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CE-QUAL-W2 MODEL CALIBRATION/VALIDATION

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CE-QUAL-W2 Workshop

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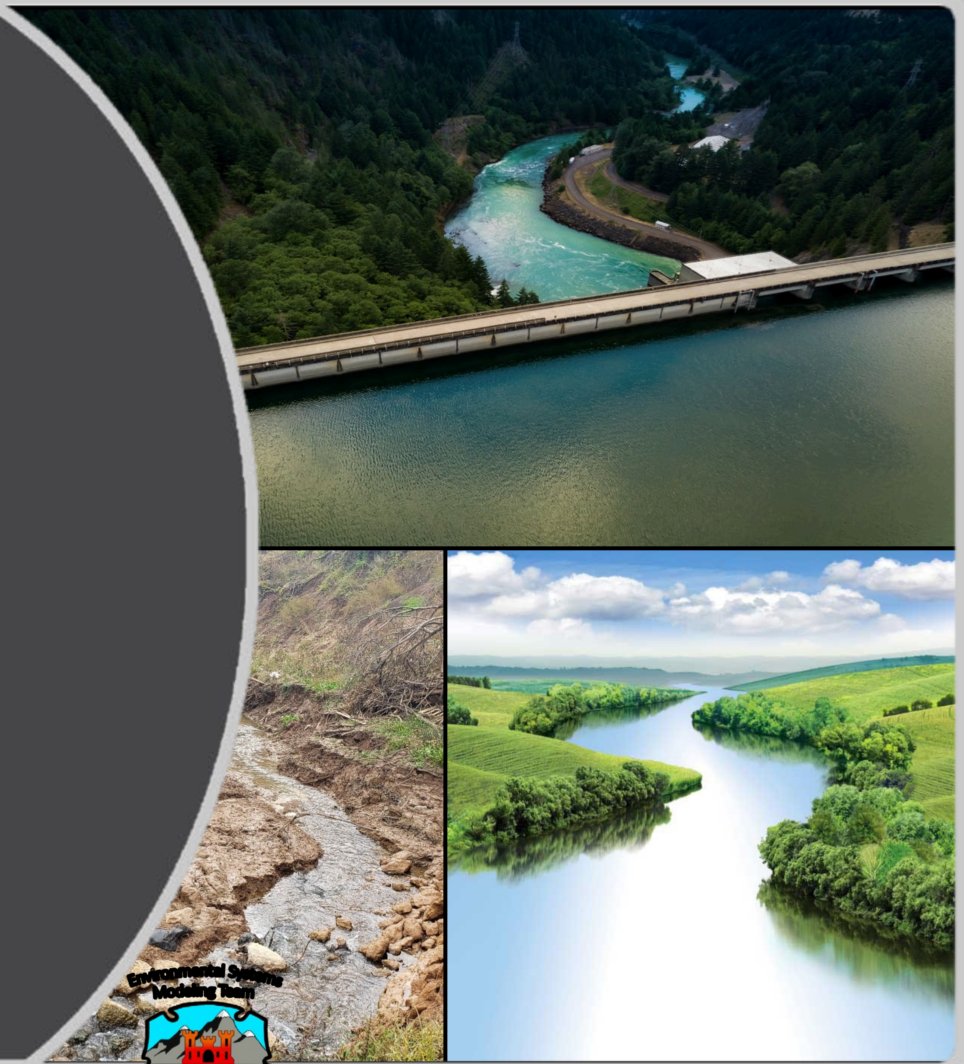

Environmental Systems Modeling Team

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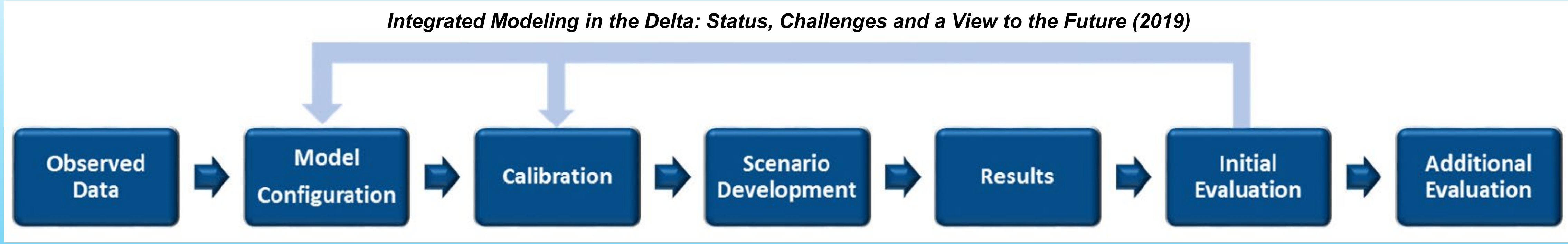
Water Quality Model Application Processes



- Use observed data from the field to configure and calibrate the model
- Apply to various scenarios
- Report results
- Model results are compared against field data and can be subjected to a variety of tests to evaluate performance
- Additional evaluation such as sensitivity and uncertainty analysis maybe required.

Model Calibration/Validation

- 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).
- A portion of the simulation period will be reserved for model validation. Data availability may impact calibration and validation periods.
- 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/Validation

- 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.

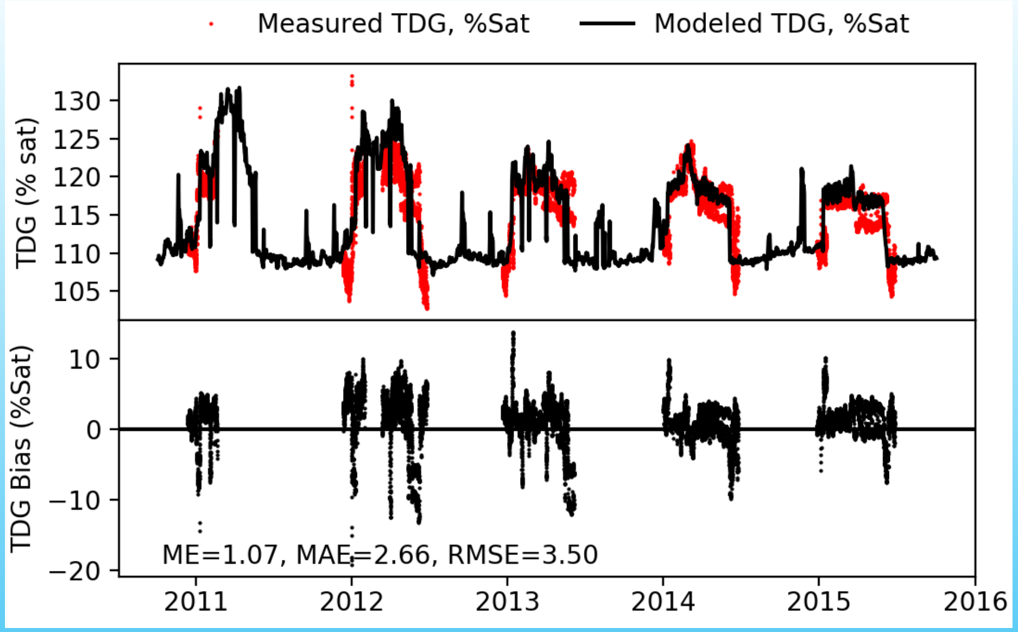
Model Calibration Process

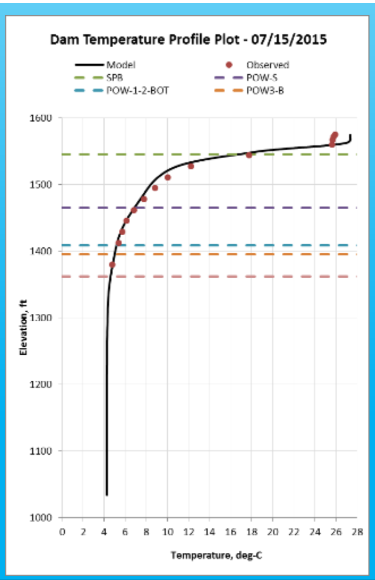
- Begin with literature values for model parameters
  - Adjust within acceptable ranges, until…
  - Model results “match” observed data
- Start with hydrodynamics
  - Fluid and energy balance checks
  - Ensuring the model reproduces flow and water level at various control points in the model domain
- Get temperature right
  - Assessed with water temperature profiles
  - Ensuring accurate meteorological data
- Proceed to water quality
  - Inorganic suspended solids
  - Phytoplankton
  - Dissolved oxygen
  - N and P

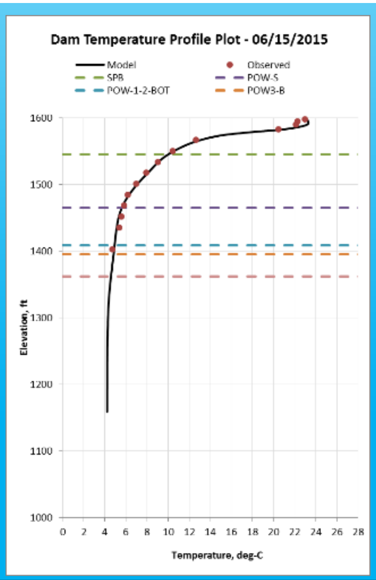
Model Performance Evaluation

- Model results will be presented graphically and statistically for assessment
  - Graphical plots of model vs. data
  - Calculate model performance statistics

- 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 45º linear regression line displayed, for state variables or fluxes
  - Profile plots







Model 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

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

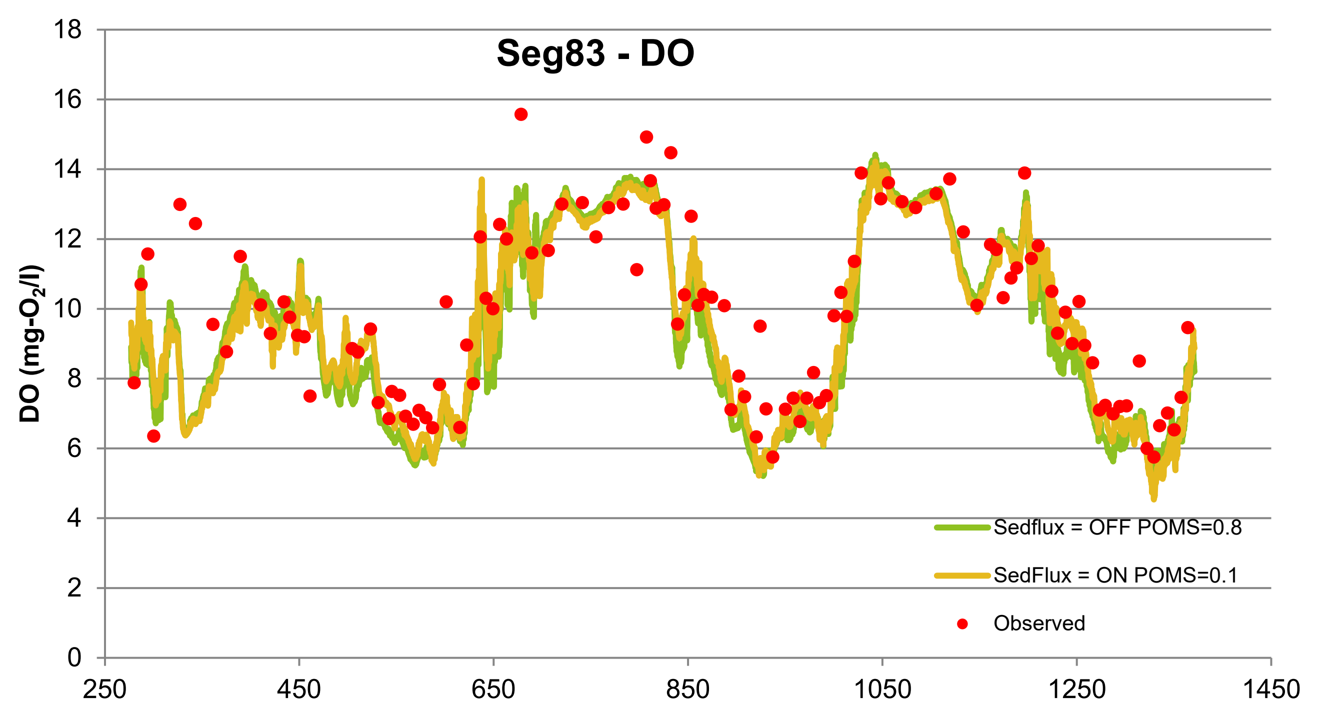
Model Performance Error Statistics

- Performance statistics:
  - Mean absolute error (MAE) determines the average magnitude of the difference between simulated and observed values
  - Relative error (RE) averages the differences between each simulated value and the observed value
  - Root mean square error (RMSE) is the measure of the differences between values predicted by a model and the observed or measured values.
  - R^2 describes the degree of collinearity between simulated and measured data
  - Nash-Sutcliffe efficiency (NSE) determines the relative magnitude of the residual variance compared to the measured data variance

- There is no single accepted performance statistic or standard that determines whether a model is valid.
  - Temperature: MAE < 1^oC, ME close to 0^oC

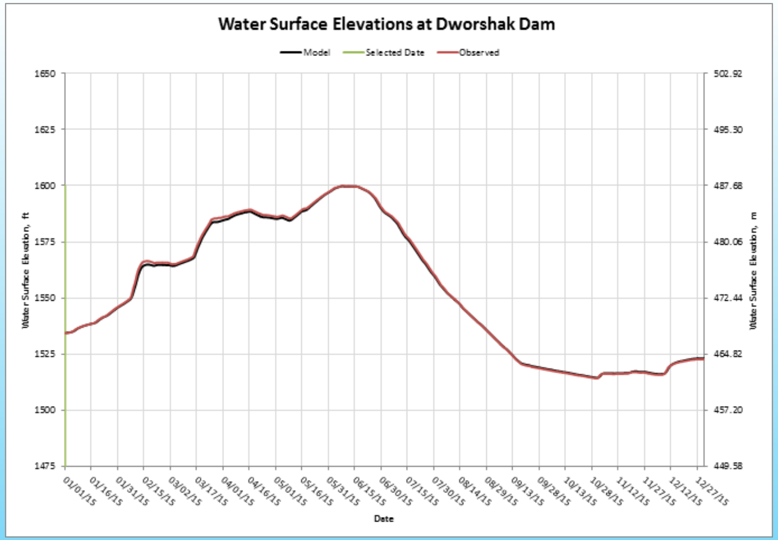
Model Sensitivity Analysis

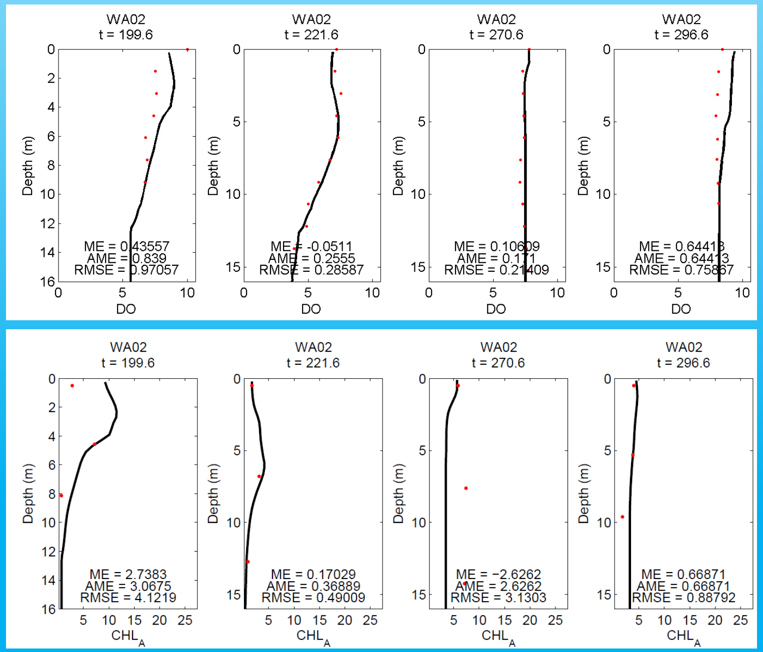
- Quantify the effect of error on state (model) variables
- Identify sensitive parameters or variables that have on predicting water quality
- Indicate the relationship between control variables and decision (or state) variables to help ensure that a change in control variable can have a desirable effect on the decision variables

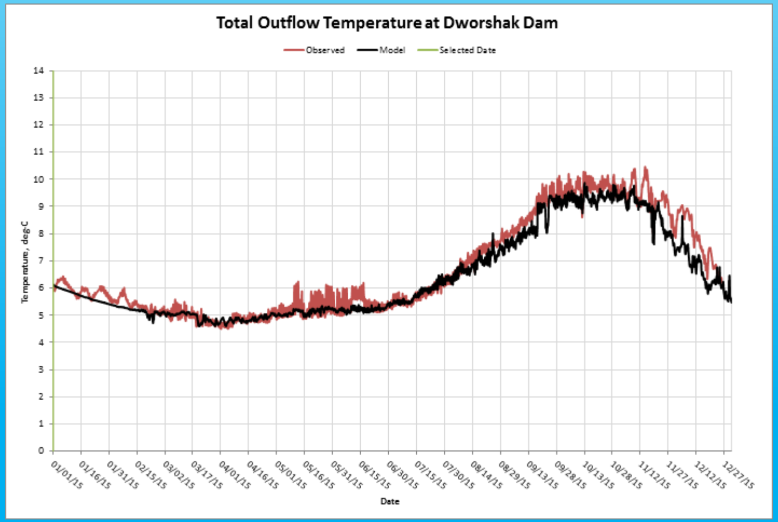


Model Calibration Data

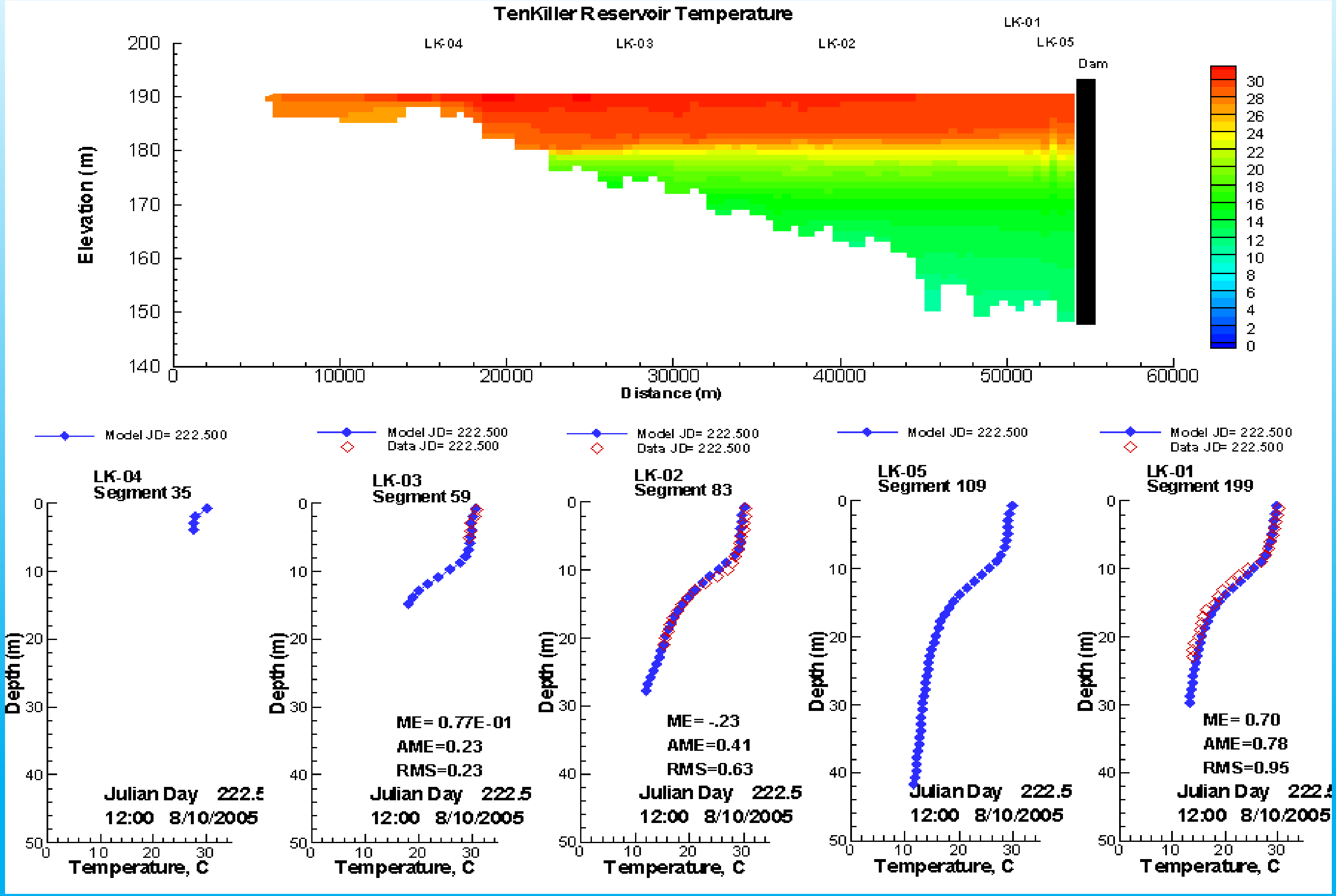
- Observed data records are fundamental during the calibration and validation phases of W2 model.
- Time Series
  - ▶ Flow and water level data
  - ▶ Water temperature and water quality data
- In-reservoir or in-river temperature and water quality profile data
  - Temperature profiles
  - Secchi disk depth
  - Dissolved Oxygen
  - Nutrient profiles
- Algae data
  - Biomass for algal species
  - Chlorophyll a concentration



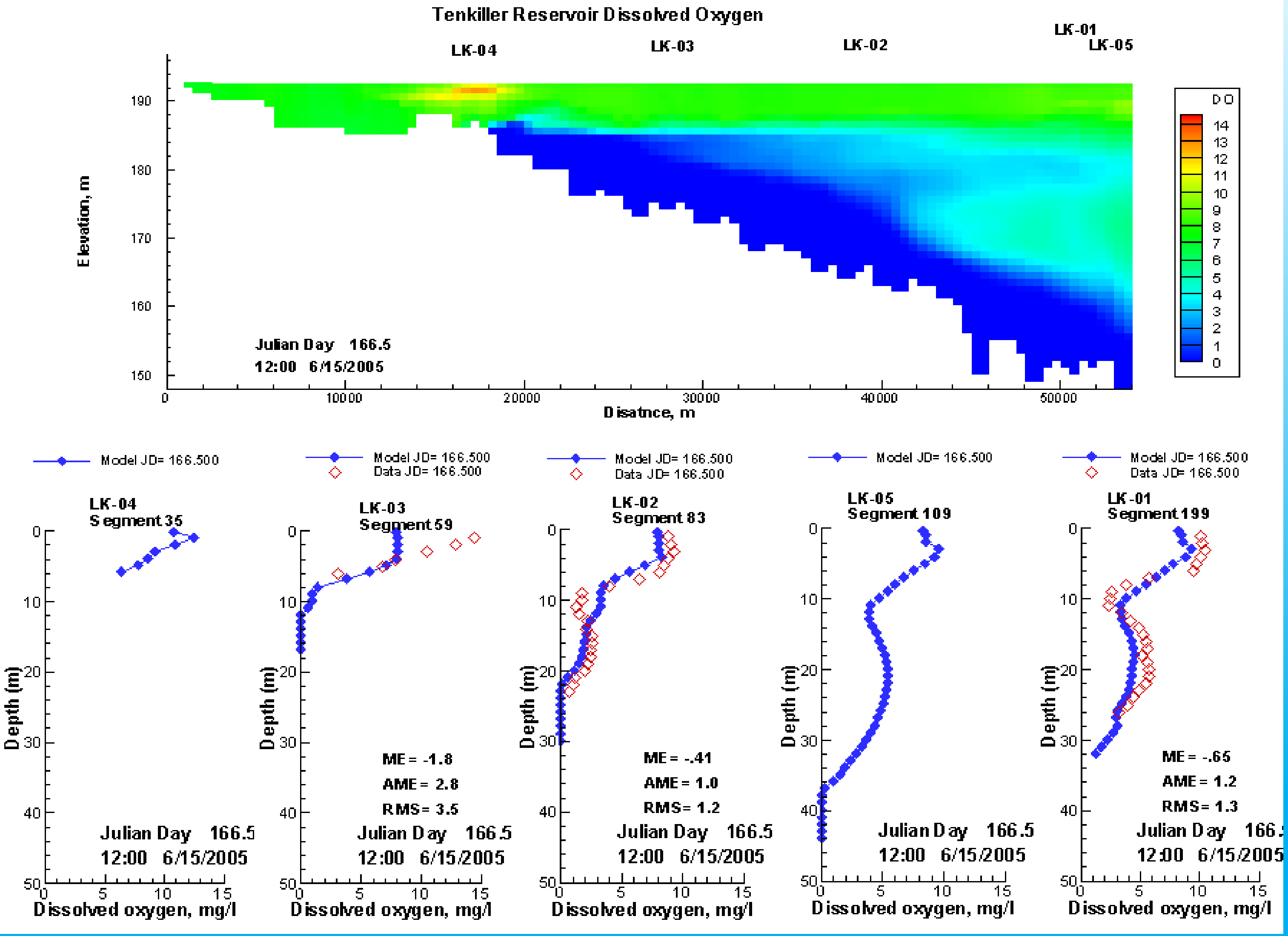




Calibration Data



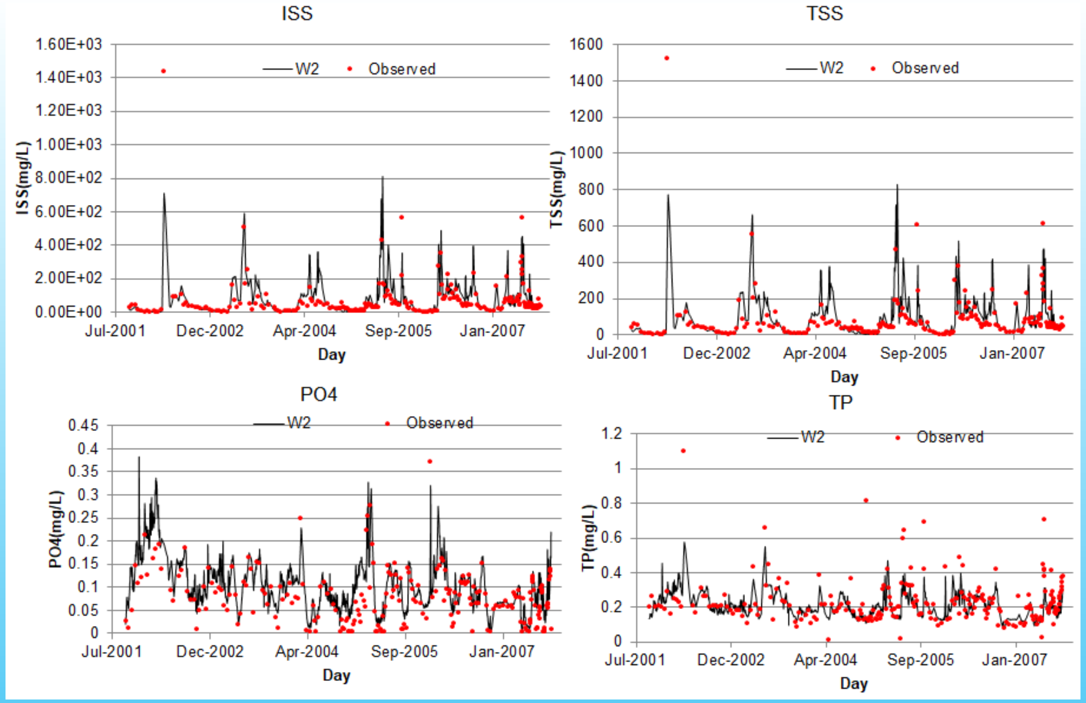
Calibration Data

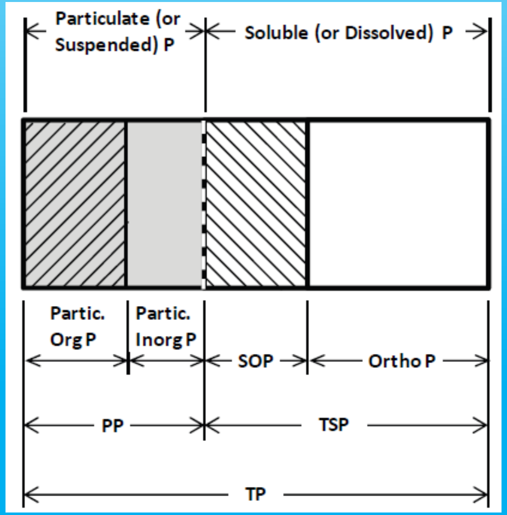


Calibration Data

Suspended Sediment is a mixture of
- clay particles
- silt particles
- sand particles
- organic material

Chemical forms of phosphorous (P):
- TP = total P
- PP = particulate P
- Partic. OrgP = organic P associated with particulates
- Partic. InorgP = inorganic P associated with particulates
- TDP = total dissolved P
- Ortho P = inorganic P
- SOP = soluble organic P





$$TISS = TSS - VSS$$

$$POM = VSS - r_{da}Chla$$

Hydrodynamics/Water Temperature Calibration Parameters

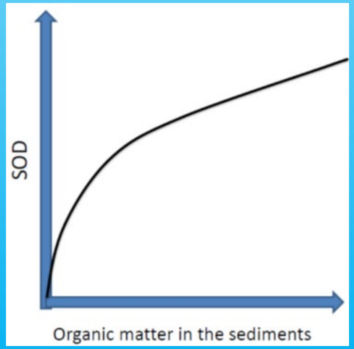
- longitudinal eddy viscosity (*Ax*)
- vertical eddy viscosity (*Az*)
- bottom friction
- sediment heat exchange
- wind-sheltering coefficient that varies by segment and time
- interaction with density field - SS, TDS, etc.
- bathymetry of the model

The W2 model is relatively insensitive to hydraulic parameters, dispersion coefficients, and bottom friction parameters for the Chezy friction model and default values are often used.

Water Quality Calibration Parameters

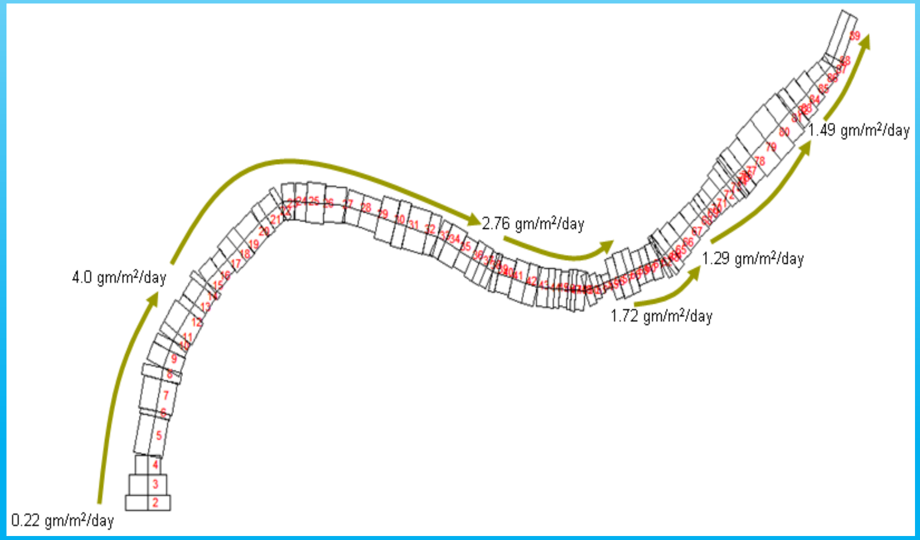
For water quality simulations, calibration parameters are varied widely, , it is preferable to obtain actual measurements of water quality coefficients …

- CBOD decay rates
- Decay rates of organic matter (carbon)
- SOD is known to vary spatially in reservoirs, SOD typically ranges from 0.1 to 1.0 $gO_2\ m^{-2}\ day^{-1}$, but can be higher.
  - ▶ Zero-order
  - ▶ First-order
  - ▶ Sediment diagenesis



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

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

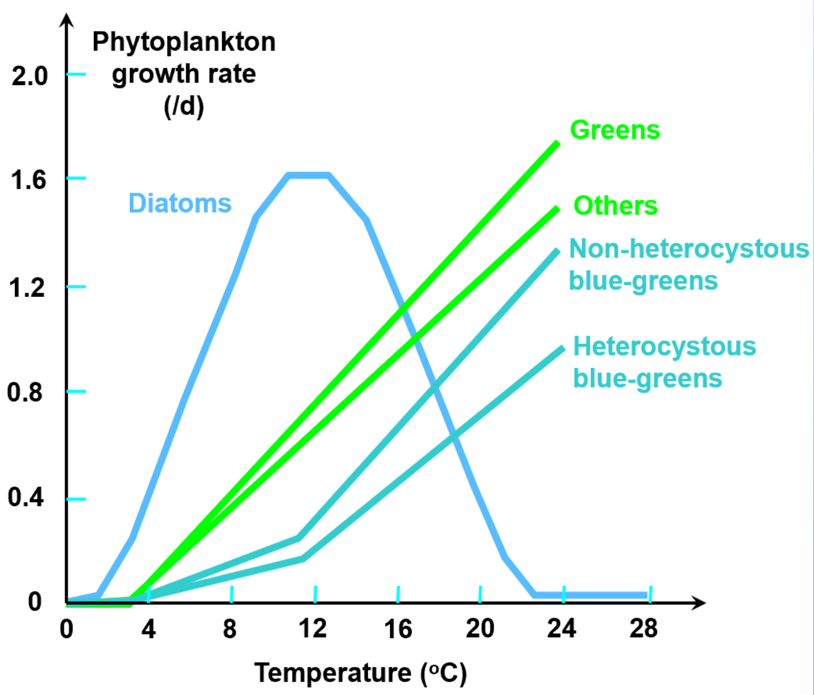


Courtesy of Dr. Chapra

Water Quality Calibration Parameters

- The measurements of algal biomass are usually available in the form of chlorophyll *a* which needs to be converted into biomass
- ACHLA is the ratio between algae (as dry weight organic matter) and chlorophyll a.
  - A wide range of chlorophyll-a-to-carbon ($Chla:C$) ratios has been reported in the literature across laboratory and field studies
  - $Chla:C$ is a function of temperature, light, and nutrient limitation.
- Stoichiometric relations

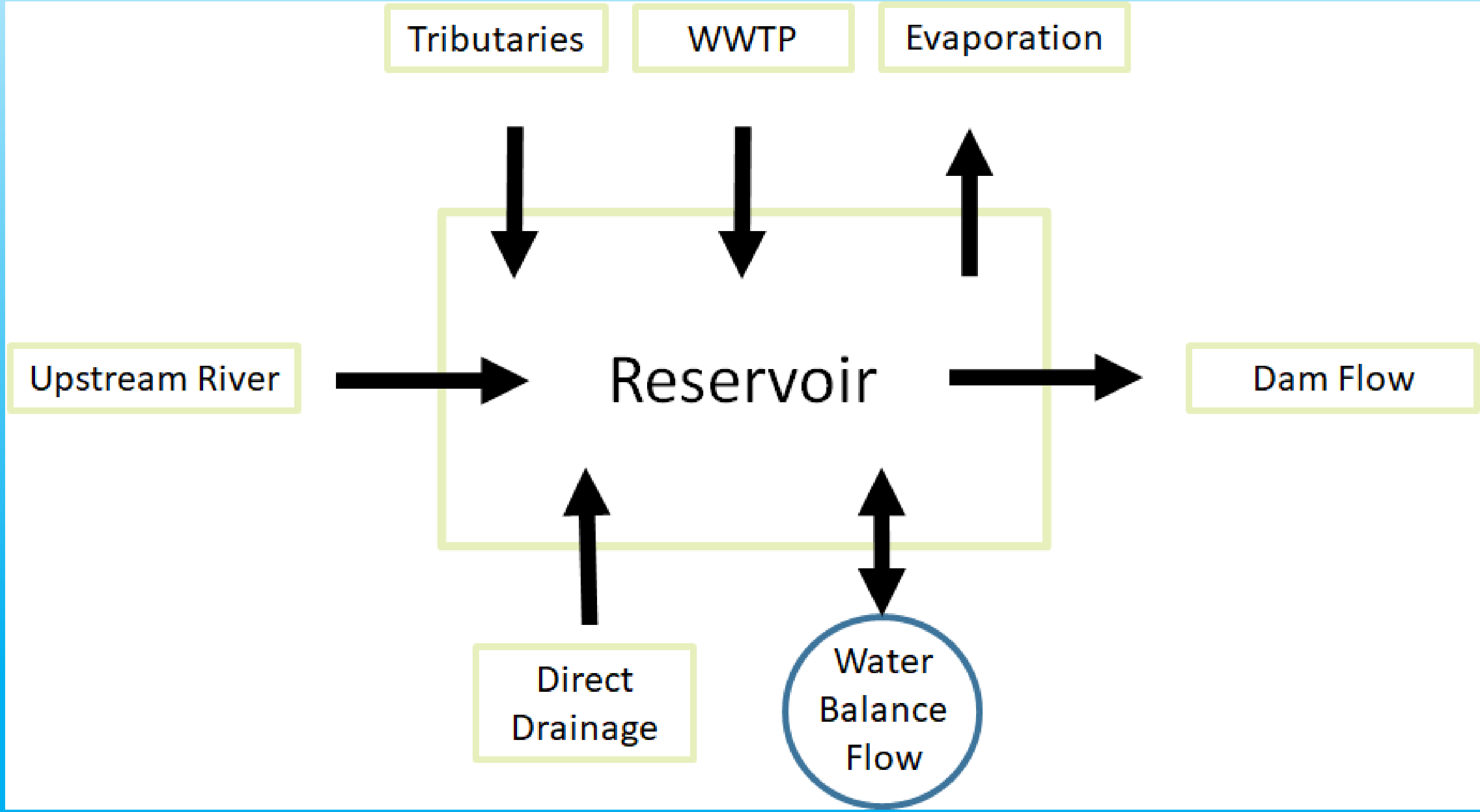
***100** g-D **: 40** g-C **: 7.2** g-N **: 1.0** g-P **: (0.4 ~ 1.0)** g-Chla*



Courtesy of Dr. Chapra

Fluid, Mass and Energy Balance

- Involve detailed evaluation of inflows and outflows, boundary conditions
- Have you accounted for all water?

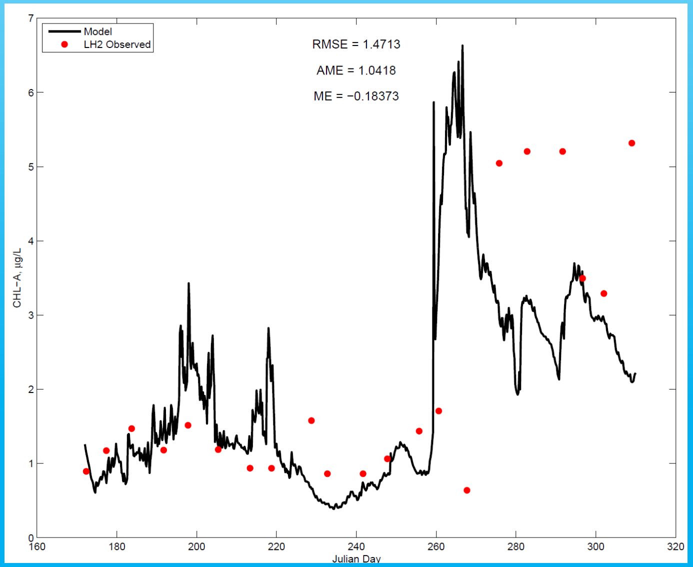


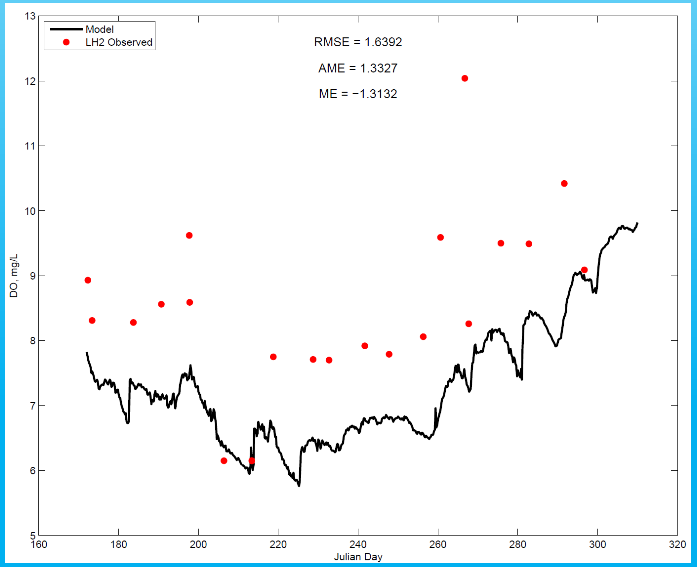
Water Quality Model Calibration Suggestions

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

Water Quality Model Calibration Suggestions (cont.)

- Use sensitivity analysis to investigate relations between observations, parameters, and model predictions
- For water quality simulations, it is important the user provide accurate initial and time-varying boundary conditions.
- If nutrient loadings are not adequately characterized, then it will be impossible for the model to accurately reproduce phytoplankton/nutrient/DO dynamics.





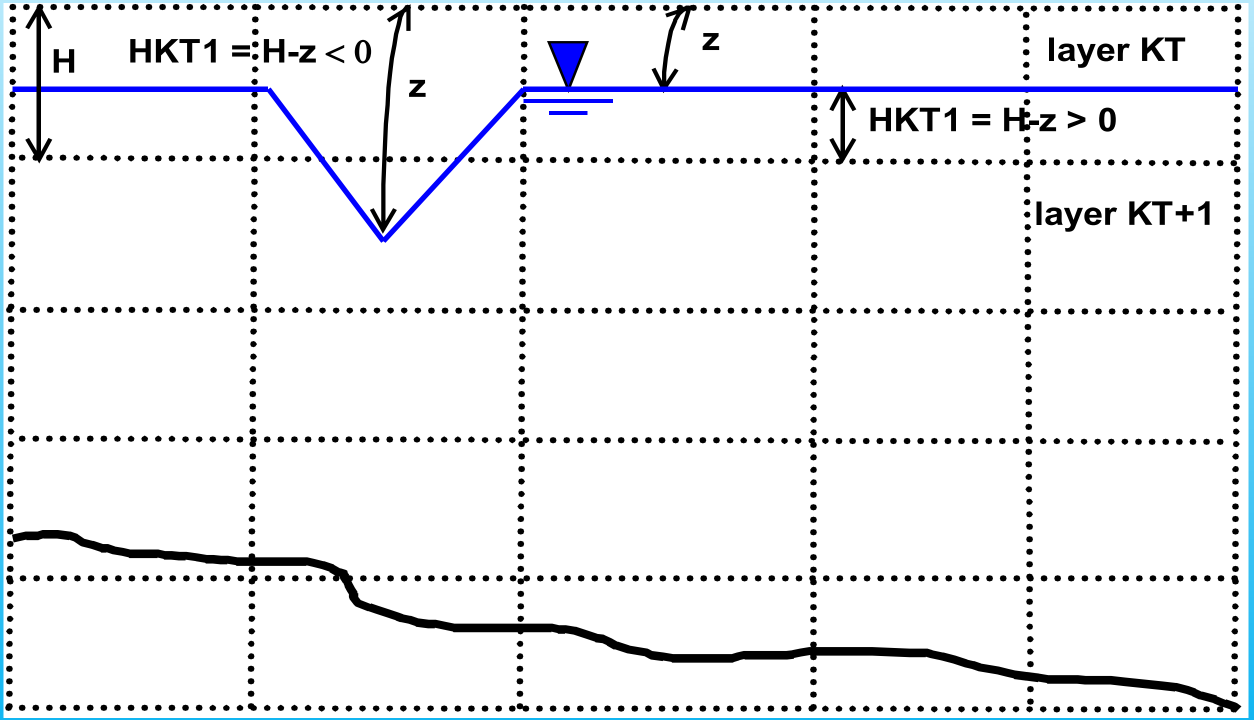
W2 Model Stability

- The W2 model works with dynamic time steps. Auto-time-stepping does not guarantee numerical stability.
- The W2 model uses the minimum timestep necessary to maintain numerical stability throughout the entire system.
- Time step selection will be based on the size of the grid cells and velocity of water in the cells.
  - 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.
  - For the times or regions with too many fluctuations in flow, the model uses a smaller time step and increases that when a small time step is not necessary.

W2 Model Stability

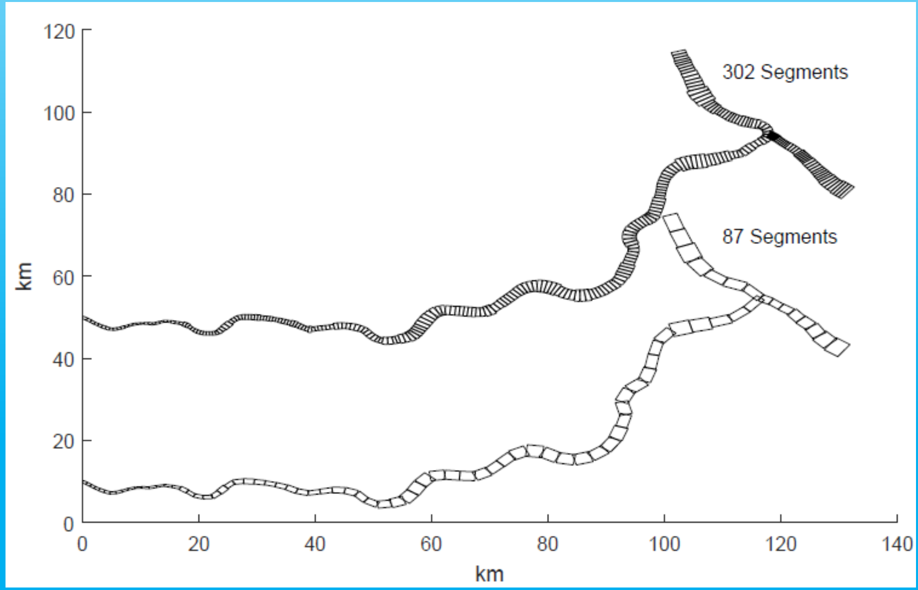
- If the current timestep is less than or equal to the minimum timestep, then the model run is stopped
- Unstable water surface elevation - negative surface layer thickness
- the user can reduce the maximum timestep **[DLTMAX]** and/or the fraction of the timestep **[DLTF]**

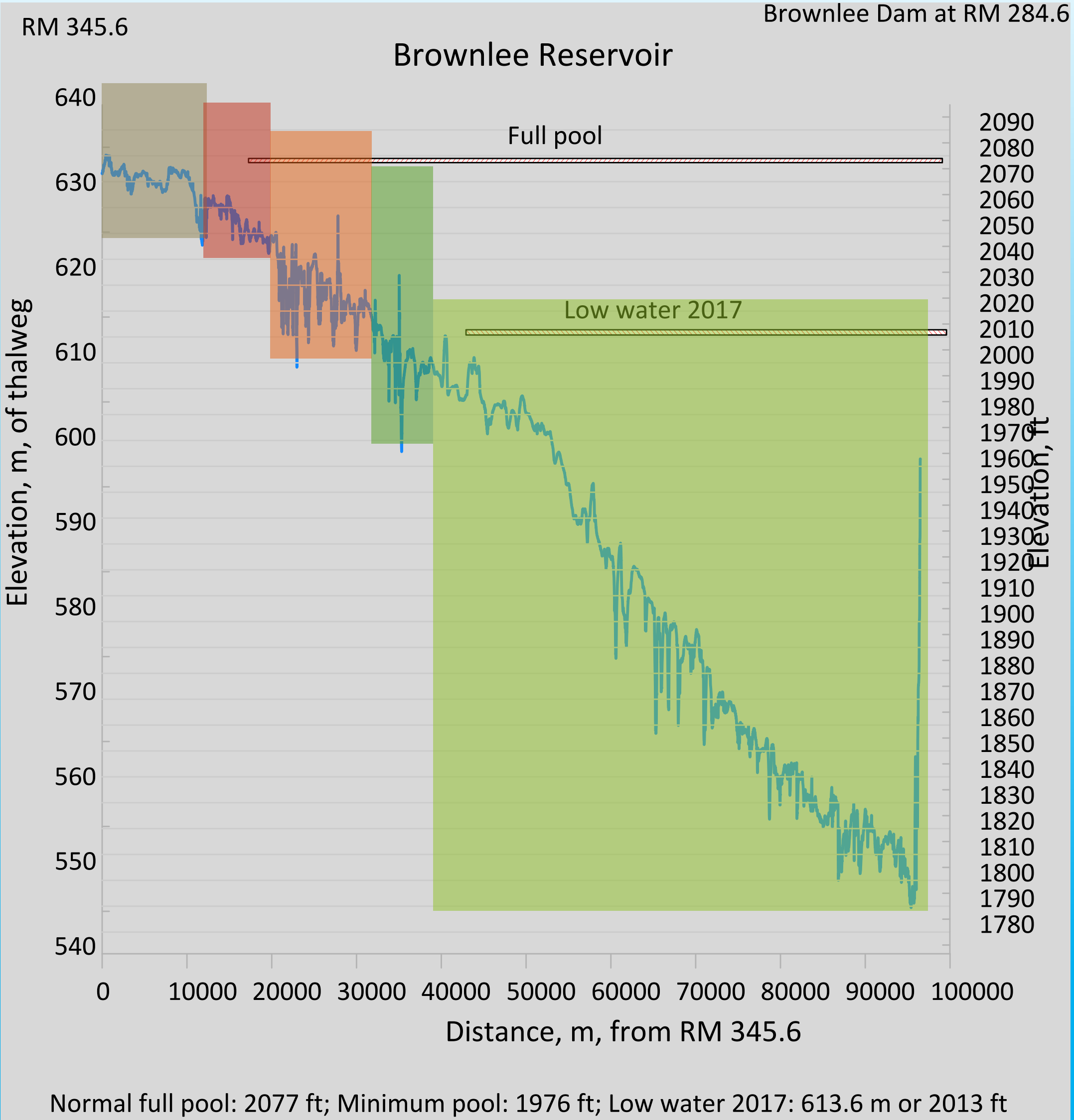
$$\Delta t \le \frac{1}{2\left(\frac{A_x}{\Delta X^2} + \frac{A_z}{\Delta Z^2}\right) + \frac{Q}{V} + \frac{\sqrt{\frac{\Delta\rho}{\rho}\frac{gH}{2}}}{\Delta X}}$$



W2 Model Stability

- Numerical solution scheme: UPWIND, QUICKEST, or ULTIMATE with the latter being the recommended option.
- W2 model grids: the conceptual model and grid resolution affect the model's stability.
- Riverine section may need to be a separate branch with a branch slope to keep it hydrated rather than having it wet and dry.





Hands-on Exercises

- Review the model inputs from "Minnesota River W2 Project"
- Review the model outputs of DO, CHLA, NH4, NO3, PO4 from Segment 83 and corresponding observed data
- Change the water quality parameters in the control file and rerun the model and see the difference of DO, NH4, PO4 from Segment 83

Questions?