INTRODUCTION TO MODELING

Todd Steissberg, PhD, PE

**U.S. Army Engineer Research and Development Center,
Environmental Laboratory**

CE-QUAL-W2 Workshop, 2024

July 08 – 09, 2024

US Army Corps of Engineers®

Environmental Systems Modeling Team

ERDC
ENGINEER RESEARCH & DEVELOPMENT CENTER

DISCOVER | DEVELOP | DELIVER

Systems Modeling: Guiding Principles

George Box:

*... all models are approximations. Essentially, **all models are wrong, but some are useful.** However, the approximate nature of the model must always be borne in mind....*

<u>Paraphrased</u>:

"All models are wrong, but some are useful."

Albert Einstein:

It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience.

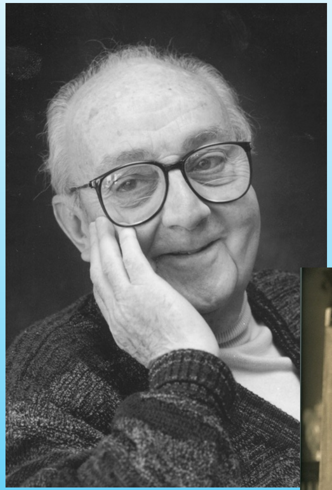
<u>Paraphrased</u>:

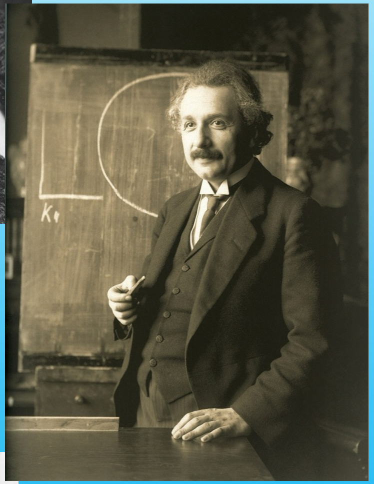
"Everything should be made as simple as possible, but no simpler."

Hans Albert Einstein (Hydraulic Engineer):

You can assume anything you want. The water won't!

<u>Moral</u>: Be careful with your assumptions.





Albert Einstein, said of his son's career, "He is working on a more difficult problem."

The Tea Leaf Paradox

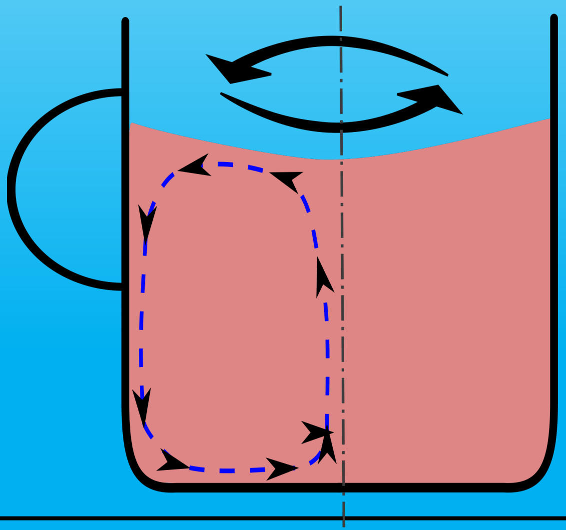
- Question: When you stir a cup of tea with tea leaves in the bottom of the cup, do they move towards the center of the cup or towards the sides?

The Tea Leaf Paradox

- Question: When you stir a cup of tea with tea leaves in the bottom of the cup, do they move towards the center of the cup or towards the sides?
- It seems simple: centrifugal force should cause the tea leaves to collect along the sides of the cup. But do they?

The Tea Leaf Paradox

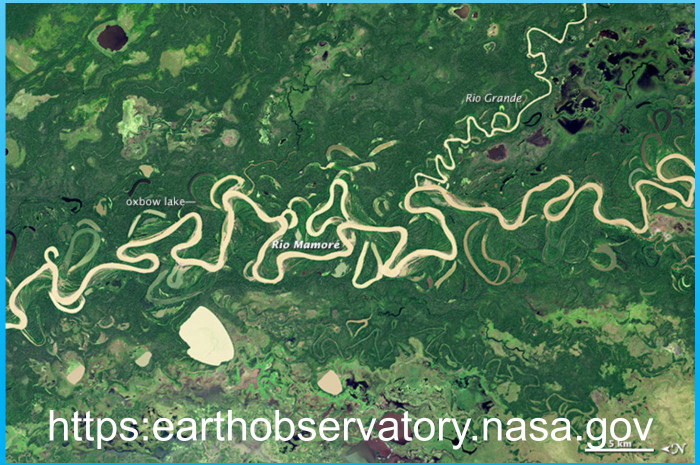
- Question: When you stir a cup of tea with tea leaves in the bottom of the cup, do they move towards the center of the cup or towards the sides?
- It seems simple: centrifugal force should cause the tea leaves to collect along the sides of the cup. But do they?
- Albert Einstein solved this problem in 1926 in a paper he wrote on meandering rivers. Einstein was the first person to describe how *helical flow* helps to determine the length and migration of meander bends in rivers.



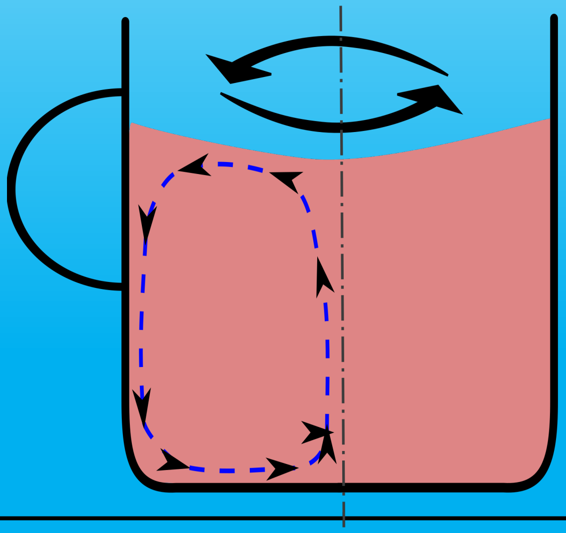
The Tea Leaf Paradox

- Question: When you stir a cup of tea with tea leaves in the bottom of the cup, do they move towards the center of the cup or towards the sides?
- It seems simple: centrifugal force should cause the tea leaves to collect along the sides of the cup. But do they?
- Albert Einstein solved this problem in 1926 in a paper he wrote on meandering rivers. Einstein was the first person to describe how *helical flow* helps to determine the length and migration of meander bends in rivers.

Amazon River, 1985

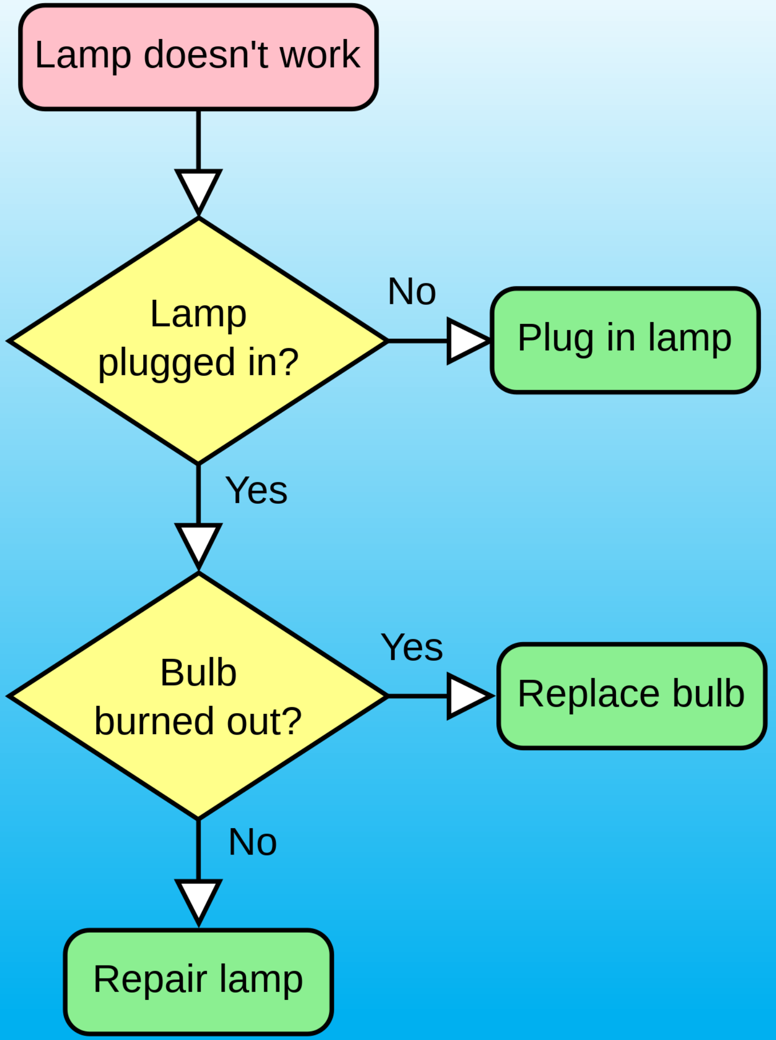


Amazon River, 2014



Modeling Definitions

- Mathematical modeling is the process of developing a mathematical representation of a system using mathematical concepts and techniques to describe the processes, interactions, and parameters of that system.
- Computer modeling is the process of developing mathematical algorithms that describe a system and then developing the computer code to simulate them.
- Modeling vs. Simulation:
  - Modeling is the process of *building* a model
  - Simulation is the process of *using* a mathematical model to study the behavior of a system *for a particular time period*.



Source: https://en.wikipedia.org/wiki/Flowchart

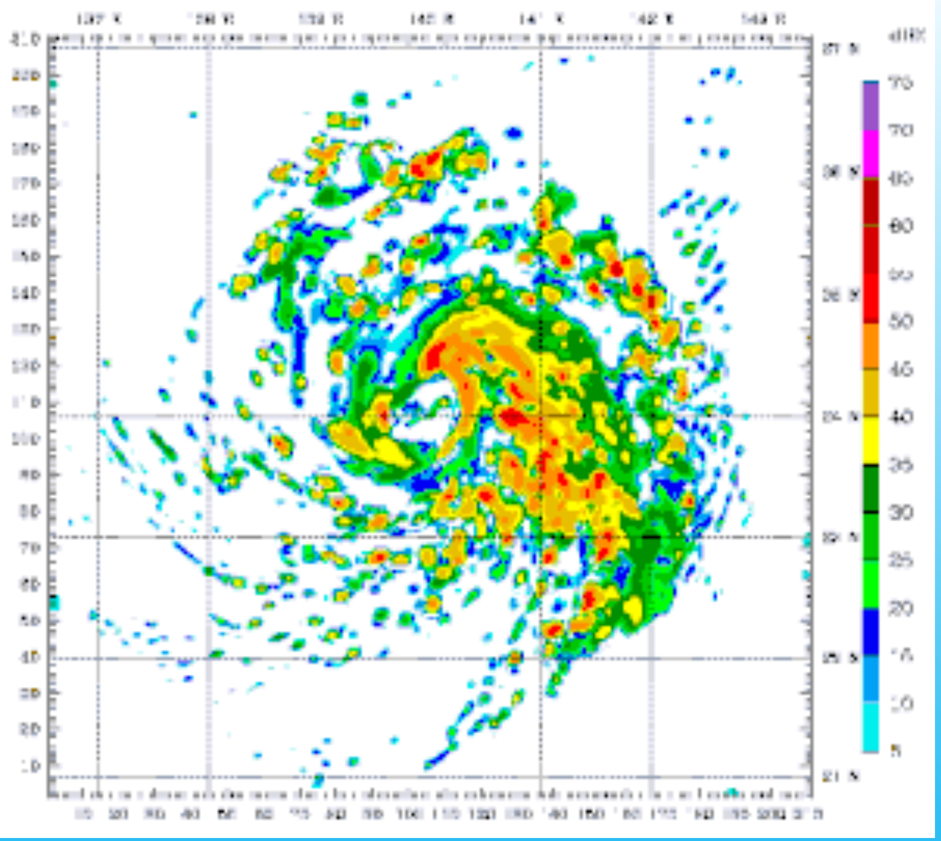
Modeling Definitions

- *Empirical* modeling uses an inductive approach, based on observations (data) and the relationships between system components, such as determined through linear and non-linear regression.
- *Mechanistic* (process-based) models use a deductive approach, based on the principles of physics, chemistry, and biology.
- Most water quality models use a mixture of empirically-derived relationships combined with iterative calculations that describe the physical and biogeochemical processes.

Source: Steven C. Chapra (1997). Surface Water-Quality Modeling. Waveland Press, Long Grove, IL.

Computer Models & Programming

- Early computer models were custom-developed applications programmed for a specific purpose, such as a water quality model of a particular lake or reservoir.
- The first *mathematical* water quality model was developed by Streeter and Phelps in 1925. It predicted the dissolved oxygen “sag curve” in rivers.
- In the 1960’s, computer models began to be developed. By the early 1970’s, general-purpose models began to emerge.
- Today’s general-purpose water resources models, e.g., HEC-RAS, HEC-ResSim, and CE-QUAL-W2, typically do not require the modeler to do any programming.
  - CE-QUAL-W2 is a general-purpose model, but it allows custom computations through modifying and enhancing the *source code*.
  - HEC-ResSim allows custom computations through “scripting.” Modelers cannot alter the source code.
  - Scripting (Python, R, MATLAB) is increasingly used for visualization and analysis of the results.



A 48-hour computer simulation of Typhoon Mawar using the Weather Research and Forecasting model.

Source: https://en.wikipedia.org/wiki/Computer_simulation

Water Quality Modeling

- Water quality modeling combines mathematical descriptions of the physical and biogeochemical processes to characterize behavior of a waterbody or water resource.
- Water resource and water quality models have been developed to understand and predict the processes in reservoirs, rivers, and watershed runoff.
- The following fields comprise the body of knowledge required for accurate water quality modeling and analysis:
    - Hydrodynamics (physical limnology)
    - Meteorology
    - Aquatic chemistry (chemical limnology)
    - Aquatic biology (biological limnology)
    - Geology (sedimentation, sediment settling, resuspension, and transport)
    - Mathematics and numerical methods
    - Statistics

Flows influence water quality

Water quality must influence flows

Benefits of Water Quality Modeling

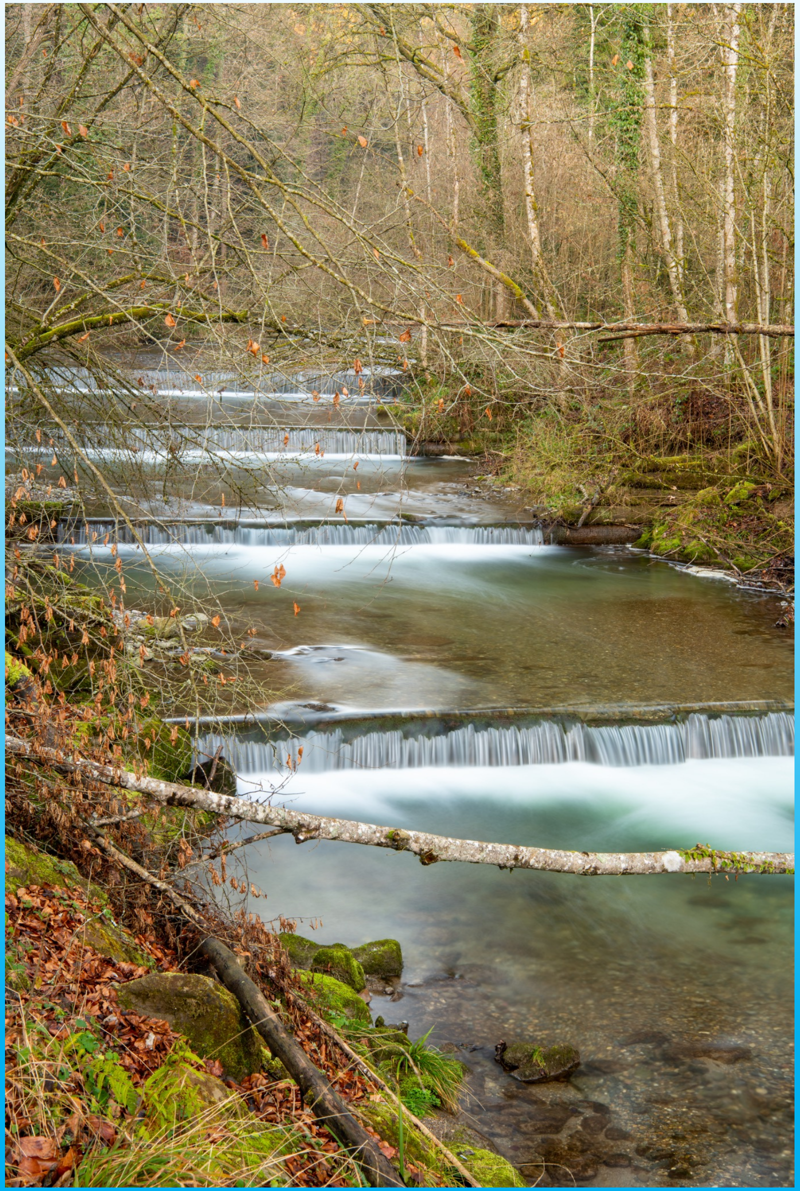
- Interpolation
  - Observed data is sparse in space and time.
  - Interpolation addresses questions like:
    - Where are the best locations for sampling?
    - Where are the most severe water quality problems occurring?
- Extrapolation
  - Forecast water quality in the future.
  - Predict water quality for different water management scenarios
  - Extrapolation answers questions like:
    - How will the watershed function under different climate forcing conditions?
    - How will the ecosystem respond if flow allocations are changed, hydropower withdrawals increased, and releases altered to meet ecosystem restoration targets (e-flows)?
- Improved understanding of the system.

Detroit Dam, Oregon

Dworshak Dam, Idaho

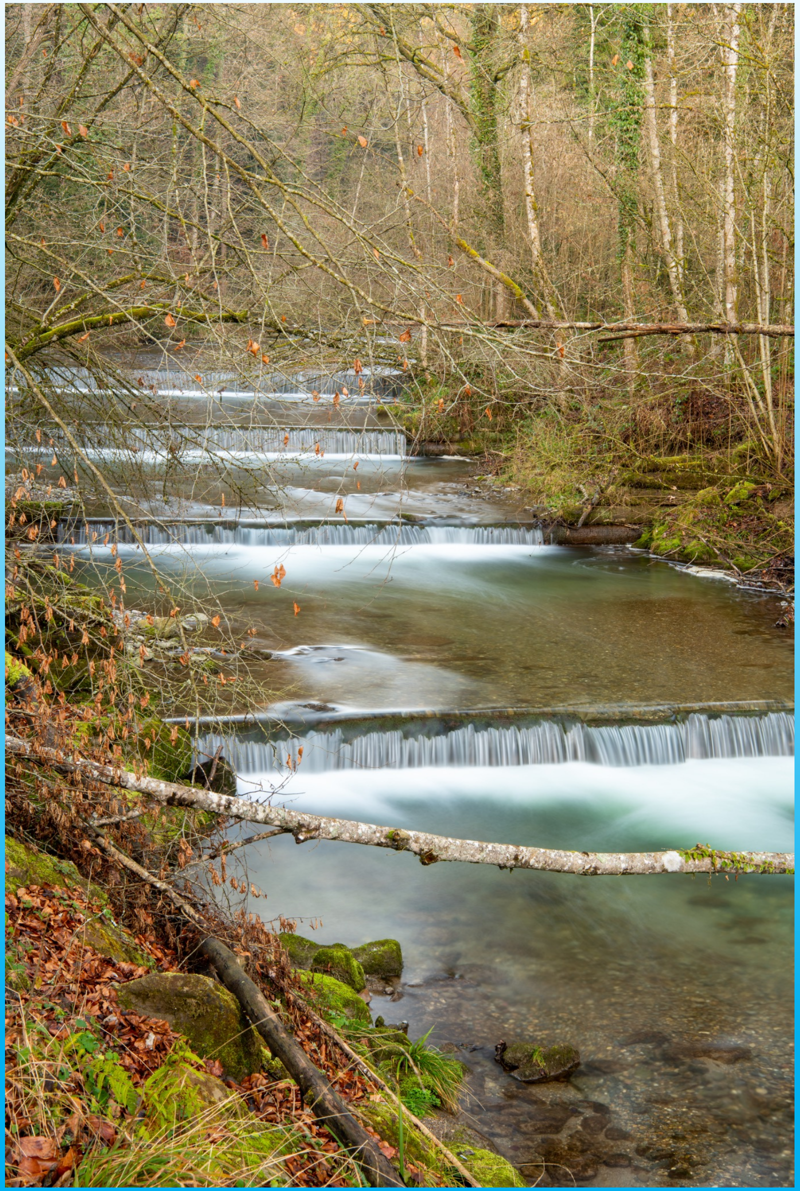
Essence of Water Quality Modeling

- Purpose: The primary goal is to understand and predict how various factors, including pollution, land use, and climate change, impact water quality.
- Simplifications: Models often use simplified representations of reality. This can include averaging data over time and space, using empirical relationships, or neglecting minor processes. Simplification helps in making models computationally feasible and easier to interpret.
  - We neglect the Coriolis force in reservoirs
  - We focus on gradually varied flow
- Assumptions: Models rely on numerous assumptions to simplify the complex interactions within water bodies.
  - We may assume that a paper mill discharges continuously at their maximum permitted level
  - We assume that lateral variations in flow and WQ are small or unimportant to the overall project goals



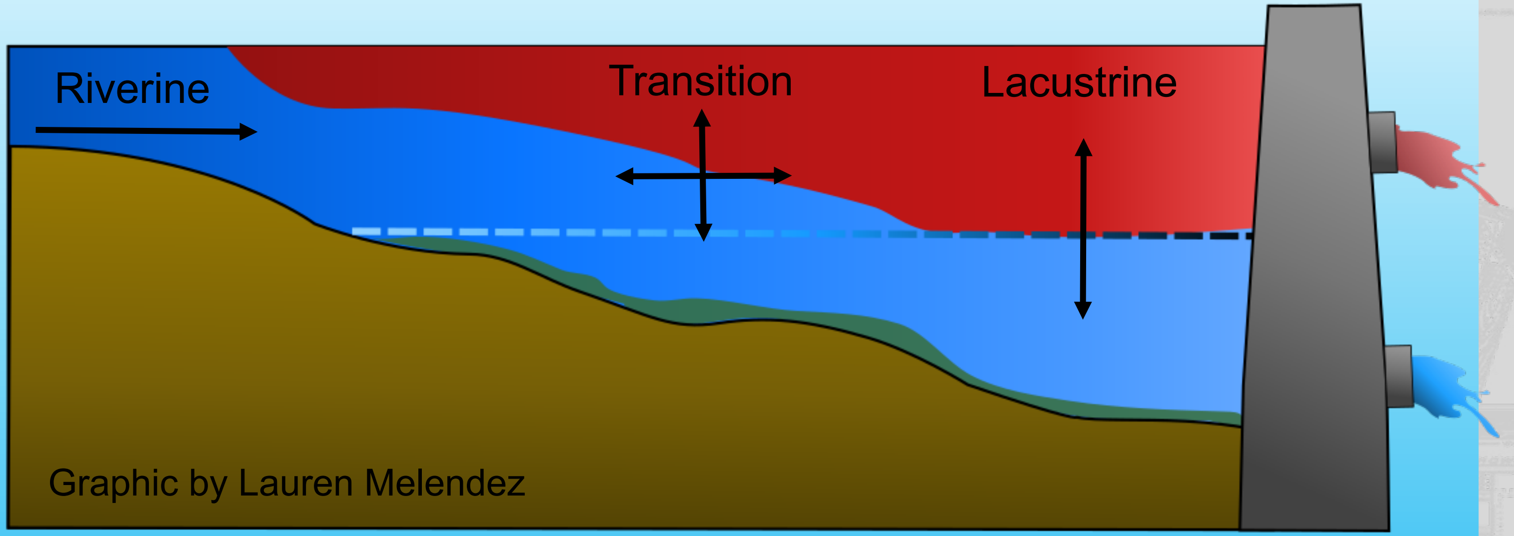
Essence of Water Quality Modeling

- Model Structure: Water quality models are typically structured into several components, including hydrodynamics (flow and transport processes), water quality constituents (e.g., nutrients, oxygen levels), and biological interactions (e.g., growth of algae). The structure and choice of model depend on the specific objectives and the scale of the study.
- Data and Calibration: Accurate and extensive data are crucial for developing reliable models. For WQ modeling, this includes data on hydrology, meteorology, water chemistry, and biological communities. Models must be calibrated and validated against observed data to ensure their accuracy and predictive capability.
- Uncertainty and Sensitivity: Uncertainty is inherent in modeling due to limited data, assumptions, and simplifications. Sensitivity analysis helps in understanding how changes in model parameters affect outcomes, highlighting the most critical factors that influence water quality.



Reservoir Processes and Zones

- Riverine zone
  - River-like flows within channel
  - Minimum requirement: 1D river model (segments)
- Lacustrine zone
  - Lake-like system, vertically stratified, slow flows
  - Minimum requirement: 1D reservoir model (layers)
- Transition zone
  - Stratification and downstream flows important
  - Minimum requirement: 2D model (layers and segments)

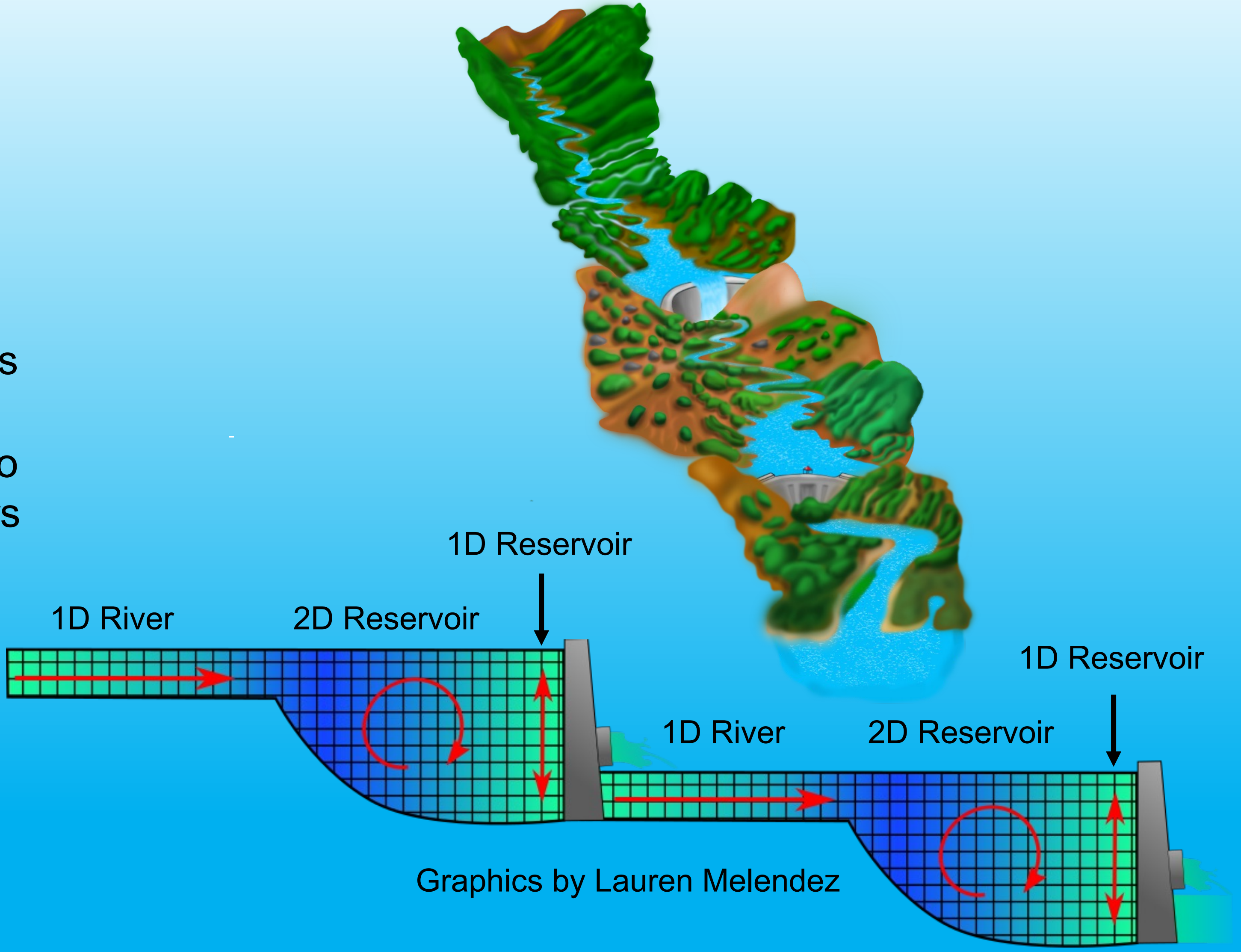


Reservoir system with important flow, WQ, and ecosystem processes for each of three zones.

Notes:
- 1D river model used for channels in a reservoir system
- 2D river model used for floodplain simulation
- 2D reservoir model used for large stratified reservoirs

Model Dimensions, River-Reservoir System

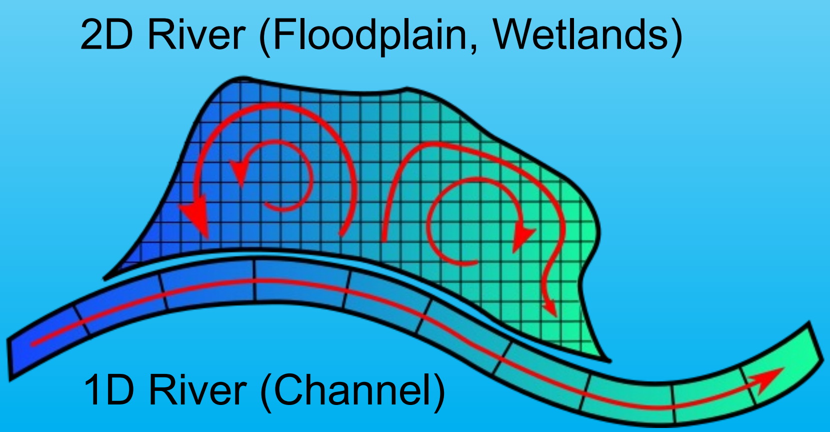
- Unstratified river/reservoir reaches:
  - May be modeled as 1D water bodies (segments)
- Stratified reaches:
  - May be modeled as 1D reservoirs (layers) for real-time release decision-making to meet downstream objectives
  - To characterize and understand in-reservoir processes, reservoirs need to be modeled as 2D water bodies (layers and segments)
    - Ensures accuracy, capturing important in-reservoir processes (mixing, pollutants, inflows, etc.)
    - Identifies vulnerabilities and restoration/management options (e.g., velocities and temperature for HAB management)

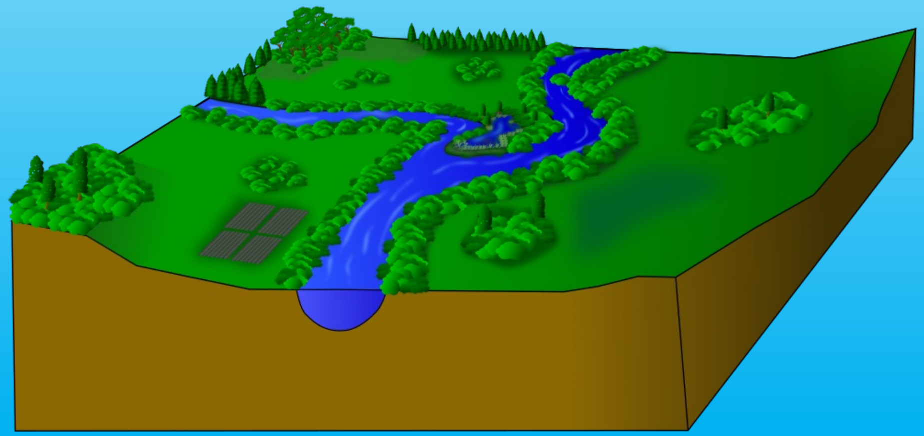


Graphics by Lauren Melendez

Model Dimensions: River-Floodplain System

- Unstratified river channels are often modeled as 1D water bodies, varying from upstream to downstream
- Hydrologic connectivity across the floodplain is important
- Floodplains need to be modeled as 2D water bodies, varying in all directions across the landscape

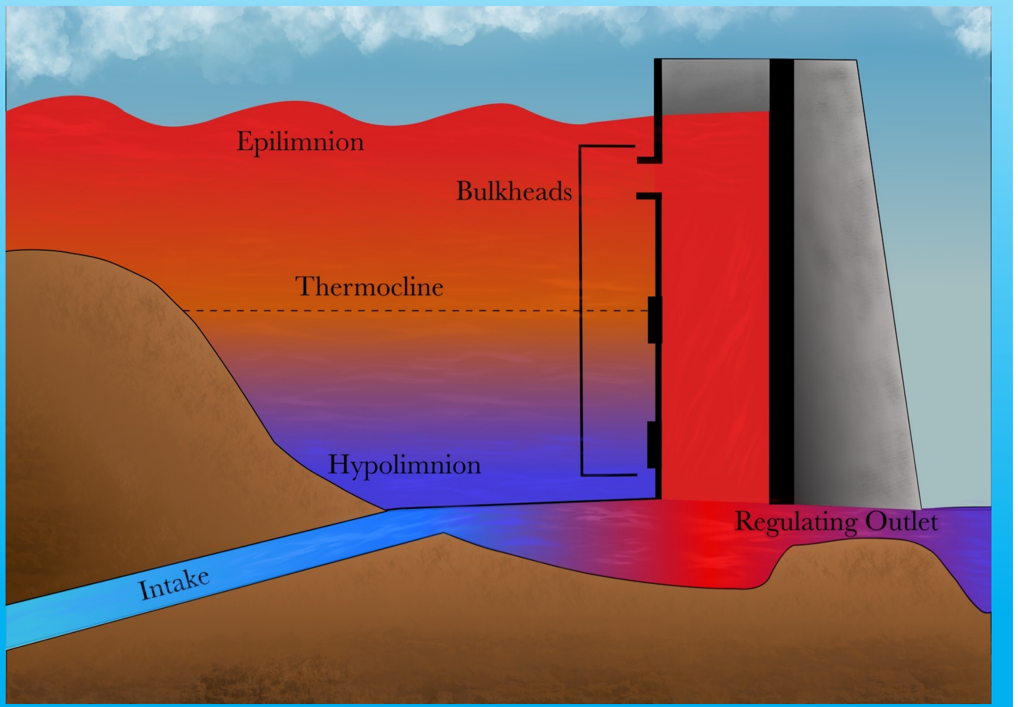


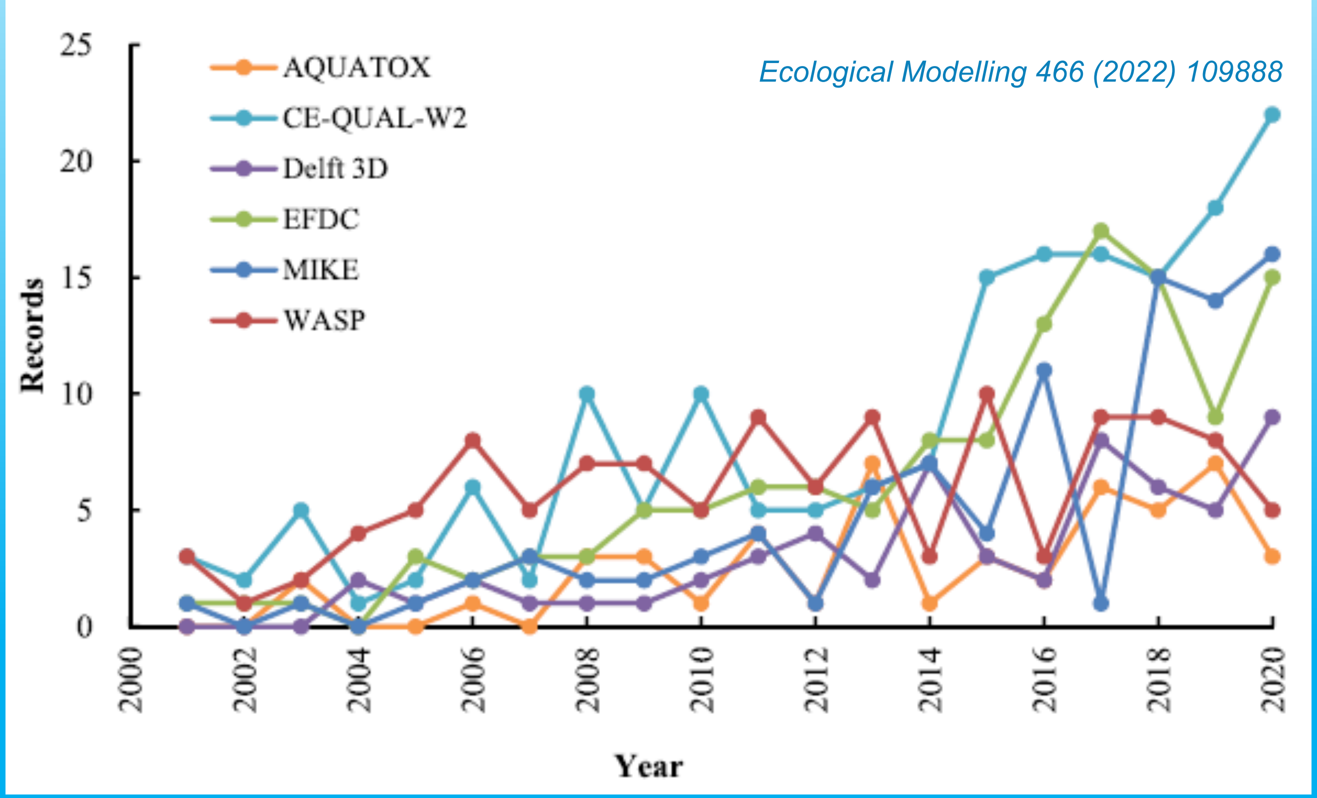


Graphics by Lauren Melendez

CE-QUAL-W2

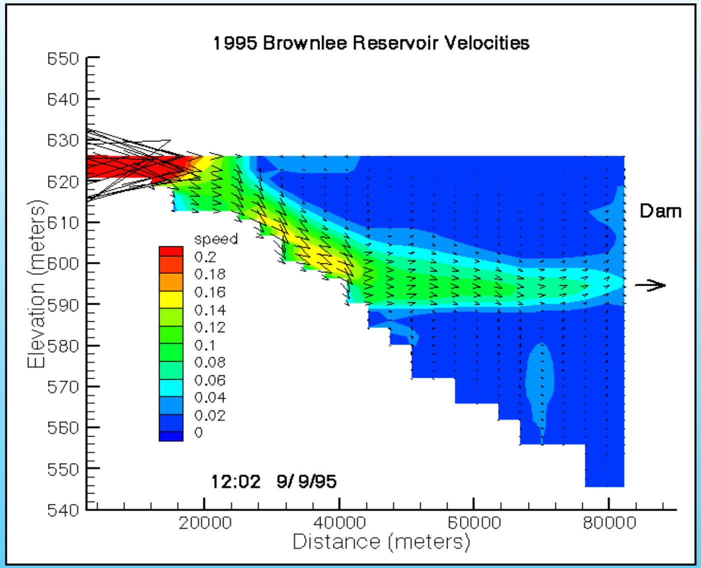
- CE-QUAL-W2 is a two-dimensional (2D), longitudinal/vertical, hydrodynamics and water quality model that enables characterization of vertical and longitudinal changes in reservoirs.
- The model assumes reservoirs are *well mixed* laterally, with no variation from one channel side to the other in a layer (vertical) and segment (longitudinal).
- CE-QUAL-W2 has been applied to rivers, lakes, reservoirs, and estuaries.

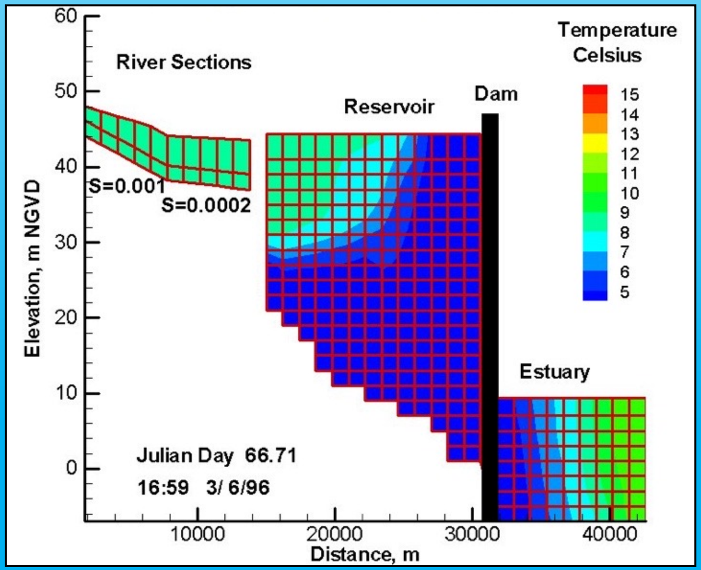




CE-QUAL-W2 Capabilities

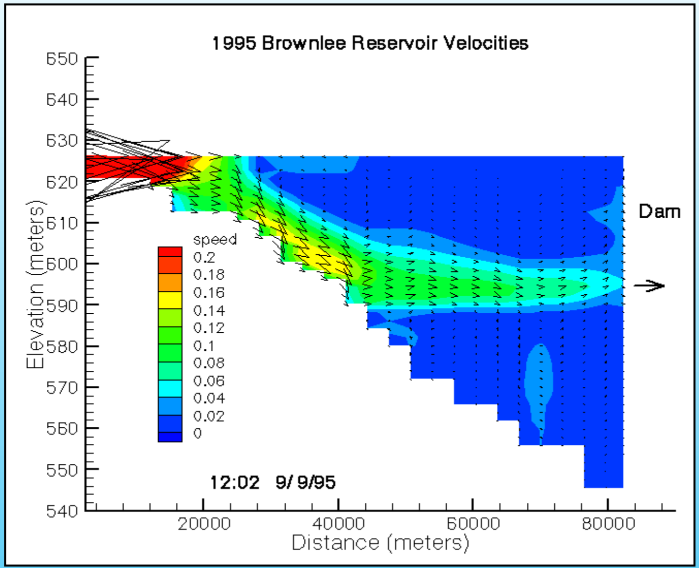
- Longitudinal-vertical hydrodynamics and water quality in stratified and non-stratified systems
- Nutrients-dissolved oxygen-organic matter interactions
- Fish habitat
- Selective withdrawal from stratified reservoir outlets
- Hypolimnetic aeration
- Multiple algae, epiphyton/periphyton, zooplankton, and macrophytes
- CBOD
- Sediment diagenesis model
- Generic water quality groups
- Internal dynamic pipe/culvert model
- Hydraulic structures (weirs, spillways) algorithms, including a dynamic shading algorithm based on topographic and vegetative cover.
- Water age

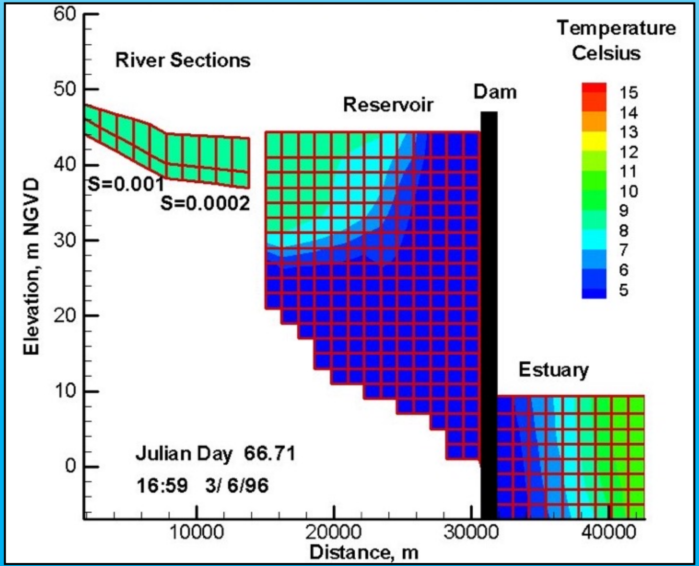




CE-QUAL-W2 Capabilities, Continued

- The hydraulic structures algorithms include submerged and two-way flow over submerged hydraulic structures as well as a dynamic shading algorithm based on topographic and vegetative cover.
- Variable density as affected by temperature, salinity, Total Dissolved Solids (TDS), and Total Suspended Solids (TSS) to simulate stratified flow.
- 28 water quality constituent state variables
    - Any combination of constituents can be included or excluded from a simulation.
    - The effects of salinity or total dissolved solids/salinity on density, and thus hydrodynamics, are included only when simulated in the water quality module.
    - The water quality algorithm is modular, allowing constituents to be easily added as additional subroutines.



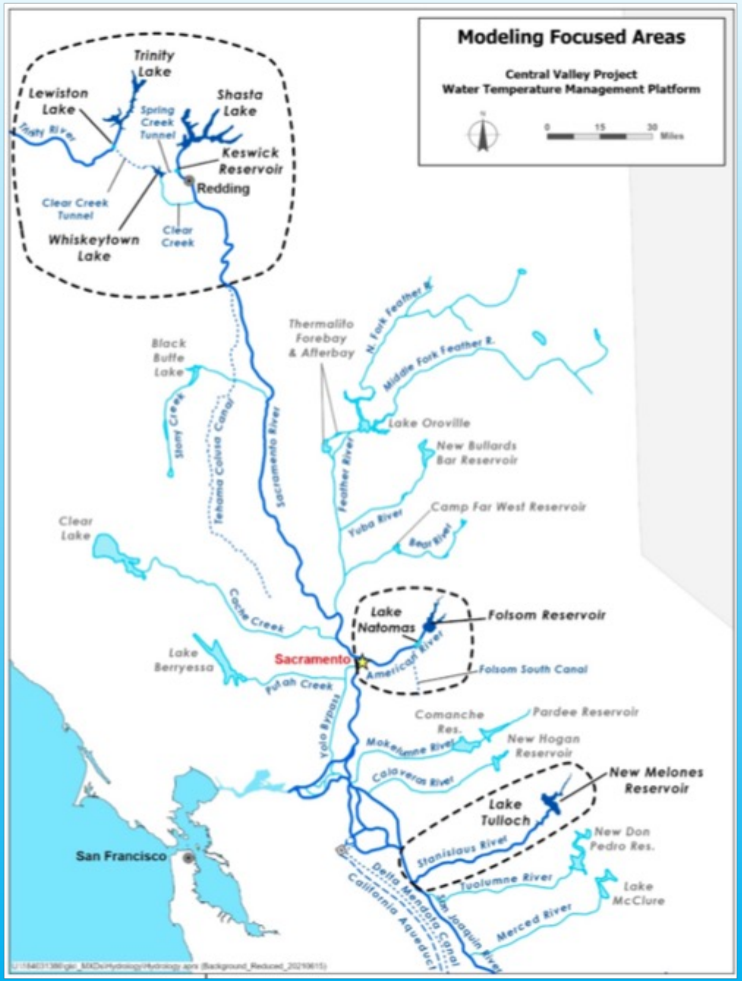


Past and Current Applications of CE-QUAL-W2

- CE-QUAL-W2 is widely used by USACE and other federal, state, and local agencies for environmental impact assessments, planning studies, etc. Agencies that use CE-QUAL-W2 as their standard reservoir water quality model include:
  - U.S. Geological Survey (USGS)
  - U.S. Bureau of Reclamation
  - U.S. Environmental Protection Agency (EPA)
  - State of California
- More than 1,100 model applications have been developed worldwide for reservoirs, rivers, estuaries, and other water bodies since CE-QUAL-W2 was released in 1986.
- CE-QUAL-W2 is also used as a research tool by researchers at universities and other organizations.
- At least 1,500 publications utilized or cited CE-QUAL-W2 in the year 2022 alone.

Recent Studies:

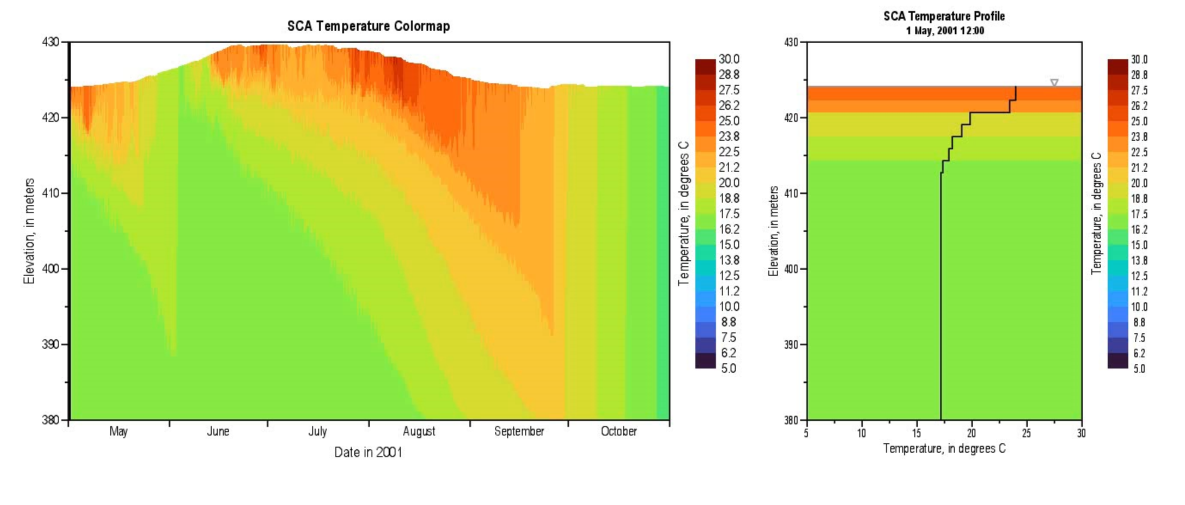
- Water Temperature Modeling Platform, California Central Valley Project (USBR and State of California): This platform applies CE-QUAL-W2 for ongoing and future operations decision-making
- USACE Northwest Division, Columbia and Snake River Watershed
  - ▶ Columbia System Reservoir Operation (CRSO) Project
  - ▶ Columbia River Treaty (CRT) Project
- Philadelphia District, Lehigh River Water Quality Modeling

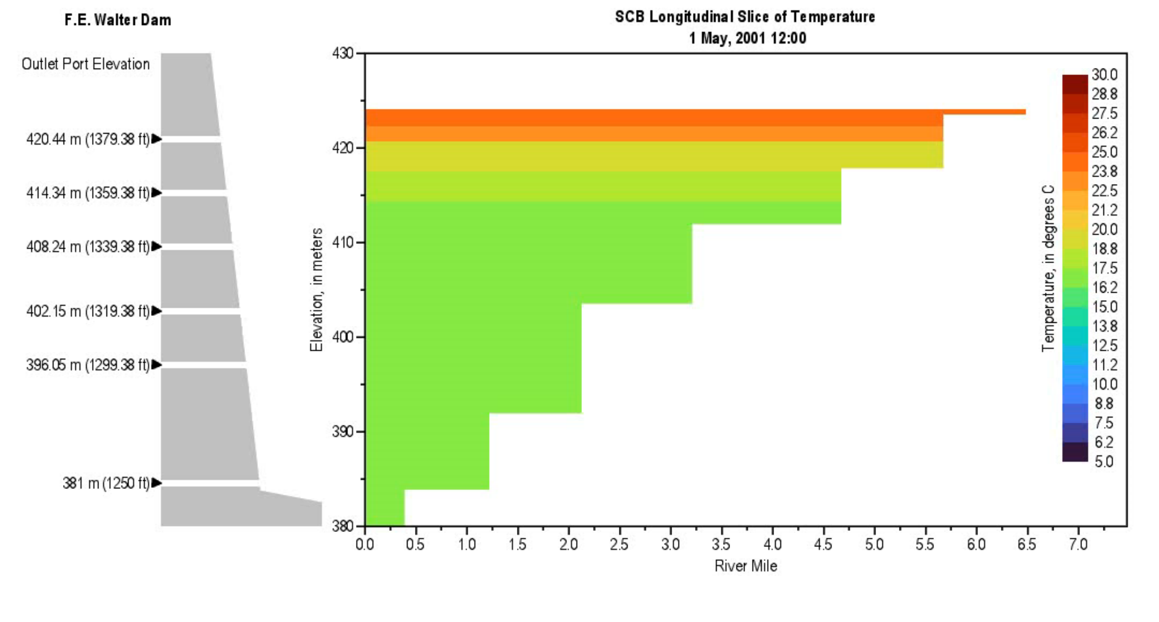


Region of Application:
Water Temperature Modeling Platform
California Central Valley Project

CE-QUAL-W2 Model Benefits

- CE-QUAL-W2 has been extensively used and tested on over 1,100 water bodies since it was first released in 1986.
- CE-QUAL-W2 enables detailed study of temperature stratification, contaminant distribution, and nutrient dynamics across diverse aquatic environments including rivers, reservoirs, lakes, and estuaries.
- In contrast with reservoir models with 1D hydrodynamics, CE-QUAL-W2 accurately simulates vertical and *longitudinal* transport of constituents, which can be as important as chemical kinetics in accurately simulating water quality.
    - This is important where thermal and/or water quality gradients exist due to pollutant inflows and/or short reservoir retention times.
- The model also incorporates advanced features relevant to fish habitat, selective withdrawal strategies, hypolimnetic aeration, and the dynamics of various algae types, as well as sediment diagenesis processes critical for understanding harmful algal bloom dynamics.





Acknowledgements

CE-QUAL-W2 Team:
- Todd Steissberg, Lead Developer, USACE ERDC
- Lauren Melendez, Course Coordinator, USACE ERDC
- Scott Wells, Professor, Portland State University
- Zhonglong, Zhang, Developer, Portland State University
- Isaac Mudge, Developer, USACE New Orleans District

Funding and Support:
- USACE Numerical Model Maintenance Program, Hydraulics, Hydrology, and Coastal Community of Practice (HH&C CoP)
- Ecosystem Management and Restoration Research Program (EMRRP)
- Aquatic Nuisance Species Research Program (ANSRP)

Graphics by
Lauren Melendez

Questions?