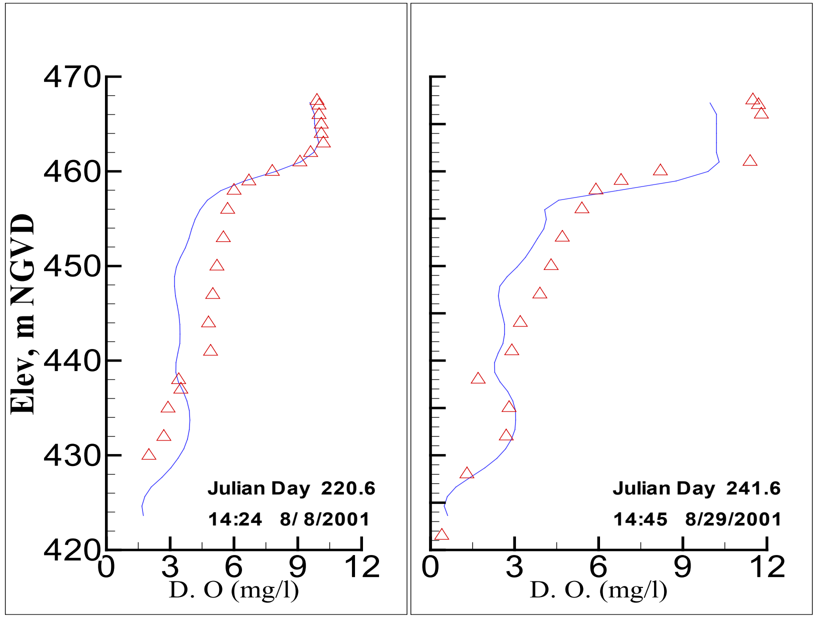
WQ Calibration Constituents

- Temperature
- Dissolved Oxygen
  - BOD (multiple types)
  - Reaeration
  - Sediment Oxygen Demand
- Nutrients
  - Nitrogen/Phosphorus
    - Nitrification and mineralization rates
    - Sorption
- Algal
  - Growth/death/settling rates
  - Nutrient Re-Cycling
  - Light
- Sediment Interaction
  - Sorption/Settling
  - Sediment Nutrient Fluxes

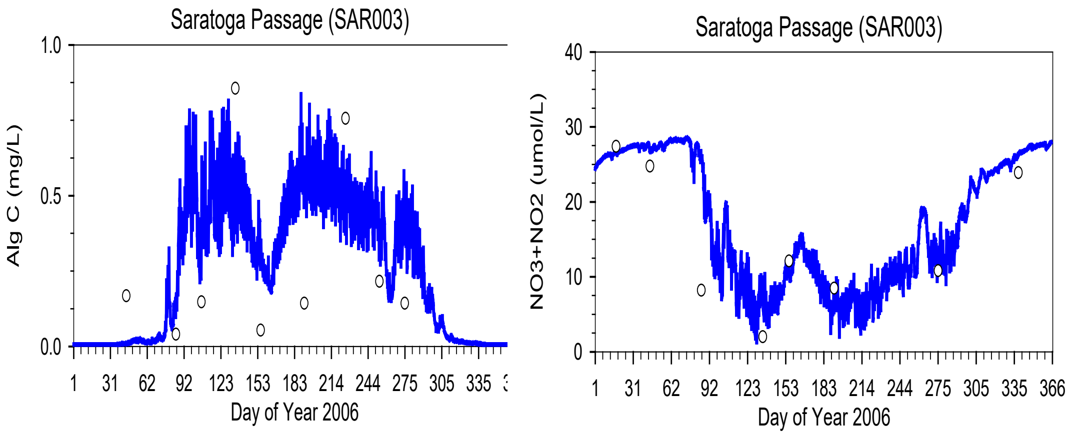
Iterative process

Water Quality Calibrations

Reservoir – Vertical Dissolved Oxygen Profiles



Estuary – Surface Algae and Nitrate



Model Scenarios & TMDL Development

Why we build models

Scientific benefits of having a model

- Improves understanding of the system
- Allows extrapolation of known to unknown (spatially & temporally)

For TMDLs, models allow us to:

- Define current conditions more fully (calibration run)
- Assess relative contributions of sources to WQ impairment
- Determine load reduction required to meet TMDL endpoint or WQ standard
- Evaluate placement & performance of BMPs

Model may not be well-calibrated to all conditions

- Can still inform decisions – depends on endpoint definition & objectives

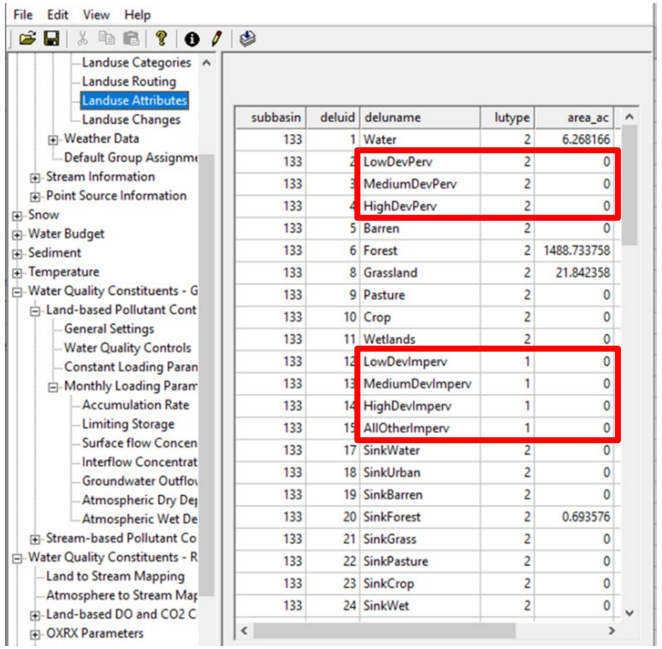
General model scenarios

Current condition

- Use calibrated model to simulate concentrations / flows under current conditions (land use, weather, and point source loads)
- Serves as baseline

Natural condition

- Revert anthropogenic land uses to natural state
    - forest / grassland / wetland
- Eliminate anthropogenic point sources, SSOs, & withdrawals
- Represents background load & concentration
- Assesses if endpoints are achievable under best-case scenario



Loading scenarios

Watershed load reduction scenario

- Apply load / concentration reduction to land use type(s)
- Re-run watershed model & pass output to WQ model
- Location of BMPs can be informed by subbasin nutrient budget

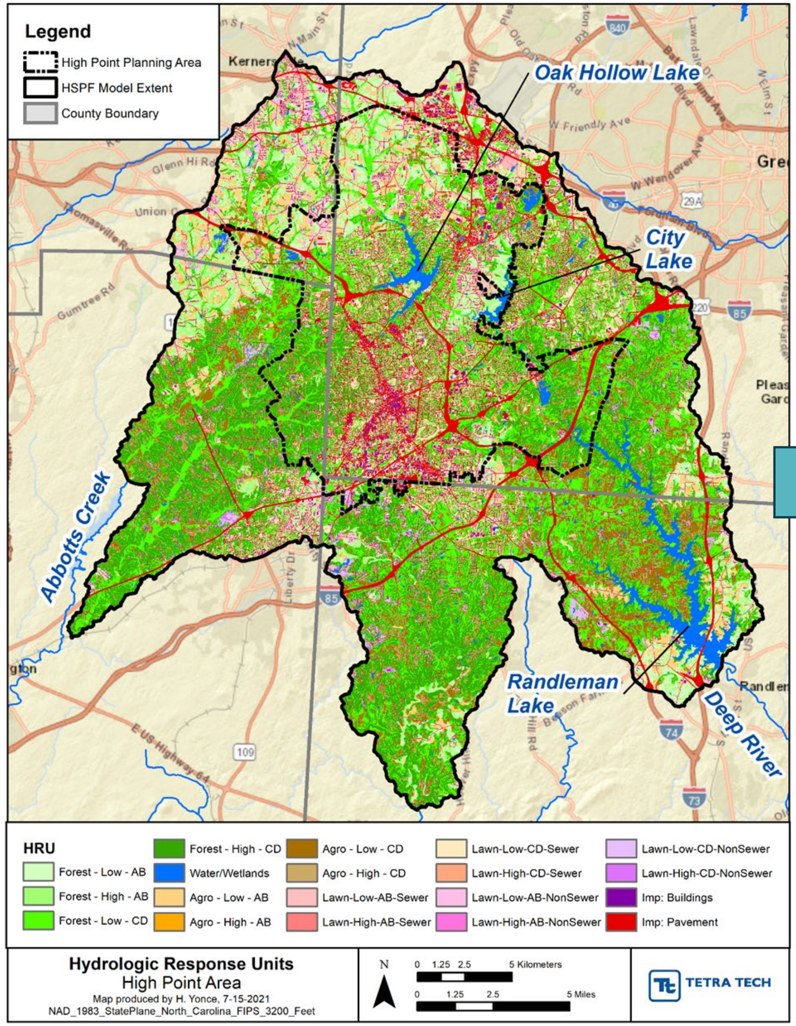
Permit limit scenario

- Reset point source discharge / concentrations to permit limits
- Evaluates instream responses under maximum allowable loads
- Can be starting point for TMDL reductions

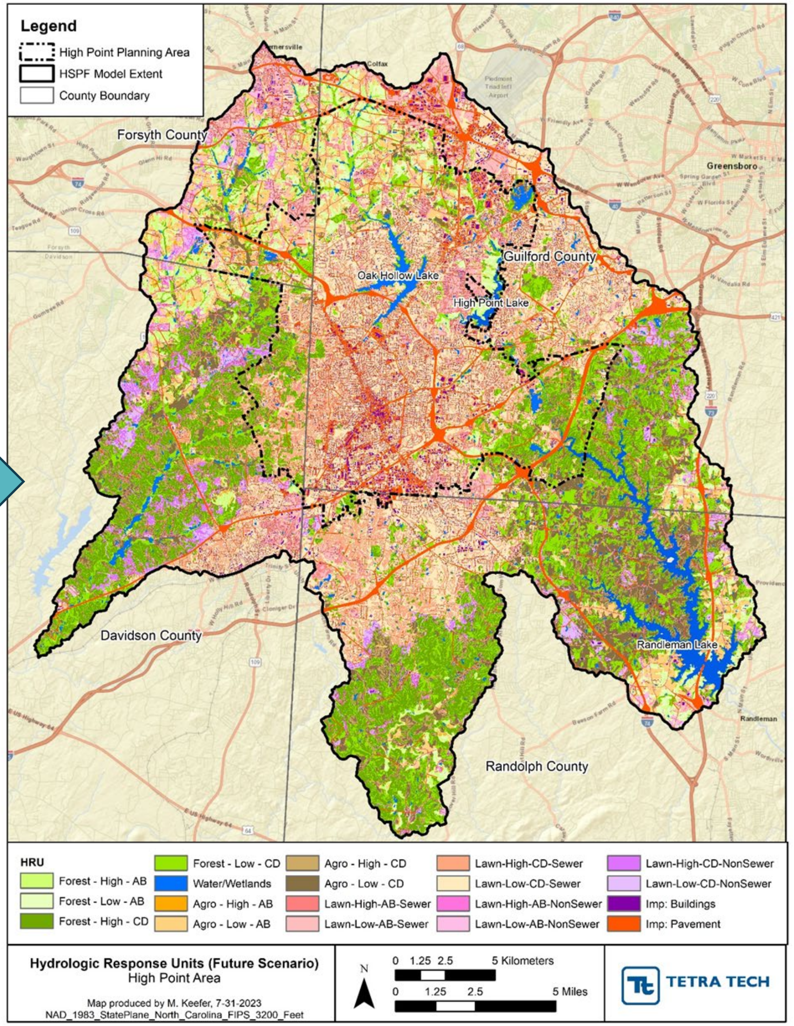
Point source reduction scenario

- Apply flow / load / concentration reduction to point source(s)
- Assess contribution of discharger to instream responses
- May be iterative search to identify loads that meet the WQS

Model scenarios: future planning



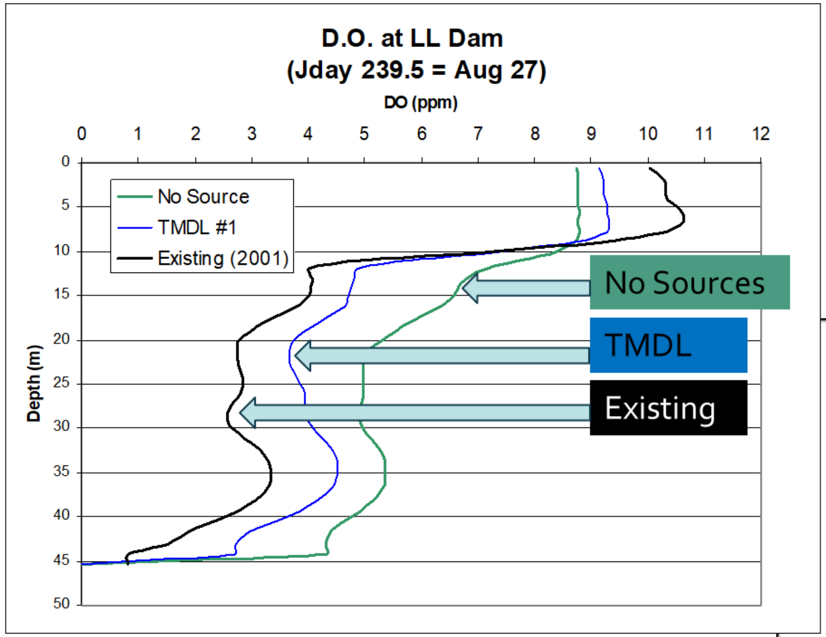
Current Condition HRU Classification



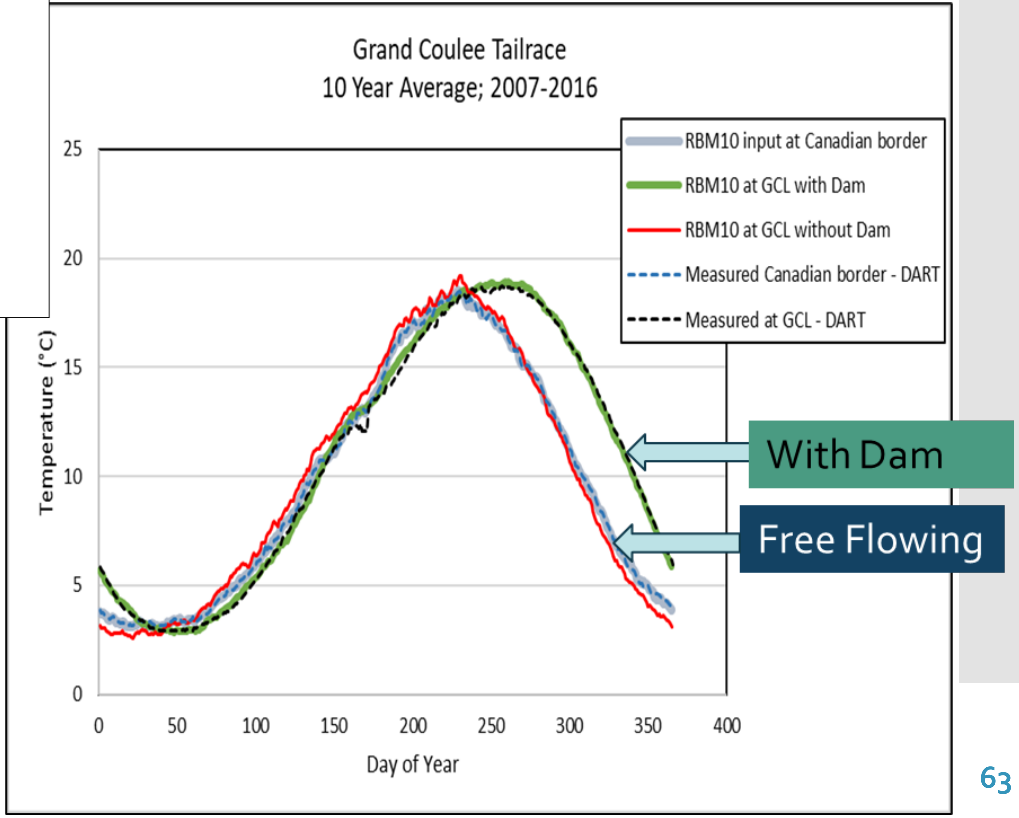
Future Condition HRU Classification

Scenario Examples

Reservoir – 2D model
Vertical DO Profiles

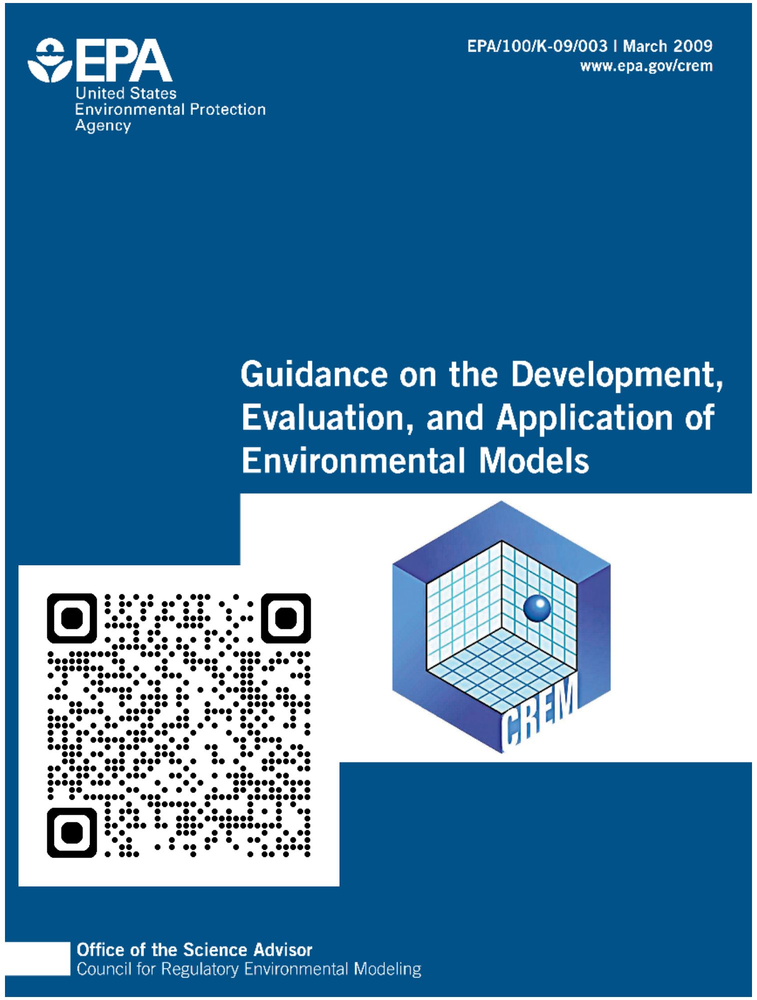


River – 1D model
Temperature below a dam



Modeling Resources

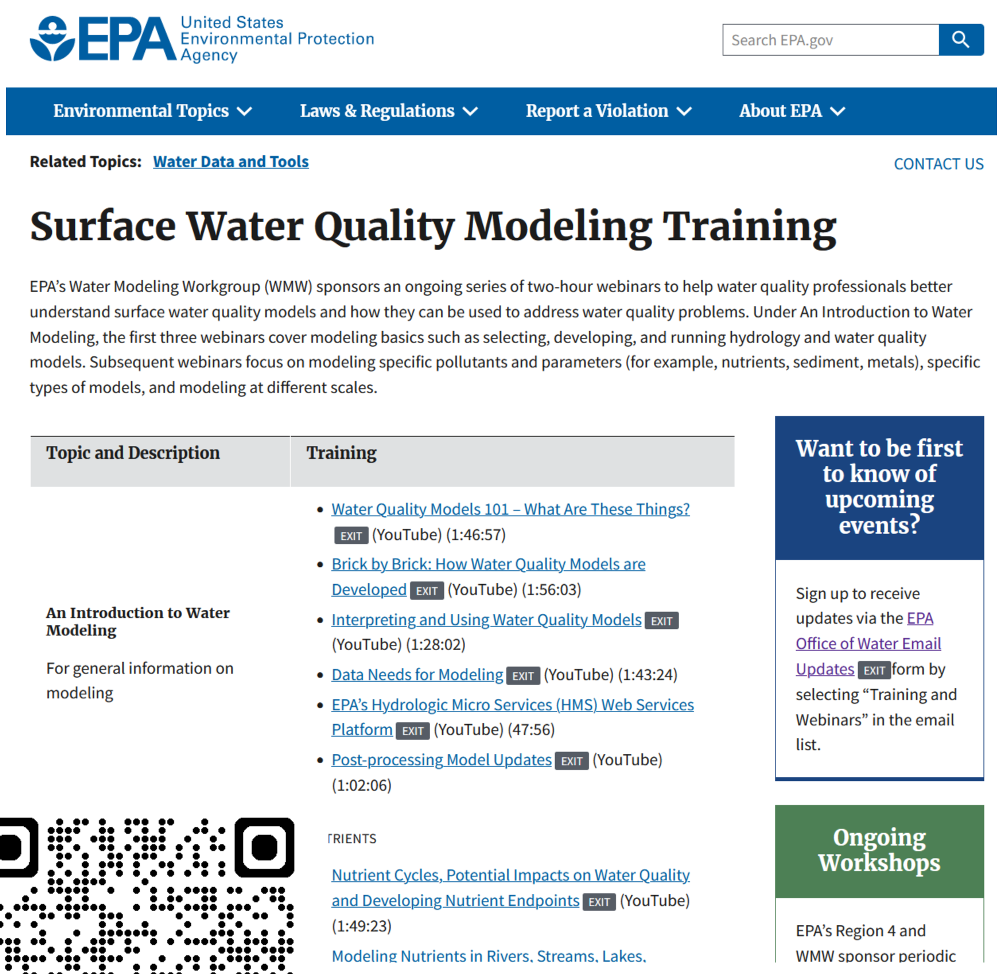
Guidance on Best Practices



https://www.epa.gov/

Water Modeling Webinars

- Archived webinars available on EPA website
- Variety of modeling topics and intros to many specific models
- Over 50 hours of training material



https://www.epa.gov/waterdata/surface-water-quality-modeling-training

Information about models and practice

EPA United States Environmental Protection Agency

EPA/600/R-18/270
September 2018

ASSESSMENT OF SURFACE WATER MODEL MAINTENANCE AND SUPPORT STATUS

Prepared by

Tetra Tech, Inc.
10306 Eaton Place, Suite 340
Fairfax, VA 22030

Contract Number #EP-C-14-016, Work Assignment 3-24

Prepared for
U.S. Environmental Protection Agency
Water Modeling Workgroup

https://www.epa.gov/waterdata/surface-water-quality-modeling

Summary of current status of common water quality models, including references and training materials

Summary of values for rates and constants used in nutrient modeling studies

EPA Doc #EPA/600/R-19/241
EPA Office of Research and Development
EPA Regions 6 and 10
December 2019

Literature Review on Nutrient-Related Rates, Constants, and Kinetics Formulations in Surface Water Quality Modeling

U.S. Environmental Protection Agency

Office of Research and Development

Regions 6 and 10

December 2019

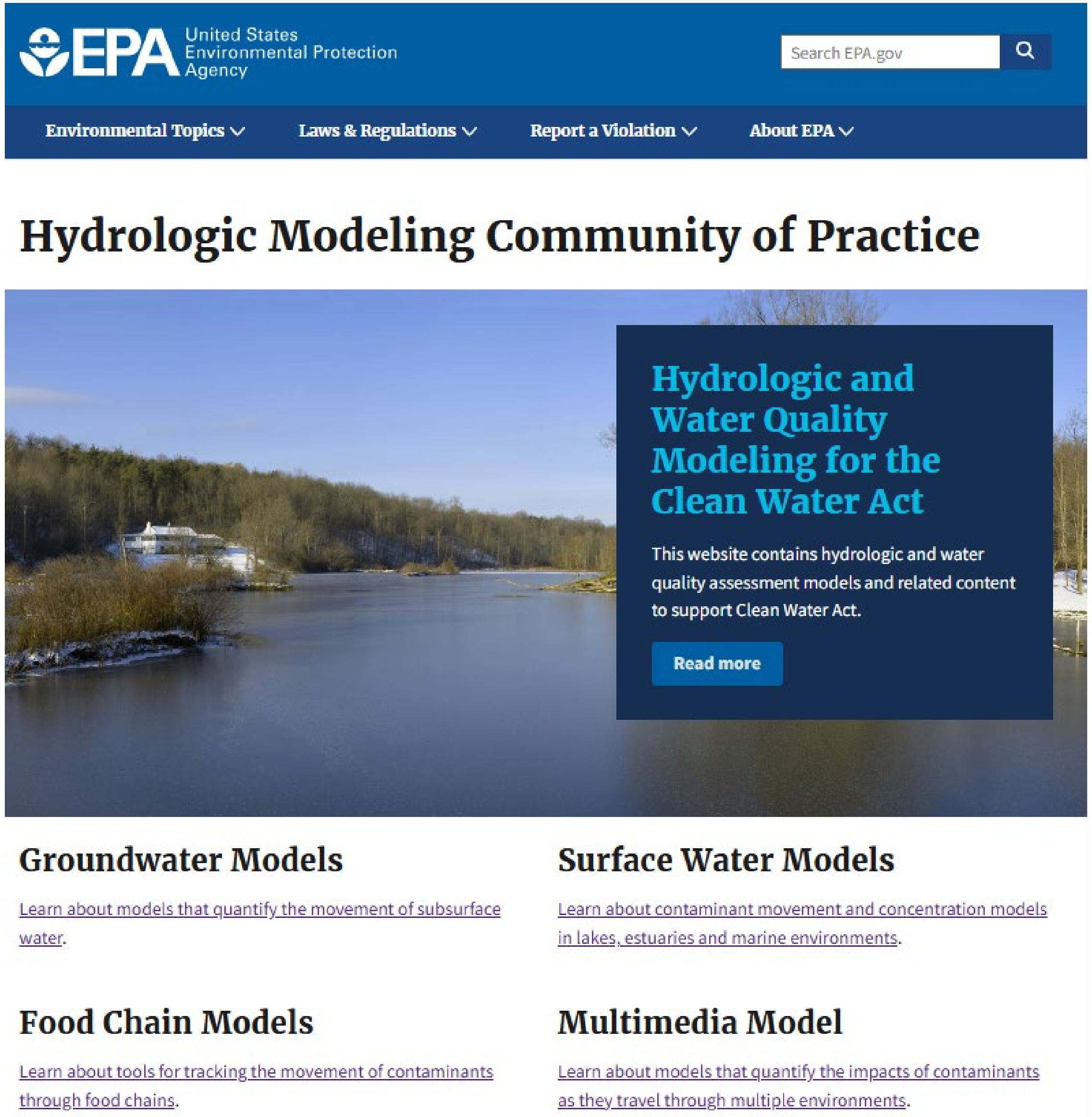
https://cfpub.epa.gov/si/

EPA Office of Research and Development

Model Software Download Site

Easy access to models & utilities

https://www.epa.gov/hydrowq



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QUESTIONS?