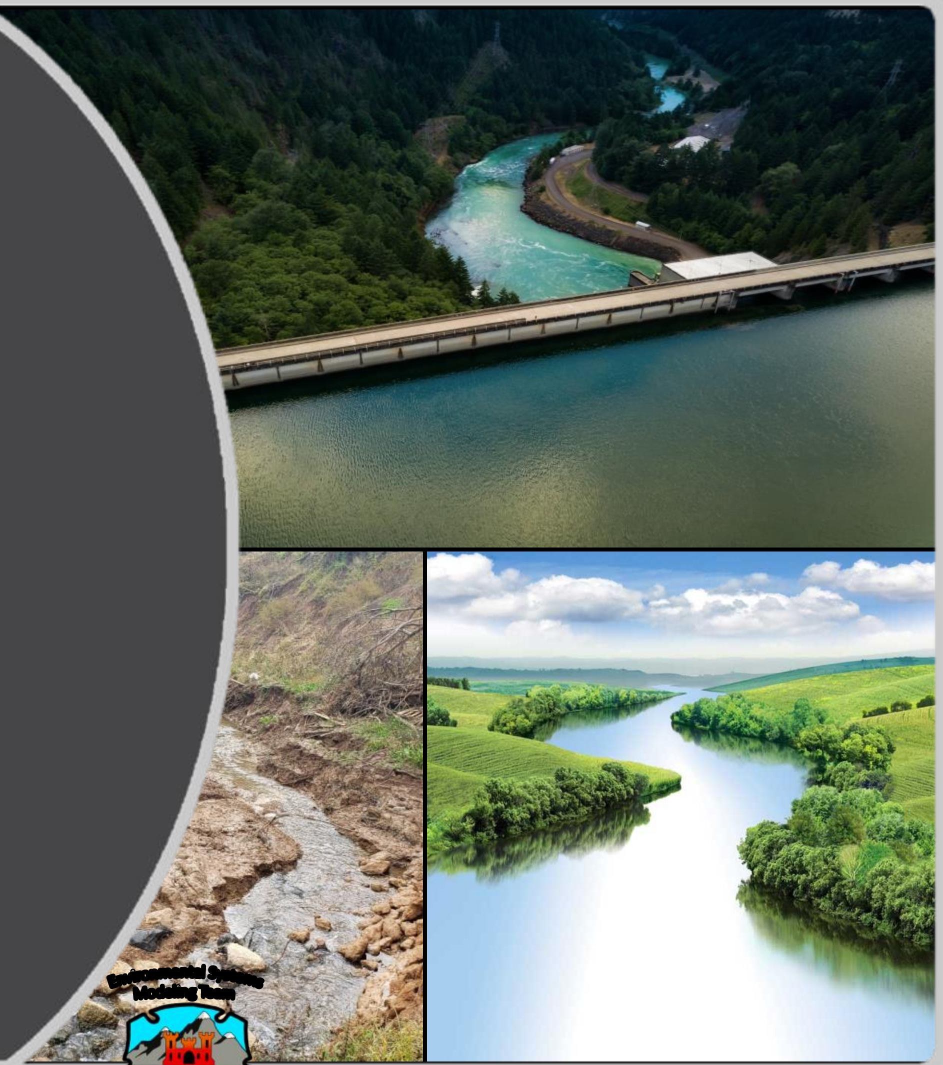
CE-QUAL-W2 CALIBRATION/VALIDATION



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Water Quality Model Application Processes

Phase I	Data collection Model input preparation Parameter evaluation
Phase II	Calibration Validation
Phase III	Analysis of alternatives

Model Calibration

- In EPA guidance, calibration is defined as the process of adjusting model parameters within physically defensible ranges until the resulting predictions give the best possible fit to the observed data (EPA 1994).
- In some disciplines, calibration is also referred to as parameter estimation (Beck et al. 1994).
- Calibration parameters are parameters whose values are uncertain.
- Adjustments for calibration parameters should be constrained by physically sensible limits.
- Calibration is an iterative process whereby model coefficients are adjusted until an adequate fit of observed versus predicted data is obtained.

Model Calibration

- Model parameter/coefficient values are adjusted manually by trial and error. This requires the user to do multiple runs of the model.
- Sufficient observed data must be collected to allow for an accurate calibration as well as analysis of different alternatives in the system.
- The model cannot be expected to be more accurate than the errors (confidence intervals) in the input and observed data. You cannot calibrate the model to any greater accuracy than the inherent uncertainty associated with the data used to develop the model.

Calibration Process

- Begin with literature values for model parameters
  - Adjust within acceptable ranges, until…
  - Model results “match” observed data

- Start with hydrodynamics

- Get temperature right
  - Assessed with water temperature profiles

- Proceed to water quality
  - Inorganic suspended solids

- Assess visually, as well as statistically
  - Graphical plots of model vs. data
  - Mean absolute error, percent bias, relative percent error

Calibration Performance Evaluation

- Both graphical comparisons and statistical evaluation are used in model calibration and validation
- Graphical comparisons
  - Time series plots of modeled results and observed data for state variables (e.g., nutrient concentrations) or fluxes (e.g., flow x concentration)
  - Modeled and observed scatter plots, with 45^{o} linear regression line displayed, for state variables or fluxes

Calibration Performance Evaluation

- Performance statistics:
  - Error statistics, e.g., mean error (ME), absolute mean error (AME), relative bias (PBIAS), standard error of estimate, etc.
  - Correlation tests, e.g., Coefficient of determination (R^2), Nash-Sutcliffe efficiency (NSE), etc.
- There is no single accepted performance statistic or standard that determines whether a model is valid.

Performance Error Statistics

Mean Absolute Error (MAE)

$$MAE = \frac{1}{n}\sum_i \left|\left(OV_i - MV_i\right)\right|$$

Mean Error (ME)

$$ME = \frac{1}{n}\sum_i \left(OV_i - MV_i\right)$$

Root Mean Square Error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_i (OV_i - MV_i)^2}$$

Nash-Sutcliffe efficiency (NSE)

$$NSE = 1.0 - \frac{\sum_i (OV_i - MV_i)^2}{\sum_i (OV_i - \overline{OV})^2}$$

Percent bias (PBIAS)

$$PBIAS = \frac{\sum_i \left(OV_i - MV_i\right)}{\sum_i OV_i} * 100$$

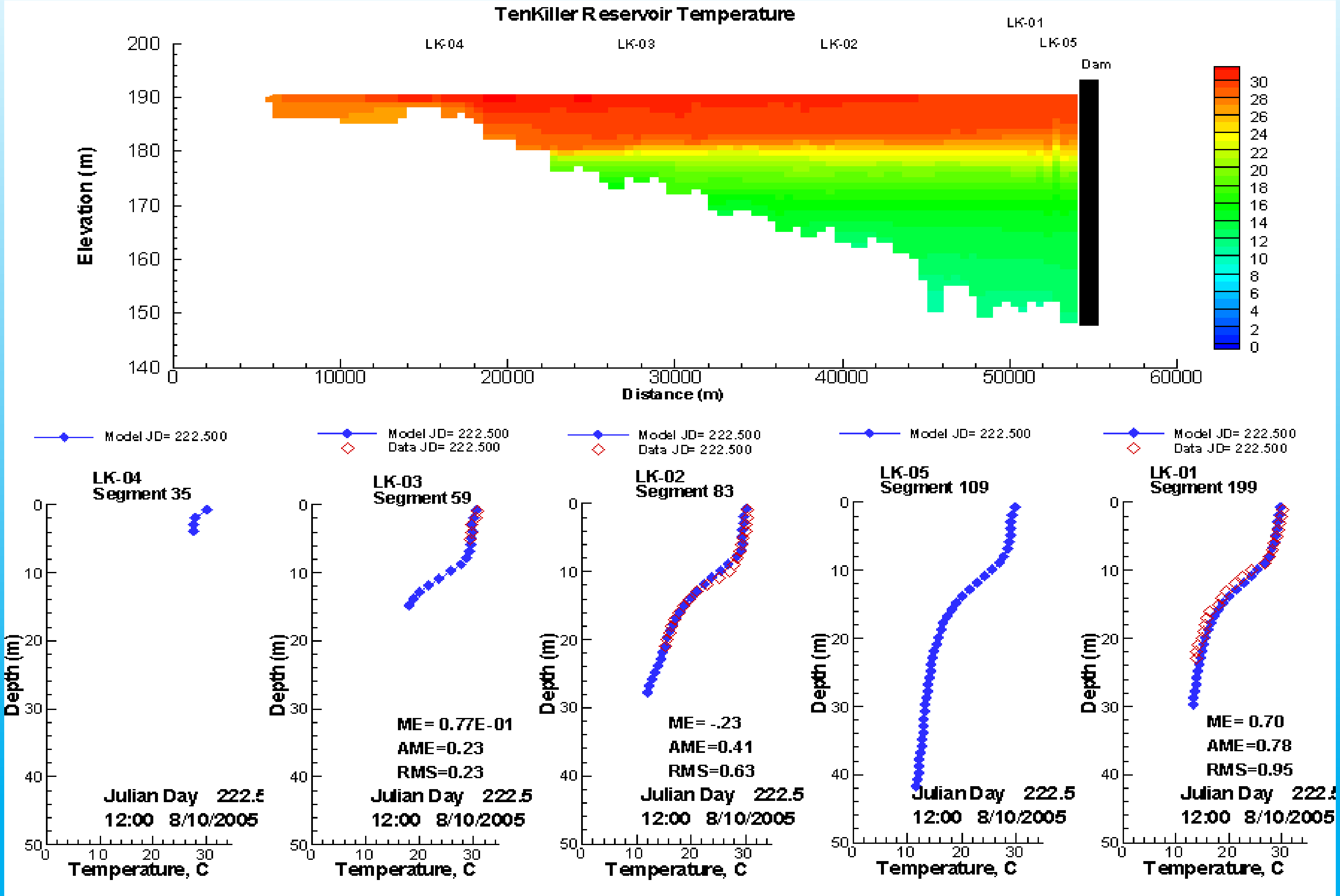
Coefficient of determination R^2

$$R^2 = \frac{\left(\sum_i (OV_i - \overline{OV})(MV_i - \overline{MV})\right)^2}{\sum_i (OV_i - \overline{OV})^2 \sum_i (MV_i - \overline{MV})^2}$$

Calibration Data

- Flow and water level data
- Outflow temperature and water quality data
- In-reservoir or river temperature and water quality data
  - Temperature profiles
  - Dissolved Oxygen and Nutrient profiles
  - Time Series
- Algae data
  - Algal speciation
  - Functional groups
- Secchi disk depth

Calibration Data



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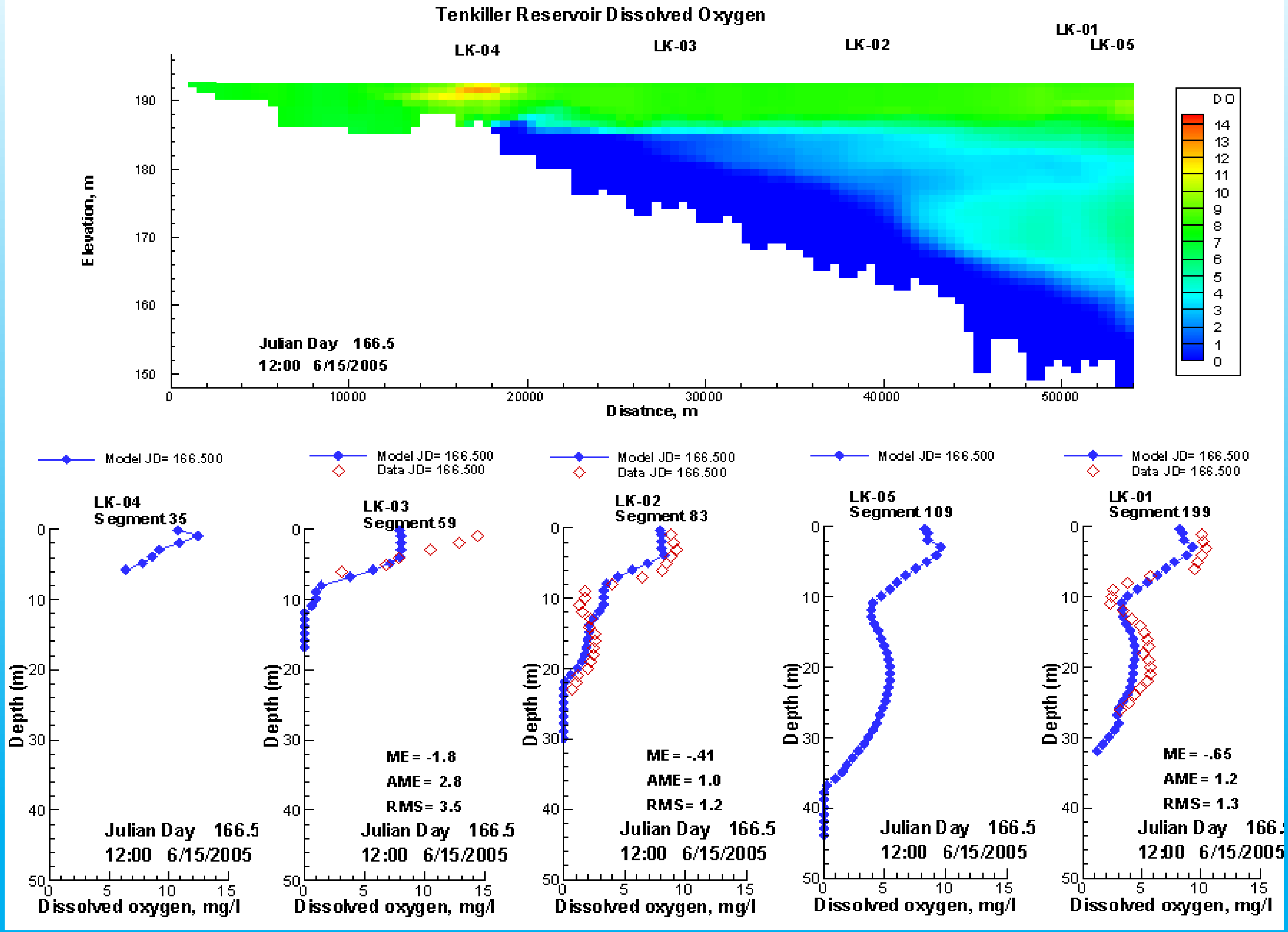
Calibration Data



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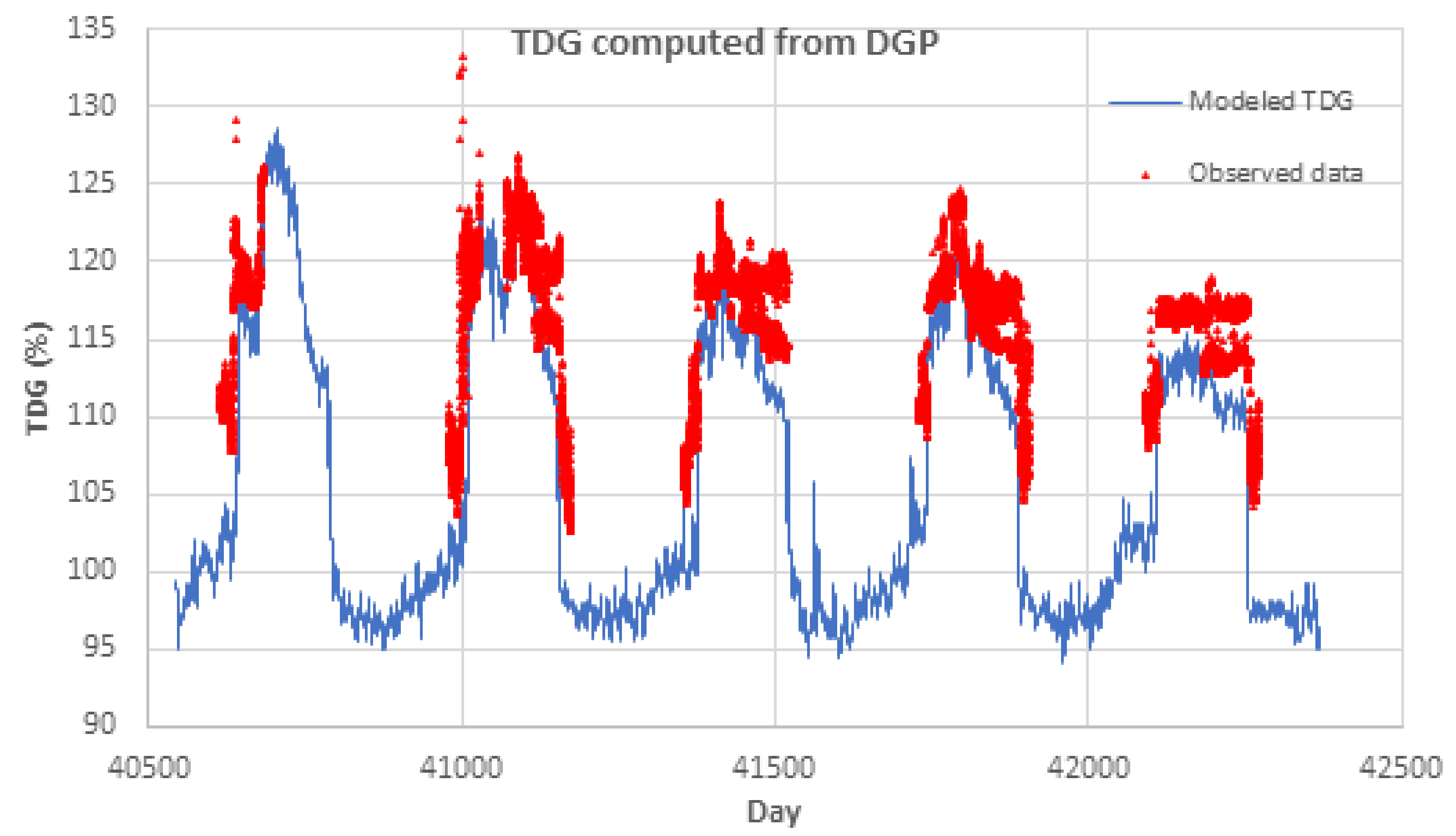

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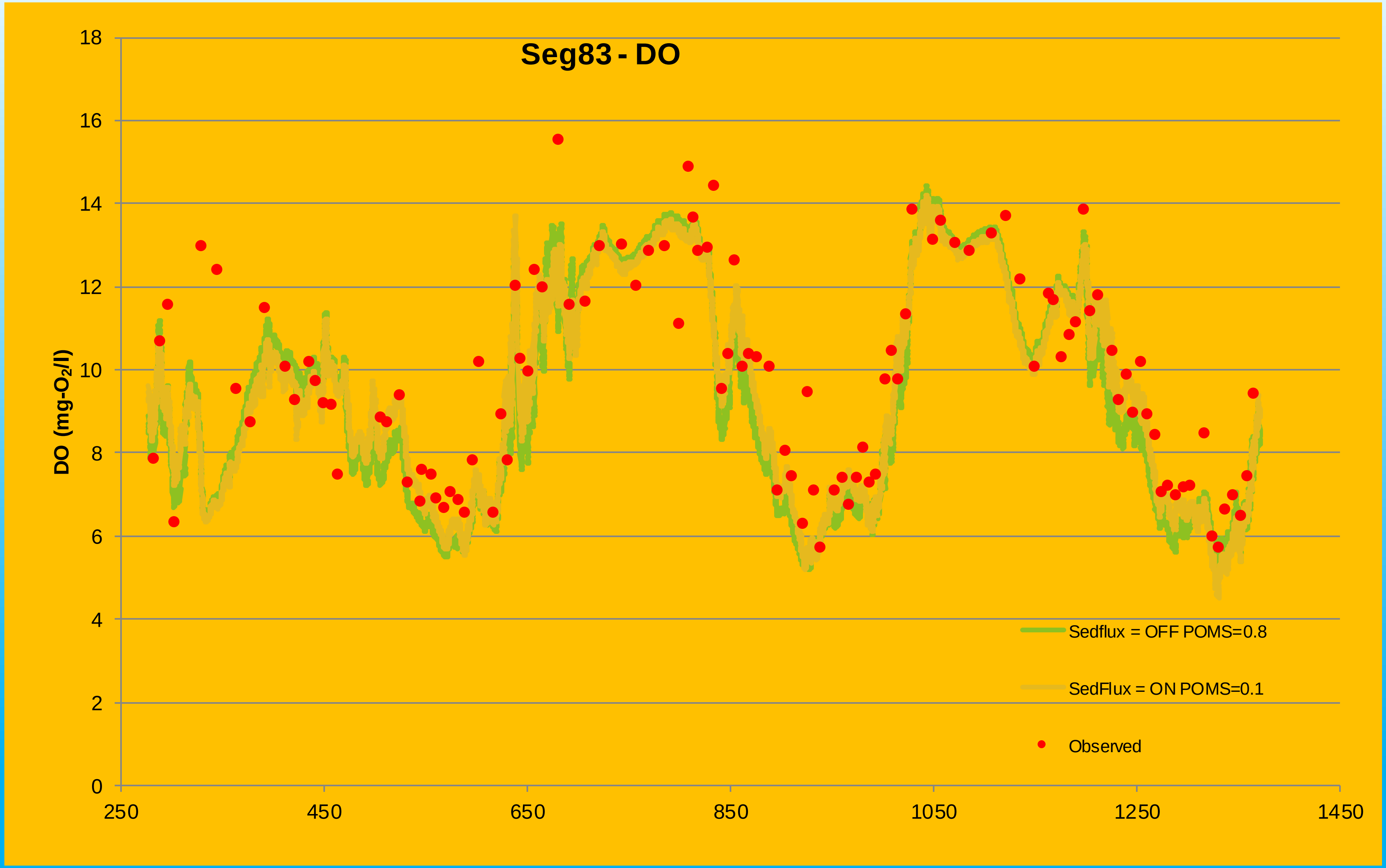


Hydrodynamics/Water Temperature Calibration Parameters

- longitudinal eddy viscosity (*Ax*)
- vertical eddy viscosity (*Az*)
- bottom friction
- sediment heat exchange
- wind-sheltering coefficient
- interaction with density field - SS, TDS, etc
- bathymetry of the model

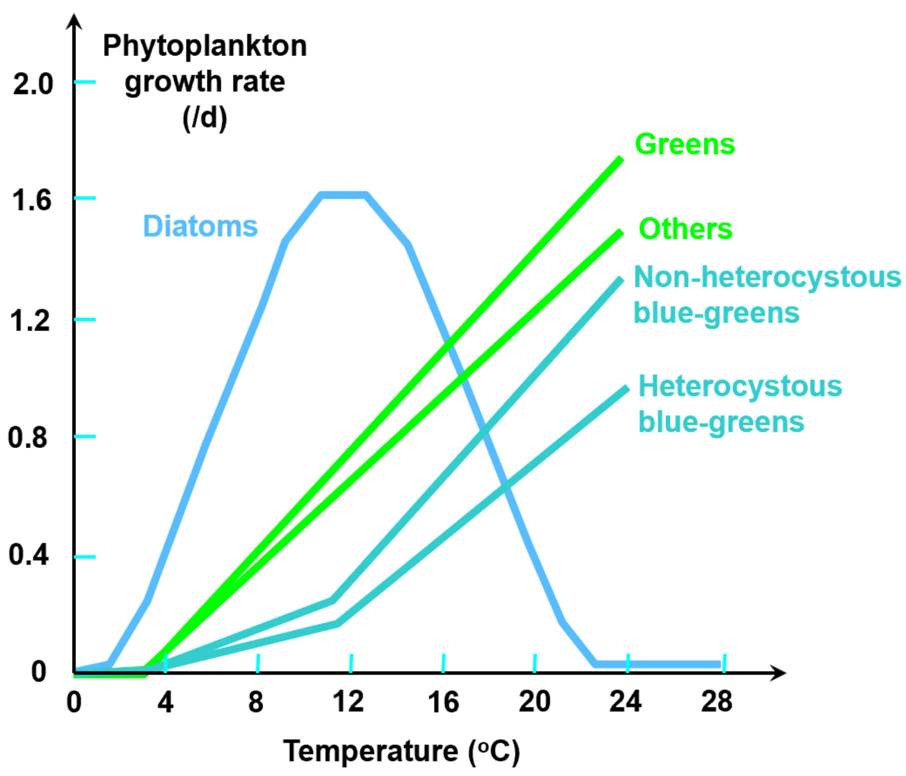
Water Quality Calibration Parameters

For water quality simulations, calibration parameters are varied widely, , it is preferable to obtain actual measurements of water quality coefficients such as CBOD decay rates…

$$CBOD_5 = CBOD_u\left(1 - e^{-k_d(5)}\right)$$

$$CBOD_u = \frac{CBOD_5}{1 - e^{-k_d(5)}}$$

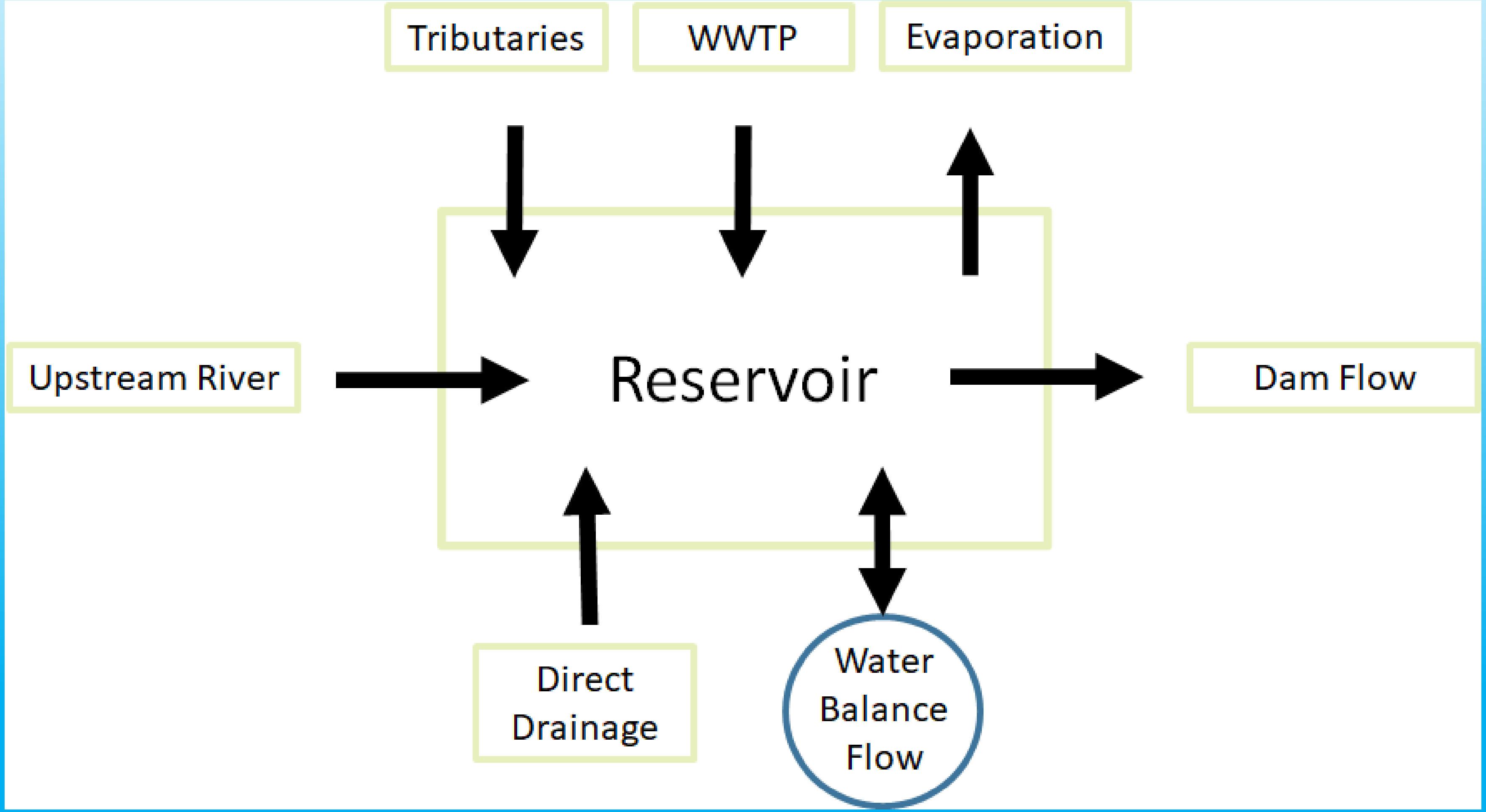
- Phytoplankton
- Dissolved oxygen
- Zooplankton
- Inorganic N and P



Courtesy of Dr. Chapra

Fluid, Mass and Energy Balance

Have you accounted for all water?



Water Quality Model Calibration Suggestions

- Make sure model output is appropriate.
  - Averaged vs instantaneous
- Only tweak appropriate model input parameters/coefficients.
  - Physically relevant
- Begin with literature values for model parameters.
- Start with water temperature and proceed to other water quality constituents.
  - All reactions are temperature dependent

Water Quality Model Calibration Suggestions (cont.)

- Do not force a calibration to fit with unrealistic water quality parameter’s values

- Use sensitivity analysis to investigate relations between observations, parameters, and model predictions

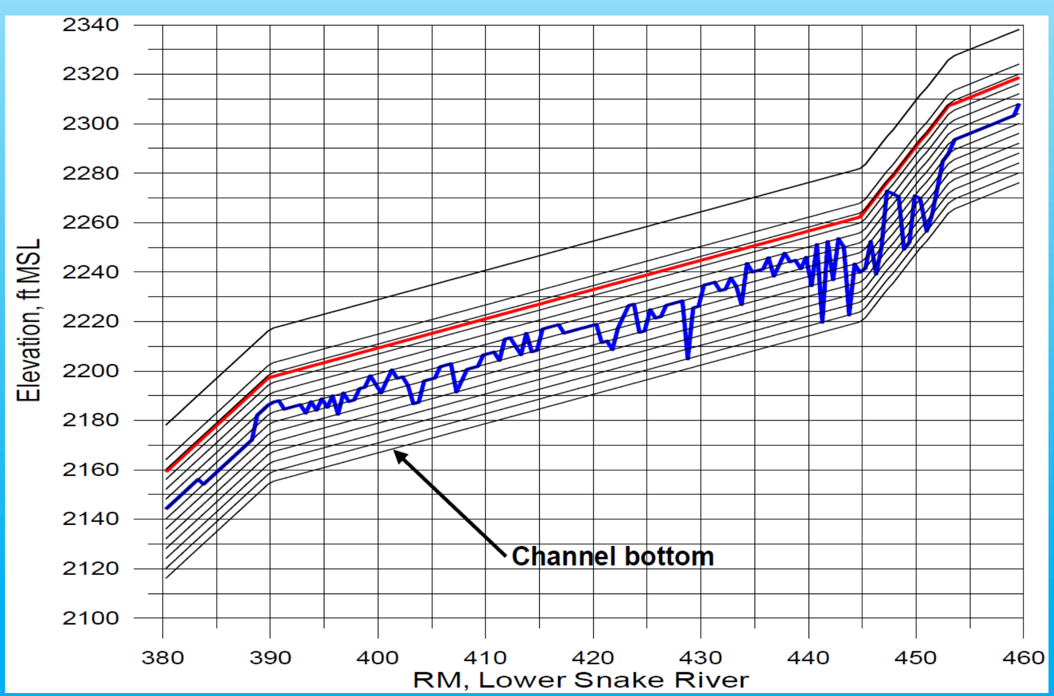
W2 Model Stability

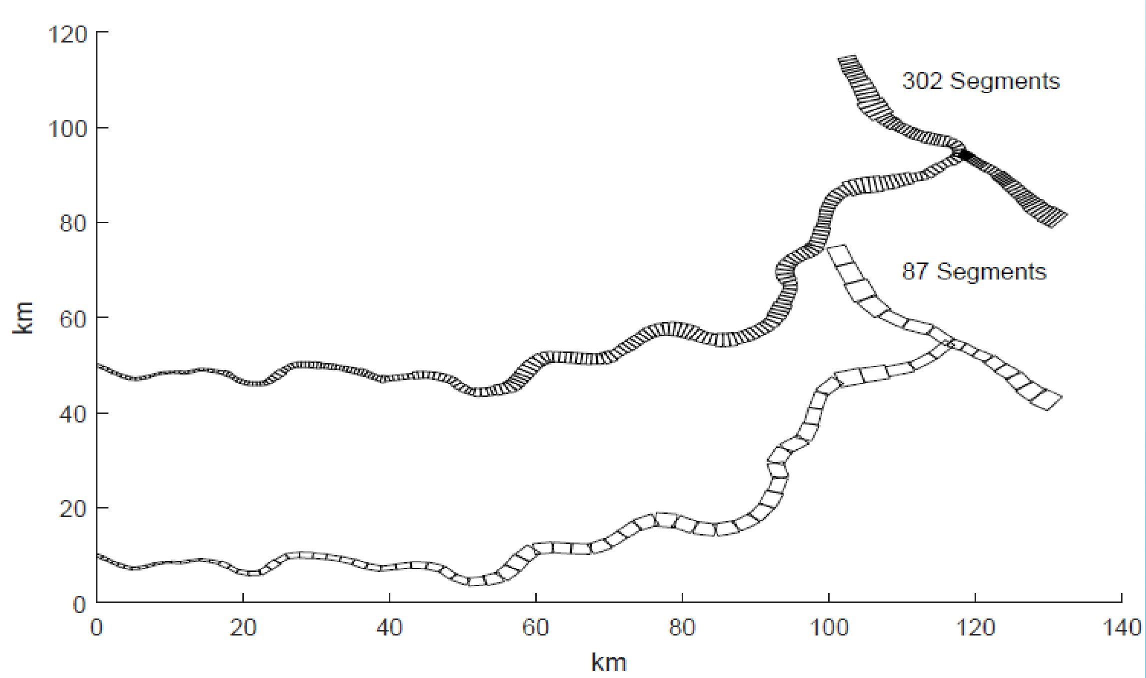
- The W2 model works with dynamic time steps. Auto-time-stepping does not guarantee numerical stability.

- Defining the time steps for calculations is a key factor.
  - Large time steps lead to stability violation and very small time-steps increase the computation time.
  - To have the stability, the spatial and temporal steps (Δx and Δt) should be fine enough.
  - The timestep adjustment is based on the characteristics of the waterbody and boundary conditions.

W2 Model Stability

- The minimum timestep is useful during periods of extremely high flows.
- UPWIND, QUICKEST, or ULTIMATE with the latter being the recommended option.
- W2 grid resolution affects the model's stability





Questions?