

CE-QUAL-W2: A Two-Dimensional, Laterally Averaged, Hydrodynamic and Water Quality Model, Version 4.5

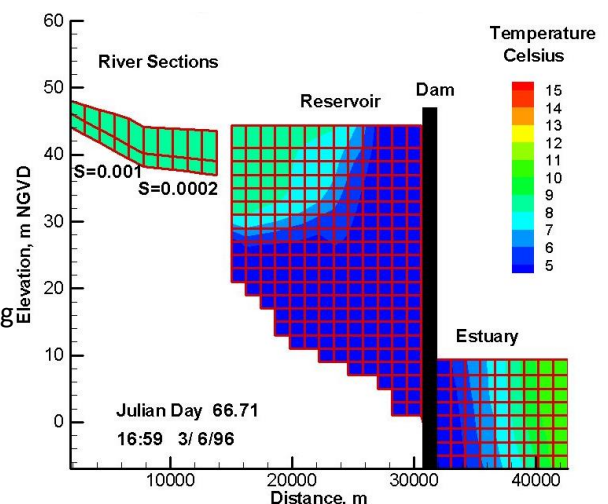
User Manual: Part 1 Introduction, Model Download Package, How to Run the Model

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Preface

This manual documents the two-dimensional, laterally averaged, hydrodynamic and water quality model CE-QUAL-W2. As in all complex models, there have been many contributors. This re-write of the User Manual was based on prior User Manuals: Environmental and Hydraulic Laboratories (1986), Cole and Buchak (1995) Version 2, and Cole and Wells (2000) Version 3.0 through Cole and Wells (2019) Version 4.1. Hence, one can think of the primary author as merely an editor of past documents, rather than reflecting one person's sole authorship. This updated User Manual contains numerous corrections, new figures, new sections, additional documentation, and improvements in organization and presentation of information compared to Cole and Wells (2019).

This section of the User Manual Part 1 introduces the model, its capabilities and limitations, an overview of the data preparation, the model download package, how to run the model for the first time, and other details about the model set-up.

The other sections of the User Manual are divided into multiple sections for ease of updating and editing:

- User Manual Part 1: Introduction to CE-QUAL-W2, Model download package, how to run the model, model versions, changes between model versions
- User Manual Part 2: Theoretical basis for CE-QUAL-W2: hydrodynamics and water quality, particle transport and numerical scheme
- User Manual Part 3: Model input and output file descriptions and input/output file examples
- User Manual Part 4: Model examples
- User Manual Part 5: Release notes, bug fixes, differences in model versions, history of bug fixes, and other user manuals such as for the GUI interface, the Waterbalance algorithm, and other external codes.

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or if a specific section with a different primary author:

Cole, T. (2022) "Overview of Data Preparation" in "CE-QUAL-W2: A two-dimensional, laterally averaged, hydrodynamic and water quality model, version 4.5, user manual part 1, introduction," ed. by S. Wells, Department of Civil and Environmental Engineering, Portland State University, Portland, OR.

1. Introduction to CE-QUAL-W2

Model Overview

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, estuaries, and combinations thereof including entire river basins with multiple reservoirs and river segments. Typical applications include stratified reservoirs, such as Brownlee Reservoir in ID/OR, USA, as shown in Figure 1. Also, the model has been applied to river basins that may or may not include reservoir or lake-like pools, such as the Tualatin River, OR, USA, shown in Figure 2.

CE-QUAL-W2: Corps of Engineers-Quality-Width Averaged 2D

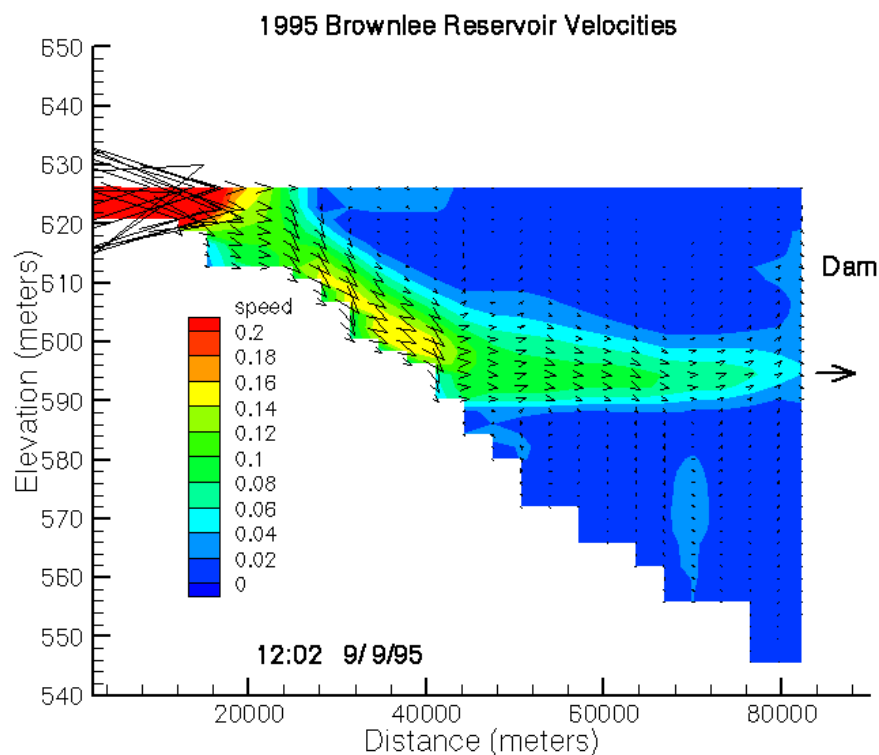


Figure 1. Brownlee Reservoir, USA, predicted velocities (m/s) showing plunging inflow of the Snake River moving as an interflow through the reservoir.

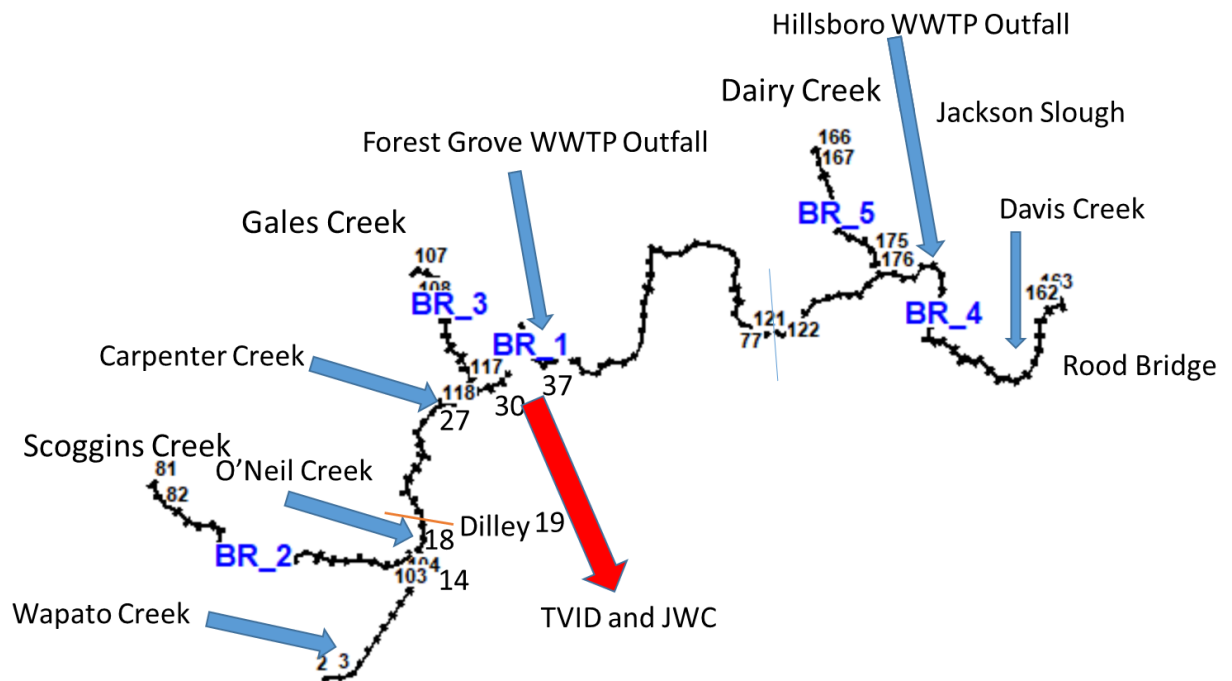


Figure 2. Layout of the Upper Tualatin River CE-QUAL-W2 model showing model segment layout, branch layout, tributaries (blue) and withdrawals (red). This model was composed of 2 waterbodies (BR1-3 and BR4-5). The mainstem was composed of 2 branches (BR1 and BR4) from RM 62.4 to RM 38.4. There were 3 side branches including Scoggins Creek BR2, Gales Creek BR3, and Dairy Creek BR4.

Terminology used in the CE-QUAL-W2 model

The CE-QUAL-W2 model discretization uses the following definitions:

Waterbodies, Branches, Segments, Layers

- **Waterbodies:** a collection of model branches that have similar turbulence closure and water quality parameter values and the same meteorological forcing. A typical example would be a reservoir and a river as separate waterbodies. One can also have one reservoir with separate waterbodies designated by different meteorological forcing.
- **Branches:** a collection of model segments with variable model slope. In a river waterbody, there can be multiple branches of variable slope; or in a reservoir, the sidearms of the reservoir can be different model branches.
- **Segments:** a longitudinal segment of length Δx .
- **Layers:** a vertical layer of height Δz .

An example is shown in Figure 3 for a reservoir in Oklahoma. In this figure the model is quasi-3D because of its use of branches for side arms. Each segment then is also composed of multiple vertical layers as shown in Figure 4.

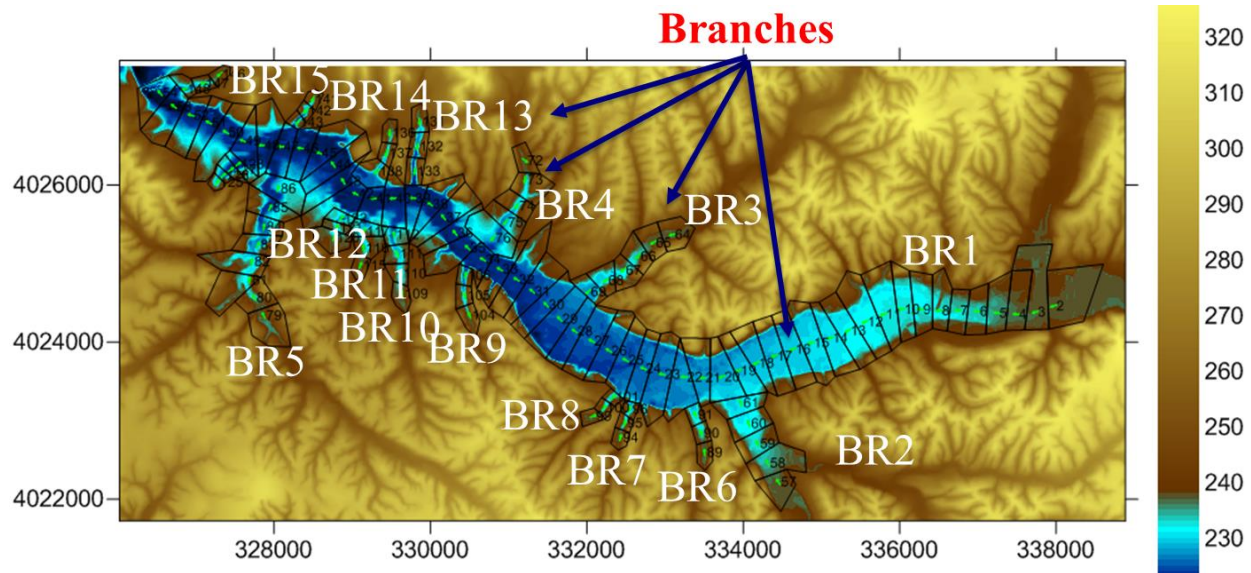


Figure 3. Grid layout for Eucha Reservoir, OK. Model segments and branches (BR) are numbered for this one waterbody model. The main branch is BR1 followed by side branches 2 through 15.

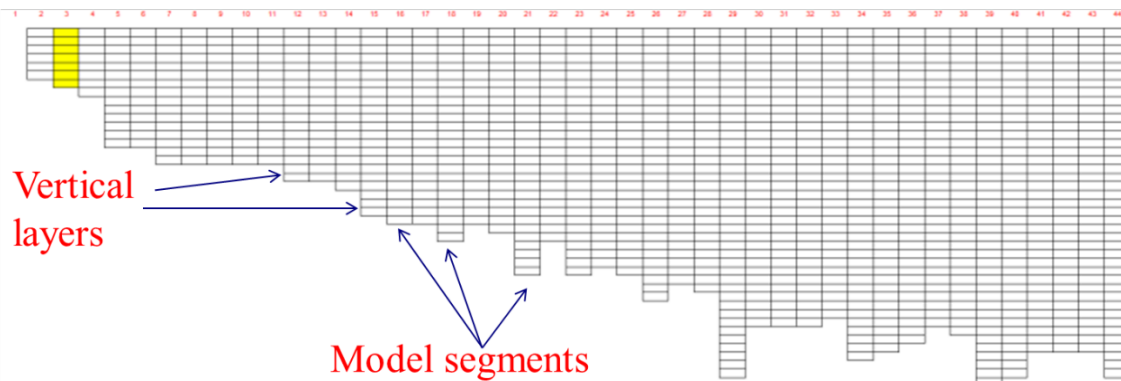


Figure 4. Vertical grid layout for Eucha Reservoir, OK. Note the vertical layers for each model segment in Branch 1.

CE-QUAL-W2 Historical Background

The development of such a complex model is a result of the collective effort of many researchers. As you will see in the historical background, this development has its origin with the Corps of Engineers. Hence, the name is based on that origin: CE: Corps of Engineers; QUAL: Quality; W2: Width averaged 2D.

Many people have contributed to the model development – a partial list is shown in Appendix A.

Version 1.0. The original model that was the foundation for CE-QUAL-W2 was known as LARM (**L**aterally **A**veraged **R**eservoir **M**odel) developed by Edinger and Buchak (1975, 1978, 1980, 1983). The first LARM application was on a reservoir with no branches. Subsequent modifications to allow for multiple branches

and estuarine boundary conditions resulted in the code known as GLVHT (**G**eneralized **L**ongitudinal-**V**ertical **H**ydrodynamics and **T**ransport Model). Addition of the water quality algorithms by the Water Quality Modeling Group at the Corps of Engineers Waterways Experiment Station (WES) resulted in CE-QUAL-W2 Version 1.0 (Environmental and Hydraulic Laboratories, 1986).

Version 2.0. Version 2.0 was a result of major modifications to the code to improve the mathematical description of the prototype and increase computational accuracy and efficiency. These changes were summarized in the Cole and Buchak (1995) User Manual. Numerous new capabilities were included in Version 2.0, including:

1. an algorithm that calculated the maximum allowable timestep and adjusted the timestep to ensure hydrodynamic stability requirements were not violated (autostepping)
2. a selective withdrawal algorithm that calculated a withdrawal zone based on outflow, outlet geometry, and upstream density gradients
3. a higher-order transport scheme (QUICKEST) that reduced numerical diffusion (Leonard, 1979)
4. time-weighted vertical advection and fully implicit vertical diffusion
5. step function or linear interpolation of inputs
6. improved ice-cover algorithm
7. internal calculation of equilibrium temperatures and coefficients of surface heat exchange or a term-by-term accounting of surface heat exchange
8. variable layer heights and segment lengths
9. surface layer extending through multiple layers
10. generalized time-varying data input subroutine with input data accepted at any frequency
11. volume and mass balances to machine accuracy
12. sediment/water heat exchange

Version 3.0. Version 3.0 is a result of additional improvements to the numerical solution scheme and water quality algorithms, as well as extending the utility of the model to provide state-of-the-art capabilities for modeling entire waterbasins in two-dimensions. The new capabilities included in Version 3 include:

1. an implicit solution for the effects of vertical eddy viscosity in the horizontal momentum equation
2. addition of Leonard's ULTIMATE algorithm that eliminates over/undershoots in the numerical solution scheme
3. inclusion of momentum transfer between branches
4. the ability to model multiple waterbodies in the same computational grid including multiple reservoirs, steeply sloping riverine sections between reservoirs, and estuaries
5. additional vertical turbulence algorithms more appropriate for rivers
6. additional reaeration algorithms more appropriate for rivers
7. variable vertical grid spacing between waterbodies
8. numerical algorithms for pipe, weir, and pump flow
9. internal weir algorithm for submerged or skimmer weirs
10. three algal groups
11. arbitrary constituents defined by a decay rate, settling rate, and temperature rate multiplier
12. nine inorganic suspended solids groups
13. dissolved and particulate biogenic silica

14. age of water
15. derived constituents such as total DOC, organic nitrogen, organic phosphorus, etc. that are not state variables
16. a graphical pre/postprocessor
17. converted to FORTRAN 90/95 with Dynamic Array Allocation eliminating the need to recompile the code for each application
18. user defined evaporation models including the Ryan-Harleman model

Version 3.1. Version 3.1 is a result of additional improvements to the numerical solution scheme and water quality algorithms, as well as extending the utility of the model to provide state-of-the-art capabilities for modeling entire waterbasins in two-dimensions. The new capabilities include:

1. any number of user defined arbitrary constituents defined by a decay rate, settling rate, and temperature rate multiplier that can include
 - a. conservative tracers
 - b. coliform bacteria
 - c. water age
 - d. contaminants
2. any number of user defined phytoplankton groups
3. any number of user defined epiphyton/periphyton groups
4. any number of user defined CBOD groups
5. any number of user defined inorganic suspended solids groups
6. dissolved and particulate biogenic silica
7. derived constituents such as total DOC, organic nitrogen, organic phosphorus, etc. that are not state variables
8. kinetic fluxes
9. graphical preprocessor

Version 3.2. Version 3.2 is a result of additional improvements to the model. These new capabilities include:

1. Internal code rewrite to reduce code size, simplify code maintenance, and improve model execution speed
2. New screen display during model run-time. The new screen display allows for controlling the processor usage, examining output variables, and stopping, starting and restarting a model run on the fly. This allows the model user to stop a code, then make changes in the control file or any input file, and then restart the model at the point that it was stopped.
3. Addition of a new algorithm to estimate suspended solids resuspension as a result of wind-wave action.
4. Reorganization of the graph.npt file to allow more output control formatting possibilities.
5. New turbulent kinetic energy-turbulent dissipation turbulence closure model was added to the model.

Version 3.5. Version 3.5 is a result of significant enhancements to the model. These new capabilities include:

1. Addition of the macrophyte model of Berger and Wells (2008) with a user-defined # of species

2. Addition of a zooplankton model with a user-defined # of species based on an updated version of the CE-QUAL-R1 model (Environmental Laboratory, 1995)
3. Addition of a new focusing or settling velocity for sediments that accumulate in the first order sediment model. In earlier versions, sediment focusing occurred at the velocity given for POM. In this version, a user can specify that focusing velocity. This means that sediments can still migrate toward the bottom of the channel over time even after they have hit the sidewalls of the channel.
4. User-defined time-variable input of P and N associated with organic matter inputs. In earlier versions, the P or N associated with organic matter was based on a static stoichiometric coefficient specified in the control file. Now, the user provides in the input files the dynamic P and N associated with organic matter inputs from tributaries or inflows. This is essentially allowing for variable stoichiometry in the input boundary conditions.
5. Based on the above refinement, the organic matter fractions within the model now have variable stoichiometry for P and N. This preserves P and N mass balances. The stoichiometry given in the input files is merely the initial value of the C-N-P stoichiometry of POM and DOM compartments. Hence, organic P and organic N are tracked correctly in the code.
6. The first order sediment model also tracks C-N-P correctly and has a dynamic stoichiometry as it accumulates organic matter in the sediment. Prior versions of W2 had a user-defined value of fixed stoichiometry for the 1st order sediment model. Also, instead of a fixed decay rate for the sediments, the decay rate is dynamic based on the decay rates of the accumulated organic material. A mass weighted average is used.
7. CBOD groups now have a user-defined settling velocity. Hence, the user can define organic matter groups as particulate and dissolved based on specification of the settling velocity. As in prior versions, CBOD has associated stoichiometry and if there is settling, it will accumulate in the 1st order sediment compartment.
8. A Monod formulation was implemented for the initiation of anaerobic processes and reduction of aerobic processes. In earlier model versions there was a specified oxygen concentration that acted like a step function turning these processes on or off.

Version 3.6. This version is file compatible with version 3.5. Hence no changes need to be made to any input files. Even though there are some new features in the input files, these are not required for users of V3.5 and can be kept blank. The primary change is allowing the code to run on multiple processors. The following changes have been made in the code from V3.5 to V3.6:

1. The code has been rewritten into smaller subroutines to allow better code compilation and optimization.
2. The code has been revised with the goal of improving the computational speed. This new compiled code using Intel Visual Fortran 11 should be faster on a single processor than the V3.5 code compiled on a PC with CVF 6.6.
3. The code now has OPENMP commands embedded to allow for limited parallelization of some of the routines. Current tests show that going from 1 processor to 2 can result in up to 20-40% speed improvement. The user can specify the # of processors the code will use in NPROC. *Note that this has been disabled in later versions in order to improve numerical precision between simulations.]*
4. The TKE algorithm has been updated with new algorithms that match experimental tank data for kinetic energy and dissipation. This is based on a Master's degree project by Sam Gould

(2006) at Portland State University. A new user option is the TKE1 algorithm, in addition to the legacy algorithm TKE.

5. The roughness height of the water for correction of the vertical velocity wind profile is now a user-defined input, z_0 . Prior to this the model had hardwired the value of $z_0=0.003$ m for wind speed correction at 2m (for evaporation where wind height at 2 m is typical) and $z_0=0.01$ m for wind at 10 m (for shear stress calculations where wind height of 10 m is typical). For consistency, both conversions now use the same value of roughness height. If the user does not specify the value of z_0 (for example if he/she leaves the spaces blank for z_0 using a V3.5 control file), the code uses 0.001 m.
6. The Windows user interface no longer uses Array Viewer. The dialog box and PC executable no longer require installation of Array Viewer (which is now obsolete) nor do they need the Array Viewer DLL. The Dialog box has some minor improvements: model run directory displayed and a progress bar.
7. Fixed error with Algae/chlorophyll a ratio in user manual and fixed pre-processor. The earlier language in the user manual discussed an Algae/Chlorophyll a ratio but presented information that was the ratio of chlorophyll a/algae – this has been revised and fixed in User Manual and in preprocessor.
8. Spreadsheet output: in earlier versions put in an alphanumeric character as a space for the spreadsheet to preserve the formatting. This was changed to a default value of -99 to facilitate numeric data processing. Also, the “-Depth” output value was changed to just “Depth” since modern plotting programs can reverse an axis.
9. Preprocessor improvements. Added variable checks for new parameters, fixed bugs, new check for wsc.npt file (not checked in earlier versions).
10. For the generic constituent, added temperature dependence on 0th order decay and fixed errors in User Manual for units of zero order decay coefficient.
11. Added the kinetic flux rates to the TSR file output for easier analysis using a spreadsheet of the flux terms for specific locations in the modeled system.
12. Revised the computation of the drag coefficient for low wind speeds so that the model now agrees better with theory in this wind speed range.
13. The light extinction coefficient (in m^{-1}) is now included as an output variable in the TSR opt file. Because the model internally computes the light extinction coefficient based on water, SS, POM, algae, zooplankton, and macrophytes, this is an important parameter understanding the internal light transmission predicted by the model. This variable replaces the equilibrium temperature as an output variable.
14. A new option for output is in the format required for TECPLOT. For TECPLOT animation there is only a flag in the CPL output line. This allows for easy model animation of the variables U, W, T, RHO, and all active constituents at the frequency specified by the CPL file as a function of distance and elevation.
15. A new variable for determining the fraction of NO₃-N that is diffused into the sediments that becomes organic matter, or SED-N was introduced.
16. In V3.5 the model computed an average decay coefficient of the sediments based on what was deposited. The user now has the option to dynamically compute that decay rate or to have it

fixed and controlled by the model user. A new variable was introduced called DYNSEDK which is either ON/OFF to allow or not allow dynamic computation of the sediment decay rate.

17. Added Kinetic flux output that sums up fluxes for all cells of a waterbody at the output frequency specified in the kinetic flux output. The output filenames are called "kflux_jw#.opt" where # is the waterbody number. All active fluxes are summed for the waterbody. This is an important overall diagnostic tool to evaluate the important fluxes in the waterbody over time. Instantaneous fluxes are output in the TSR file for individual cells and a series of fluxes at given segments are shown in the Flux output file which is similar in format as the SNP file. This new file is easy to import into a spreadsheet for analysis.
18. The selective withdrawal algorithm computation was adjusted to more closely follow the Corps' model code SELECT (based on personal communication with Gary Hauser, 2008). The variable DLRHOMAX is used to compute the relative velocity profile. In V3.5 and earlier, this variable was the maximum for the entire profile above and below the outlet, i.e., $DLRHOMAX = \max(DLRHOT, DLRHOB)$. In V3.6 and later, DLRHOT is used above the outlet and DLRHOB is used below the outlet.
19. Command-line working directory specification is now active for the preprocessor, GUI, and W2 windows versions. Also, the Windows box can now be closed after a run is finished by specifying CLOSEC=ON in the control file. This makes it easier to use the Windows executable in batch file processing.

Version 3.7. This version is not file compatible with version 3.6 because of the addition of several more state variables. The release notes show where the control file differs from Version 3.6. Many of the new features to Version 3.7 are accessed through additional control files separate from the main control file, w2_con.npt. The following changes have been made in the code from V3.6 to V3.7:

1. The model has been improved to handle river flow regimes. These model enhancements for river systems include the following:
 - a. The initial water surface elevation of a river system based on the normal depth of the river is computed within the model. This allows the model to run more smoothly from the start and eliminates trying to guess an initial water surface elevation for a river system.
 - b. The model in earlier versions assumed that the initial velocity regime was 'zero'. By computing an initial velocity regime based on the initial conditions of the flows, the river model then starts with a non-zero velocity. This allows the model to run more smoothly from the very beginning of the model simulation.
 - c. The model user can choose 'Trapezoidal' or 'Rectangular' model segments. This will allow for a smoother transition as water levels move up and down in a river channel. This should also allow for a larger maximum time step for stability in the river system.
 - d. The model user can now specify 2 slopes for a model branch. One slope is the slope of the elevation grid for which all elevations are tied together. The other slope is the hydraulic equivalent slope of a channel. In other words, if a model branch includes riffles and pools, the actual grid slope may not be the equivalent hydraulic slope.
2. There is a new bathymetry file input format in comma delimited format (csv) that is easily developed using 'Excel'. This simplifies setting up the initial grid and debugging it.

3. Temperature and dissolved oxygen habitat volumes are now computed within the model for user-specified fish species.
4. There is a new automatic selection of a withdrawal port algorithm that will select the elevation of the withdrawal necessary to meet temperature targets including splitting flows between outlets to reach a target temperature.
5. Since each BOD group can have a different BOD-P, BOD-C and BOD-N stoichiometric equivalent, it was necessary to add to the model new state variables, BOD-P, BOD-N, and BOD-C that allowed for time variable inputs of BOD-P, BOD-C and BOD-N from a point or non-point source.
6. Environmental performance criteria were developed to evaluate time and volume averages over the system of state variables chosen for analysis. This is an easy method for looking at water quality differences between model runs.
7. The model now has a module for adding dissolved oxygen, such as hypolimnetic aeration, to specific locations based on a dynamic dissolved oxygen probe monitoring the dissolved oxygen levels.
8. The model has a dynamic pipe algorithm allowing a pipe to be turned ON or OFF over time, as if a gate was closed.
9. The model also has a dynamic pump algorithm that allows the model user to set dynamic parameters for the water level control over time. This is very useful in setting rule curves for operation of the reservoir water levels over time.
10. The maximum time step can now be set to interpolate its value over time rather than suddenly changing the maximum time step. This allows for a smoother change in the model time step.
11. The computation of the temperature at which ice freezes has been adjusted to account for salt water impacts. [Courtesy of Dr. Ray Walton]
12. New model output includes volume weighted averages of eutrophication water quality variables as a function of segment and for only surface conditions as specified by the model user. Other new output includes output of flows, concentrations, and temperatures from a segment for all individual withdrawals.

Version 3.71. This version is file compatible with version 3.7 but does add one new variable to the control file w2_con.npt.

1. New model input formats (free format) for many input files that were in fixed format. The new files allow for much easier model file development in Excel. These new files include the following files:
 - a. All concentration input files for inflows, tributaries, distributed tributaries and precipitation:
 - i. Cin files
 - ii. Ctrib files
 - iii. Cdtrib files
 - iv. Cpre files
 - b. Wind sheltering file
 - i. Wsc file
 - c. Meteorological input file
 - i. Met file

- d. Vertical profile file for initial condition
 - i. Vpr file
- e. Longitudinal-vertical profile initial condition
 - i. Lpr file
- f. Withdrawal flow file
 - i. Qwd file
- g. Structure outflow file
 - i. Qot file
- h. Flow and temperature input files for
 - i. Qin and Tin
 - ii. Qtrib and Ttrib
 - iii. Qdtrib and Tdtrib
- 2. New option for dynamic outlet structure elevation for each model structure. Hence, the center-line elevation of the structure can be variable over time. In the control file, there is an ON/OFF option after declaring the # of structures for each branch.
- 3. The release of a new post-processor from DSI, Inc. that uses the vector output in w2_con.npt to specify frequency of output for this post-processor.

Version 3.72. This version is file compatible with version 3.71 unless one uses the new USGS automatic port selection algorithm where the w2_selective.npt format is changed. This new version allows for using the algorithm of Rounds and Buccola (2015) for trying to meet downstream temperature targets from reservoirs with multiple outlets.

Version 4.0. This version is file compatible with Version 3.72. All the new model options are contained in new control files other than the existing model files. The new model includes the following features:

1. Sediment diagenesis model of Prakash et al. (2015) and Berger and Wells (2014). This model is described in Part 2 of the User's Manual. This model includes bubble formation and rise in the water column, sediment consolidation, and sediment diagenesis. It includes the following new state variables:
 - a. Sediment and water column CH₄
 - b. Sediment and water column H₂S
 - c. Sediment and water column SO₄
 - d. Sediment and water column Sulfide
 - e. Sediment and water column FeOOH(s)
 - f. Sediment and water column Fe⁺²
 - g. Sediment and water column MnO₂(s)
 - h. Sediment and water column Mn⁺²
 - i. Sediment organic P, sediment PO₄
 - j. Sediment organic N, sediment NO₃, sediment NH₄
 - k. Sediment Temperature
 - l. Sediment pH
 - m. Sediment alkalinity
 - n. Sediment Total inorganic C
 - o. Sediment organic C

- p. Mature fine tailings (about 70% water and 30% fine clay – can take centuries to consolidate; from oil sands mining operation) – like another inorganic suspended solids group
 - q. Turbidity based on correlation with TSS
- 2. Non-conservative alkalinity from work of Sullivan et al. (2013)
- 3. Wind induced and boundary induced shear causing scour of organic matter from sediments and resulting oxygen demand
- 4. The new sediment model largely deprecates the older state variable Fe(total) since we now have different state variables for Fe and Mn
- 5. Ice formation and ice melting now affect the water body through loss or gain of water mass. This can be turned ON/OFF.
- 6. Periphyton and macrophyte variable areal density/concentration can be set for each model cell as well as setting a global initial concentration.
- 7. Output files tsr, qwo, two, cwo, structure, gate, pipe, pump, and spreadsheet files are now in comma delimited format rather than the older fixed format.
- 8. TSR file output now includes the limiting nutrient term for N, P, and light which is between 0 and 1
- 9. Photodegradation and gas transfer (volatilization) are now options for generic constituents
- 10. N₂ gas is now an option for a generic constituent. If this is used, the model automatically computes %TDG using both N₂ and O₂ state variables
- 11. A floating skimmer weir can be used and is set up in the main control file section on internal weirs
- 12. A new output file format for longitudinal profiles of water level, temperature, flow rate and water quality are set up in the profile output section of the main control file
- 13. A new output file which gives a P and N mass balance for each waterbody including existing P/N in water column, in plants, and in sediments and fluxes in and out of the system including sediment release and P/N flux to the sediments

Version 4.1. This version is file compatible with Version 3.72. All the new model options are contained in new control files other than in the main control file. The new model includes the following features:

- 1. Particle Tracking Algorithm based on a revised and updated algorithm from Goodwin et al. (2001). There is a new input file for activating the particle tracking algorithm, 'particle.csv', and a new documentation report outlining how to use this new algorithm.
- 2. Branch active and inactive algorithm. In prior versions of the CE-QUAL-W2 model, if a branch lost water, the model would end. Now the model can activate or deactivate branches based on wetting and drying. Also, upstream inflows or tributaries are automatically added to the most downstream active segment of the inactive branch. This allows then filling and emptying a large reservoir with complex side branches with no further input of the model user.
- 3. Updates to the Sediment Diagenesis Model. These updates are focused on (1) increasing the speed of execution of the code, (2) improved input/output including adding sediment diagenesis fluxes of P and N to the massbal.csv file for analyzing big picture nutrient balance of a waterbody, and (3) Improved preprocessor checks of sediment diagenesis input parameters.
- 4. The value of Ax and Dx can now scale with the mean longitudinal velocity rather than being constants.

5. Canopy shade can be used in conjunction with the dynamic shade algorithm to estimate solar reduction when the channel has a vegetative canopy.
6. Assorted minor bug fixes and updates. [Thanks to Stewart Rounds, USGS, for suggesting several of these!]
7. New waterbalance utility as a console application. It has a few more features than the earlier windows version which is still available.
8. For withdrawal output files, precise output timing can now be used for seconds, minutes or hours.
9. The model user can now deal with a constriction between 2 model segments without having to have a very small segment between 2 larger segments.

Version 4.2. This version is file compatible with Version 3.72. All the new model options are contained in new control files other than in the main control file. The new model includes the following features:

1. Multiple waterbody cascade modeling using multiple processors. If the model is set-up for multiple independent waterbodies where flow moves from upstream to downstream, then the downstream models can run as they receive information from the upstream waterbody. This can save significant simulation time as multiple processors are used for each independent waterbody.
2. The User Manual was updated to a new format and organization with hundreds and hundreds of additions, updates, corrections.
3. The Corps of Engineers, SYSTDG, program for evaluating Total Dissolved Gas at spillways, was added to the release version of the model.
4. The restart feature with sediment diagenesis and Tecplot CPL output is now working. Prior to this version, restart did not work with sediment diagenesis nor with Tecplot CPL output.

Version 4.2.1 This version is file compatible with Version 3.72 except for the new Excel version of the control file. The new model includes the following features:

1. Multiple waterbody cascade modeling using multiple processors has been updated using code developed by Stewart Rounds (USGS). This allows for a pause while waiting for upstream information rather than a model restart allowing for more precise calculations.
2. A new control file, w2_con.csv, is now available for use in CE-QUAL-W2. This is derived from the Excel spreadsheet w2_con.xlsm which contains a macro to write the file into csv output format. This new file has many advantages compared to the fixed format file including no longer needing the graph.npt file. The User Manual, preprocessor and model executable have all been updated to allow for this input file. Also, a converter utility has been developed to transform legacy control files to the new version. This is described in the Model Utilities part of the User Manual.
3. The model examples and User Manual were updated with a new example problem from Long Lake, WA. This new example uses the new Excel form of the control file. Also, all example problems were updated with the Excel version of the control file.
4. The preprocessor now spawns a window showing the pre.err file in case there are errors detected in the preprocessor. Also, several new preprocessor checks were added.
5. Output file format has been improved for the w2.wrn and the W2errordump.opt files using suggestions from Stewart Rounds (tireless!).
6. The pump algorithm has a new enhancement allowing water to be pumped from the upstream to downstream based on downstream water level.
7. Tecplot output through the CPL output can now specify which branches to write out. A new input file, Tecplotbr.csv, is used to specify which model branches are output to the Tecplot file.

Version 4.2.2 This version is not file compatible with Version 3.72 since two new variables were added to the control file. These are described in the User Manual Part 5 showing changes in the control file between versions. This code update adds a regression equation for CO₂ global average concentration in ppm and allows the user to define an average CO₂ gas concentration. This new calculation technique is described in the User Manual Part 2. The earlier code used a relationship that was from around 1960 (and had a minor coding error that had existed since Version 2)! Hence, there was a need to update the global CO₂ atmospheric concentration for computation of CO₂ gas exchange affecting total inorganic C and pH.

Version 4.5 This version includes many new features and upgrades and is not file compatible with earlier versions because of many new variables in the control file. Differences between versions are shown in Part 5 of the User Manual. The new model includes the following features (many of these features were supported by ERDC Environmental Laboratory and Portland District of U.S. Army Corps of Engineers):

1. Atmospheric deposition of any state variable – model user provides mass loading to waterbodies. There is now no need to specify a flow, temperature, and concentration file since only a time series of mass per area per time is used as an input.
2. Ability to specify directly output of flow balance file, N and P mass balance file, water level file
3. New generic constituent source: sediment release
4. New state variables: water age, N₂, dissolved total gas pressure, bacteria, CH₄, Fe(II), FeOOH, Mn(II), MnO₂, H₂S. Many of these before were only operative using sediment diagenesis as generic constituents or were recommended generic constituents.
5. New derived variables: turbidity (correlated to TSS), Secchi disk (based on light extinction), unionized ammonia (based on temperature, pH, and total ammonia), and Total Dissolved Gas (TDG).
6. Ammonia volatilization is computed based on unionized ammonia volatilization rate and is a derived variable. pH must also be active as a derived variable.
7. Implementation of variable algal settling velocity including buoyancy effects from Overman (2019). This allows for predicting the variable velocity of cyanobacteria allowing for rise and fall of the cells during the day and night.
8. Zooplankton settling is a new zooplankton parameter.
9. Implementation of algal toxin production based on Garstecki (2021)
10. Ability to generate lake contours easily (elevation vs time for temperature and dissolved oxygen)
11. Ability to generate river contours easily (model segment or distance along river vs time) for temperature and dissolved oxygen)
12. The C groups dissolved organic C (DOC) and particulate organic C (POC) with both labile and refractory groups were added as an alternative to organic matter groups. The option is available to use either C or organic matter. This was done earlier by Zhong in an earlier version of W2.
13. Sediment diagenesis updates. Many updates were made allowing for multiple vertical layers, simplified calculation, and much faster computation than before. Now when sediment diagenesis is turned ON, both zero order and first order sediment models are turned OFF internally. Also, the sediment diagenesis input file format has been updated and integrated into the Excel master sheet. This work was performed by Dr. Zhang at PSU.
14. Removed internal minimum reaeration coefficient value and allowed model user to set a minimum value if required. For example, for waterbodies designated as 'LAKE' with zero wind, the

model will now predict zero reaeration unless a minimum value is set. The reaeration coefficient for the surface layer is now an output in the Time Series file.

15. Updates to auto-port selection
16. SYSTDG input files updated to csv input format.
17. Updates to particle settling and P adsorption onto inorganic SS. A bug was fixed where dissolved oxygen-controlled P adsorption to particles rather than just P adsorption to Fe.
18. All external control files are included in an Excel master sheet for ease of writing out as csv files.

New Features and Planned Enhancements

A partial list of significant new model features since Version 3.7 are shown below in Table 1. Planned model enhancements are shown in Table 2.

Table 1. New CE-QUAL-W2 model features since Version 3.7.

Feature	Description	Model Version first included
Post-processor released for CE-QUAL-W2	DSI released a free tool for viewing output from the CE-QUAL-W2 model.	3.71
Csv file input/output	Model input files can now be in comma delimited format rather than fixed space formatted text. Most output files can be in csv file format for ease of processing in a spreadsheet. This continued through model version 4.1.	3.71-4.1
USGS automatic port selection algorithm	A more complex automatic port algorithm than in Version 3.7.	3.72
Sediment diagenesis	Predictive sediment diagenesis model with bubble formation and dynamic pH and temperature in the sediment layers	4.0
Scour of both inorganic suspended solids and organic solids	Scour based on bottom shear stress was added to mobile not only inorganic suspended solids, but also organic solids back into the water	4.0
New state variables such as CH ₄ , H ₂ S and Fe and Mn	Since the addition of sediment diagenesis, other water state variables were added that connected to the sediments. Now metals can oxidize and precipitate and be reduced in the sediments and released.	4.0
Non-Conservative alkalinity	Using algorithm from Sullivan et al. (2013) for non-conservative alkalinity	4.0
Photodegradation for generic constituents	Generic constituents can now photodegrade based on the available light at depth.	4.0
TDG with N ₂ as a state variable	Total Dissolved Gas using N ₂ as a state variable with O ₂ . Gas generation at spillways and dams is still included in the model.	4.0

Feature	Description	Model Version first included
Post-processor released for CE-QUAL-W2	DSI released a free tool for viewing output from the CE-QUAL-W2 model.	3.71
P and N balances	P and N balances are now computed in the model and output as a diagnostic tool	4.0
Branch active/inactive	Branches can be dry and wetted without crashing the model. The model accounts for all inflows and moves them to an appropriate wetted model segment.	4.1
Particle tracking	A 3D particle tracking algorithm allows for the movement of particles based on random turbulent motion and advection, including settling or rising of particles. There are many options to track particle releases.	4.1
Ax and Dx scale with U	The longitudinal eddy viscosity and eddy diffusivity can now scale with the longitudinal velocity	4.1
Multiple processor running of multiple waterbody models	Each waterbody can be run in conjunction with an upstream waterbody to utilize different processors for significant speed improvements in bug model systems.	4.2, 4.2.1
TDG algorithm	SYSTDG algorithm from the Corps was added to the existing formulations for TDG at spillways and gates.	4.2
Excel input file	A new input file, w2_con.csv, is available for model input and legacy converter utility.	4.2.1
Variable CO ₂ atmosphere	A regression equation is used to estimate global average CO ₂ in the atmosphere. Also, the model user can input a user-defined value.	4.2.2
Algal vertical movement in water column	Vertical rise and sink of algae cells can be mechanistically modeled as a function of time. This is especially important for cyanobacteria blooms.	4.5
Algae toxin production and fate/transport	Allows for specifying production and fate and transport of algal toxins	4.5
New state variables	Water age, N ₂ , dissolved total gas pressure, bacteria, CH ₄ , Fe(II), FeOOH, Mn(II), MnO ₂ , H ₂ S.	4.5
New derived variables	Turbidity, Secchi disk, un-ionized ammonia, and total dissolved gas.	4.5
Use of C instead of organic matter	The organic matter fractions can be represented in terms of C rather than organic matter if the user wishes.	4.5
Atmospheric deposition	Allows for atmospheric deposition of any state variable to waterbody	4.5
Ammonia volatilization	Computes unionized ammonia volatilization.	4.5

Feature	Description	Model Version first included
Post-processor released for CE-QUAL-W2	DSI released a free tool for viewing output from the CE-QUAL-W2 model.	3.71
Sediment Diagenesis	Computed for every vertical layer rather than just the bottom layer	4.5

Table 2. Planned Enhancements to CE-QUAL-W2.

Enhancement	Description	Status
1	Fish Bioenergetics model	Tested and working in research code
2	Simultaneous water level solution for all branches in a water body	Tested and working in research code
3	Sediment transport	Limited algorithms already in W2
4	Smart particle tracking – Fish model	Tested and working in research code
5	Toxics	Limited algorithms already in W2 as generic constituents
6	Sediment channel bottom heating algorithm	Tested and working in research code
7	Hyporheic flow algorithm	Tested and working in research code
8	W3 – a 3D model based on the W2 algorithms	Tested and working in research code

2. Capabilities and Limitations

Capabilities

Hydrodynamic. The model predicts water surface elevations, velocities (longitudinal and vertical), and temperatures. Temperature is always included in the hydrodynamic calculations because of its effect on water density through the equation of state. Water quality computations are done after a hydrodynamic computation allowing for feedback between water quality and hydrodynamic variables.

Even though the model is quasi-3D by the use of model branching, the most severe model limitation is lateral averaging. This does not mean that a 3D model will perform better than a 2D model. In some cases, a 3D model may be necessary to understand complex 3D flow patterns.

Water quality. Any combination of constituents can be included/excluded from a simulation. The effects of salinity or total dissolved solids/salinity on density and thus hydrodynamics are included if they are defined as active constituents. The water quality algorithm is modular allowing constituents to be added as additional subroutines. The current version includes the following water quality state variables in addition to temperature:

1. any number of generic constituents defined by either or all of the following: 0 order decay rate, 1st order decay rate, settling velocity, Arrhenius temperature rate multiplier, volatilization rate, and a photo-degradation rate based on available light. This can be used to define any number of the following:
 - a. conservative tracer(s)
 - b. bacteria
 - c. toxic contaminant(s)
2. Bacteria
3. Water Age
4. N₂ gas used in Total Dissolved Gas (TDG) computation
5. CH₄
6. H₂S
7. Dissolved gas pressure
8. any number of inorganic suspended solids groups with varying settling rates
9. any number of phytoplankton groups
10. any number of periphyton/epiphyton groups
11. any number of CBOD groups, including CBOD-N and CBOD-P
12. ammonium
13. nitrate+nitrite
14. bioavailable phosphorus (commonly represented by orthophosphate or soluble reactive phosphorus)
15. labile dissolved organic matter
16. refractory dissolved organic matter
17. labile particulate organic matter
18. refractory particulate organic matter
19. total inorganic carbon
20. alkalinity
21. FeOOH(s), Fe+2, MnO₂(s), Mn+2
22. dissolved oxygen
23. organic sediments for first order sediment model
24. any number of macrophyte groups
25. any number of zooplankton groups
26. labile dissolved organic matter-P or as C
27. refractory dissolved organic matter-P or as C
28. labile particulate organic matter-P or as C
29. refractory particulate organic matter-P or as C
30. labile dissolved organic matter-N or as C
31. refractory dissolved organic matter-N or as C
32. labile particulate organic matter-N or as C
33. refractory particulate organic matter-N or as C
34. organic sediment C
35. organic sediment N
36. organic sediment P
37. sediment NO₃
38. sediment NH₄
39. sediment PO₄
40. sediment and water column CH₄
41. sediment and water column H₂S
42. sediment pH

43. sediment temperature
44. sediment alkalinity
45. sediment and water column SO₄
46. sediment and water column Sulfide
47. sediment and water column FeOOH(s)
48. sediment and water column Fe⁺²
49. sediment and water column MnO₂(s)
50. sediment and water column Mn⁺²
51. sediment Total inorganic C
52. mature fine tailings (an inorganic suspended solids group)

Additionally, over 60 derived variables such as pH, TOC, DOC, TON, TOP, DOP, TP, TN, TKN, Secchi disk depth, unionized ammonia, and turbidity, can be computed internally from the state variables and output for comparison to measured data.

Long term simulations. The water surface elevation is solved implicitly, which eliminates the surface gravity wave restriction on the timestep. This permits larger timesteps during a simulation resulting in decreased computational time. As a result, the model can easily simulate long-term water quality responses. The vertical diffusion criterion from stability requirements has also been eliminated allowing for even larger timesteps. But larger time steps do not guarantee numerical accuracy since a larger time step leads to degraded numerical accuracy. Model simulations of multiple decades can usually be performed easily within the CE-QUAL-W2 model framework.

Head boundary conditions. The model can be applied to estuaries, rivers, or portions of a waterbody by specifying upstream or downstream head or water level boundary conditions.

Multiple branches. The branching algorithm allows application to geometrically complex waterbodies such as dendritic reservoirs or estuaries.

Multiple waterbodies. The model can be applied to any number of rivers, reservoirs, lakes, and estuaries linked in series. The multiple waterbodies each responds to a unique meteorological input file.

Multiple turbulence closure schemes. The model user can choose several different turbulence closure schemes. The preferred scheme for both estuary, river and lake/reservoir systems is the k- ϵ turbulence model.

Variable grid spacing. Variable segment lengths and layer thicknesses can be used allowing specification of higher resolution where needed. Vertical grid spacing can vary in thickness between waterbodies.

Water quality independent of hydrodynamics. Water quality can be updated less frequently than hydrodynamics thus reducing computational requirements. However, water quality is *not* decoupled from the hydrodynamics (i.e., there is not a separate, standalone code for hydrodynamics and water quality where output from the hydrodynamic model is stored on disk and then used to specify advective fluxes for the water quality computations).

Auto-stepping. The model includes a variable timestep algorithm that attempts to help ensure stability requirements for the hydrodynamics imposed by the numerical solution scheme are not violated. This though does not in all cases guarantee numerical stability since exact stability criteria cannot be determined *a priori*. Hence, the model user can still limit the maximum time step.

Restart provision. The user can output results during a simulation that can subsequently be used as input. Execution can then be resumed at that point.

Layer/segment/branch addition and subtraction (wetting and drying). The model will adjust surface layer and upstream segment locations, as well as branches, for a rising or falling water surface during a simulation.

Multiple inflows and outflows. Provisions are made for inflows and inflow loadings from point/nonpoint sources, branches, and precipitation. Outflows are specified either as releases at a branch's downstream segment or as lateral withdrawals. Evaporation can also be computed based on modeled temperatures and meteorological conditions.

Ice cover calculations. The model can calculate onset, growth, and breakup of ice cover.

Selective withdrawal calculations. The model can calculate the vertical extent of the withdrawal zone based on outlet geometry, outflow, and density as shown in Figure 5.

Multiple hydraulic structure algorithms. The model can be set up to allow multiple pumps, spillways, pipes and gates between model segments.

Dynamic shading. The model computes topographic and vegetative shading for each model segment.

Particle transport. The model simulates in a Lagrangian sense the movement of particles in x, y, and z. There are options to use particles for dye studies and for tracking the time history of temperature of a particle released at a fixed time and location.

Automatic vertical port selection in a reservoir. The model can compute what vertical layer to extract water from a reservoir to meet an imposed temperature standard downstream.

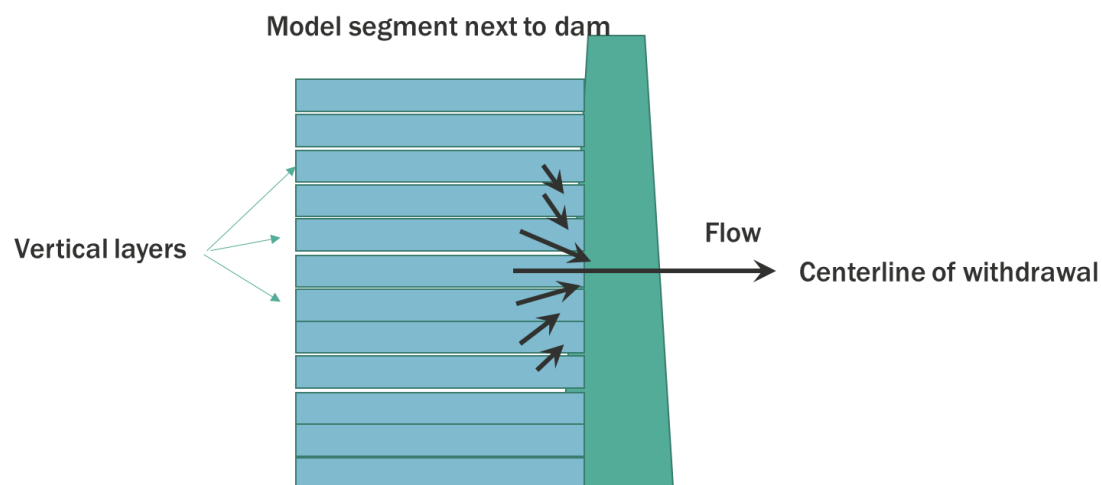


Figure 5. Withdrawal zone created in model using selective withdrawal theory.

Time-varying boundary conditions. The model accepts a given set of time-varying inputs at the frequency they occur independent of other sets of time-varying inputs.

Outputs. The model allows the user considerable flexibility in the type and frequency of outputs. The user can specify what is output, when during the simulation output is to begin, and the output frequency. A graphical postprocessor is available for plotting/ visualization.

Potential Limitations

Theoretical

Hydrodynamics and transport. The governing equations are laterally and layer averaged. Lateral averaging assumes lateral variations in velocities, temperatures, and constituents are negligible. This assumption may be inappropriate for large waterbodies exhibiting significant lateral variations in water quality. Whether this assumption is met is often a judgment call on the user and depends in large part on the questions being addressed. Eddy coefficients are used to model turbulence. Currently, the user must decide which vertical turbulence schemes is most appropriate for the type of waterbody being simulated. The equations are written in the conservative form using the Boussinesq and hydrostatic approximations. Since vertical momentum is not included, the model may give inaccurate results where there is significant vertical acceleration, but the selective withdrawal algorithms compensate for this in the vicinity withdrawals.

Water quality. Water quality interactions are simplified descriptions of complex processes. The goal of modeling is often to represent these as simple as possible to describe known phenomena. Improvements in these algorithms are often made as needed to describe complexities in the dynamics of the state variables or state variable interactions.

Sediment oxygen demand. The model includes both a user-specified sediment oxygen demand (zero order model) that is not coupled to the water column, a predictive first order simple SOD model, and a predictive sediment diagenesis model. Zero-order SOD only varies according to temperature. The first order sediment model is tied to the water column settling of organic matter. But the first order model only models labile, oxidic, sediment decay. The sediment diagenesis model models kinetics in the sediment and at the sediment-water interface. Because of the complexity of this model, data to drive this model may be a primary limitation.

Numerical

Solution scheme. The model provides three different numerical transport schemes for temperature and constituents - upwind differencing, the higher-order QUICKEST (Leonard, 1979), and Leonard's ULTIMATE algorithm. Upwind differencing introduces numerical diffusion often greater than physical diffusion. The QUICKEST scheme reduces numerical diffusion, but in areas of high gradients generates overshoots and undershoots which may produce small negative concentrations. ULTIMATE, Leonard's solution to the over/undershoots, has been incorporated into Version 3 and later. In addition, discretization errors are introduced as the finite difference cell dimensions or the timestep increase.

Computer limits. A considerable effort has been invested in increasing model efficiency including a vertically implicit solution for vertical turbulence in the horizontal momentum equation. However, the model

still places computational and storage burdens on a computer when making long-term simulations. Year-long water quality simulations for a single reservoir can take from a few minutes to days for multiple waterbodies in a large river basin. Applications to dynamic river systems can take considerably longer than reservoirs because of much smaller timesteps needed for river numerical stability.

Since the model uses dynamic allocation memory, the memory required for a simulation is determined at run-time. In most cases the memory requirements of CE-QUAL-W2 are minimal since the model opens input files and reads them record-by-record as needed rather than reading them all into memory at the beginning of the model run.

3 Overview of Data Preparation

Authors: Tom Cole, Scott Wells

The section is largely from Cole and Wells (2019) with Tom Cole as the primary author, and it provides an overview of the data preparation.

The following data are needed for model application:

1. geometric data
2. initial conditions
3. boundary conditions
4. hydraulic parameters
5. kinetic parameters
6. calibration data

A detailed discussion of these data follows.

Geometric Data

The first input task involves assembling geometric data. These data will be used to define the finite difference representation of the waterbody. The following data are needed for setting up input geometry:

1. topographic map and/or sediment range surveys
2. project volume-area-elevation table

The topographic map or sediment range surveys are used to generate bathymetric cross-sections that are input into the model. The project volume-area-elevation table is used for comparison with the volume-area-elevation table generated by the model.

Computational grid. The computational grid is the term used for the finite difference representation of the waterbody. Grid geometry is determined by four parameters:

- | | |
|---|---------|
| 1. longitudinal spacing (segment length) | [DLX] |
| 2. vertical spacing (layer height) | [H] |
| 3. average cross-sectional width (cell width) | [B] |
| 4. waterbody slope | [SLOPE] |

The longitudinal and vertical spacing may vary from segment to segment and layer to layer, but the spacing should vary gradually from one segment or layer to the next to minimize discretization errors.

Factors affecting computational grid. Several factors must be evaluated and weighed against each other when determining longitudinal and vertical spacing. These include:

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1. **Areas of strongest gradients.** This factor applies particularly to the metalimnion in fresh-water and the pycnocline in saltwater. If the model is not capturing water quality gradients in these regions, then vertical resolution may have to be increased. Similar reasoning applies to areas of longitudinal gradients.
2. **Computational and memory requirements.** The model penalizes the user in two ways when increasing grid resolution. As the number of grid cells goes up, so do computational and memory requirements. In addition, as the dimensions of a grid cell **decrease**, the timestep must also decrease to maintain numerical stability. As a rule of thumb, it is always desirable to err on the side of finer grid resolution, but the user must balance that with the available computer resources and the money and time available for completing the project.
3. **Bottom slope.** For reservoirs and some estuaries, the waterbody bottom slope is more accurately modeled as the ratio of cell thickness to cell length $[H]/[DLX]$ approaches the overall bottom slope. For sloping streams/rivers, the ratio is accurately represented by the slope or a hydraulic equivalent slope.
4. **Results.** Results should not be a function of the computational grid's resolution. With the development of the bathymetry editor, finely discretized grids can be easily coarsened. The coarser grid will have fewer computational cells and larger average timesteps resulting in decreased runtimes. The computational grid should initially be of high resolution and, if runtimes are excessive, reduced in resolution until the results change substantially. Results should never be a function of the grid resolution.

Previous applications have used a horizontal grid spacing of 100 to 10,000 *m* and a vertical grid spacing of 0.1 to 5 *m*. Regardless of the grid spacing used, the user should check to make certain that model predictions are grid independent. This is usually performed by making model simulations with varying grid resolution and using the largest grid that reproduces essentially the same results as those using the smallest grid.

Bathymetric data. The next step after determining horizontal and vertical cell dimensions is to determine average cross-sectional widths for each cell. This is an iterative procedure whereby initial bathymetry is input into the preprocessor and the volume-area-elevation table is then generated by the preprocessor. This table is compared to the project table and widths are adjusted to better match the project table.

Several methods have been used for determining average widths. Transects along the waterbody center-line can be drawn on a topographic map. A contour at the elevation corresponding to the **center** of a grid cell is located and the area encompassed by the contour line and the upstream and downstream transect is determined by planimeter. This area divided by the segment length is the average width of the grid cell. The process is repeated for each grid cell.

When no topographic information is available, the user can determine average widths from sediment range surveys for existing waterbodies. However, this method is generally not as accurate as data obtained from topographic maps since the number of available transects are usually insufficient to adequately describe the complex shape of most waterbodies. If available, sediment range surveys should be used to refine the grid generated from topographic information - particularly where significant sedimentation has occurred.

Other methods by individual investigators have been developed for generating grids using contour plotting packages such as Surfer, ArcGIS, and AUTOCAD.

Sample computational grid. A sample computational grid in the longitudinal/vertical plane with four branches is shown in [Figure 6](#). The FORTRAN variables associated with the grid are also included. The grid consists of 25 longitudinal segments $[IMX]$ and 22 vertical layers $[KMX]$. They constitute the total number

DATA PREPARATION

of cells in the computational grid. This is exactly how the model sees the grid layout even though this is not the correct physical representation of the system. Branch two and branch three join branch one. Branch setup is described in more detail below.

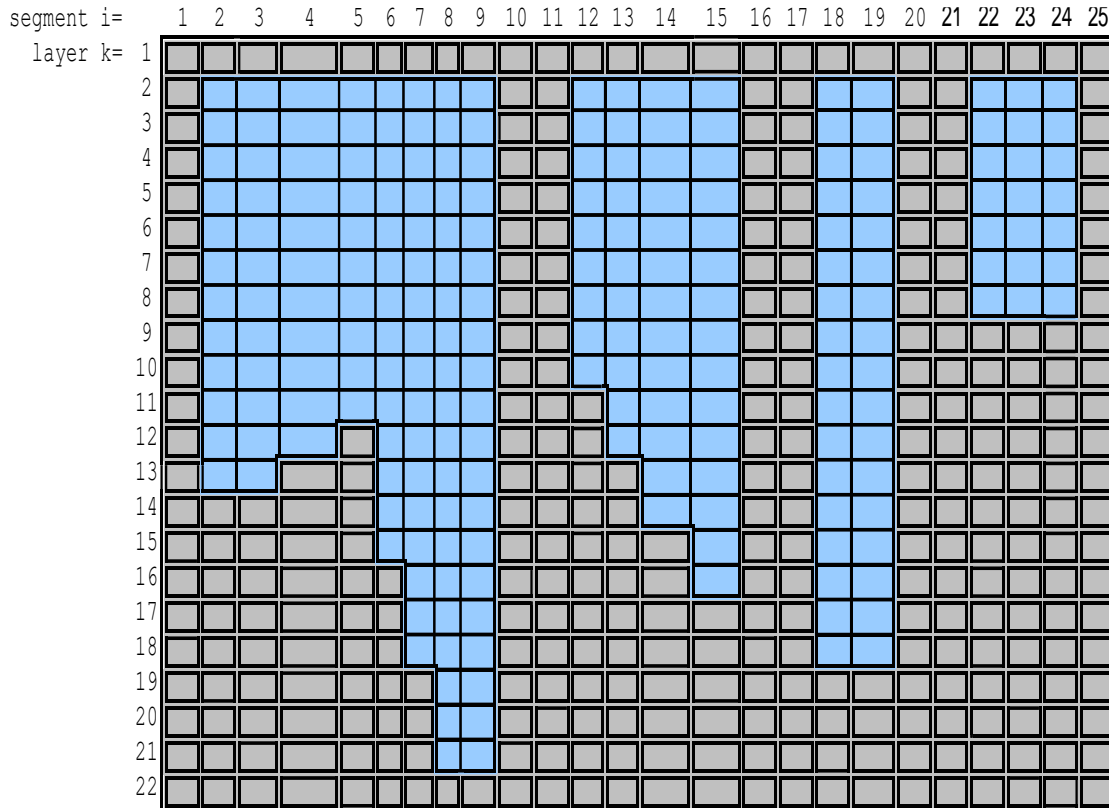


Figure 6. Sample computational grid in the x-z plane showing active and inactive cells.

Grid cell types. Figure 6 contains two kinds of cells - ones with either a single or a double line border. Cells with a single line border represent cells that may contain water during the simulation. The **active cells** are defined in the bathymetry input as having **non-zero widths**. Cells with a double border represent boundary cells located at or beyond the waterbody boundaries. The **boundary cells** are defined in the bathymetry input as having **zero widths**.

Boundary cells. There are four types of boundary cells:

1. top
2. bottom
3. upstream
4. downstream

Each segment must have a zero width for the cell in layer 1 and a zero width for every cell located below the bottom active cell. For example, cells 1 and 12-22 in segment five would have zero widths. In addition, each branch must have zero widths for upstream boundary and downstream boundary segments. Note this requirement results in **two segments** of boundary cells between each branch (segments 10-11 & 16-17).

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Branches. CE-QUAL-W2 can simulate a system with any number of waterbodies containing any number of branches. [Figure 7](#) shows a plan view of the same three branch grid of [Figure 6](#) along with the FORTRAN variables defining the geometry for each branch. For each branch, the upstream segment [US] and the downstream segment [DS] must be defined. The current upstream segment [CUS] is calculated by the model and may vary over time to meet restrictions imposed by the solution scheme. Typically segment numbers increase going from upstream to downstream in the branch.

A branch may connect to other branches at its upstream [UHS] and/or downstream segment [DHS]. In [Figure 7](#), the downstream segment of branch 2 ([DS]=15) connects to branch 1 at segment 7 ([DHS]=7).

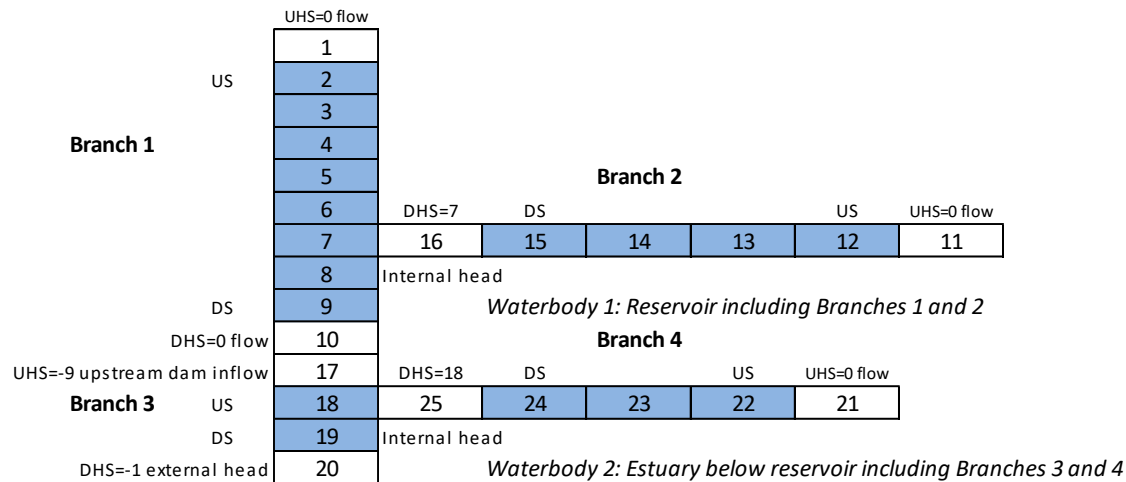


Figure 7. Sample computational grid in the x-y plane showing cell numbering and branch and water body connections.

Grid restrictions. The grid must satisfy the following restrictions:

1. Cell widths **cannot increase** with depth.
2. A **branch** may connect to other branches at its upstream or downstream segment, but a branch **may not enter or leave** itself.
3. Two branches may not connect at the same segment of another branch.

The bathymetry input file contains the longitudinal grid spacing [DLX], initial water surface elevation [WSEL], segment orientations [PHIO], vertical grid spacing [H], bottom friction [FRICT], and average cell widths [B].

After the bathymetry is generated, it should be checked to ensure the bottom elevation varies smoothly and represents the average slope over appropriate portions of the waterbody for reservoirs and estuaries. Oftentimes, minimum bottom widths are set at 5-15 *m*. This helps increase timesteps with minimal impact on the volume-area-elevation curves. However, increasing widths in the bottom layers can affect water quality since sediment oxygen demand and nutrient fluxes are dependent on bottom surface areas. Refer to the [bathymetry file](#) and [preprocessor output](#) in the sample applications for additional guidance in setting up the bathymetry.

Initial Conditions

Initial conditions are specified in the control, bathymetry, and vertical and/or longitudinal profile input files. The control file specifies the following initial conditions:

1. **Time (required).** Starting [\[TMSTRT\]](#) and ending time [\[TMEND\]](#) of the simulation.
2. **Temperatures (required) and concentrations (optional).** The initial temperature [\[IT2\]](#) and constituent concentrations [\[IC2\]](#). If the grid is not initialized to a single value, then a grid-wide vertical profile can be specified in the vertical profile input file [\[VPRFN\]](#). The option is also available to specify a longitudinally and vertically varying initial concentration for temperature and constituents via the longitudinal profile file [\[LPRFN\]](#).
3. **Inflows/outflows (optional).** The number and location of inflows and outflows.
4. **Restart (optional).** If a previous run with the model was made specifying restart conditions were to be written [\[RSOC\]](#) to an output file, then the user can specify the model read the file [\[RSIC\]](#) and continue the simulation from that point.
5. **Waterbody type (required).** The waterbody can be specified as either saltwater or freshwater [\[WTYPE\]](#).
6. **Ice thickness (optional).** The initial ice thickness [\[ICETHI\]](#).

Boundary Conditions

Inflows. The model recognizes the following inflows:

1. **Upstream inflows (optional).** Upstream inflows occur only at a branch's current upstream segment [\[CUS\]](#), which may vary during a simulation. The model provides the option to distribute inflows evenly throughout the inflow segment or place inflows according to density [\[PQC\]](#). *If* the upstream inflow option is used, then a separate file for inflow [\[QIN\]](#), a separate file for temperature [\[TIN\]](#), and, *if* constituents are modeled, a separate file containing constituent concentrations [\[CIN\]](#) for *each* branch is required.
2. **Tributary inflows (optional).** Tributary inflows or point source loadings [\[QTR\]](#) may enter any segment of the computational grid. If the current upstream segment [\[CUS\]](#) number is greater than the segment the tributary enters, then the tributary inflows are added into the current upstream segment to maintain the waterbody water balance. As in upstream inflows, the model provides the option to distribute tributary inflows evenly throughout the inflow segment or place inflows according to their density [\[PTRC\]](#). An additional option to place inflows between two specified elevations is also included to better describe point source inflows such as wastewater effluent discharged from a pipe. The number of tributaries [\[NTR\]](#) and their segment location [\[ITR\]](#) are specified in the control file. *If* this option is used, then file requirements for *each* tributary are the same as for upstream inflows.
3. **Distributed tributary inflows (optional).** Distributed tributary inflows or nonpoint source loadings [\[DTRC\]](#) may be specified for any branch. The flow is distributed throughout a branch weighted by segment surface areas. *If* this option is used, then file requirements for *each* distributed tributary are the same as for upstream inflows.
4. **Precipitation (optional).** Precipitation [\[PRC\]](#) can be specified for each branch and is distributed according to the segment surface areas. *If* this option is used, then file requirements for *each* branch are the same as for upstream inflows.

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5. **Internal inflows** (optional). Flows from gates, pipes, and pumps and over spillways and weirs can now be routed internally in the computational grid from one segment to another. This allows application of the model to highly engineered systems.

Outflows. The model recognizes the following outflows:

1. **Downstream outflows** (optional). Downstream outflows [QOUT] occur only at the downstream segment [DS] of a branch. Selective withdrawal where the vertical extent of and flow distribution in the withdrawal zone is calculated by the model is used for all outflows. Additionally, the bottom [KBSTR] and top layers [KTSTR] below and above which outflow cannot occur can be specified by the user to include the effects of upstream structures that restrict the selective withdrawal zone. Outflow will occur even if the outlet location is above the current water surface layer [KT]. This is a necessity when calibrating water surface elevations. A separate file for *each* branch is required.
2. **Lateral withdrawals** (optional). Lateral withdrawals [QWD] may be specified for any active cell. The number of withdrawals [NWD], their segment location [IWD], and their centerline elevation [EWD] must be specified in the control file. *If* this option is used, a separate file for *each* withdrawal is required. Version 3 now uses selective withdrawal for lateral withdrawals.
3. **Evaporation** (optional). Evaporation is calculated by the model from air [TAIR] and dew-point [TDEW] temperature and wind speed [WIND]. If a waterbody loses a significant amount of water from evaporation that is not accounted for in the inflows, then the user should include evaporation. Evaporative heat loss is *always* included in the heat budget.
4. **Internal outflows** (optional). Flows from gates, pipes, and pumps and over spillways and weirs can now be routed internally in the computational grid from one segment to another. This allows application of the model to highly engineered systems.

Head Boundary Conditions (optional). The model recognizes the following head boundary

1. **External.** The user may specify an external upstream [UHS] and/or downstream head [DHS] boundary condition for each branch. This boundary specification is intended primarily for estuarine simulations although it has also been used for river and reservoir applications. *If* this option is used, a separate file for time-varying elevations, [EUH] and/or [EDH], a separate file for vertical temperature profiles, [TUH] and/or [TDH], and, if constituents are modeled, a separate file containing vertical profiles for each constituent modeled, [CUH] and/or [CDH], *must* be specified for *each* external head boundary condition.
2. **Internal.** Internal head boundary conditions are specified wherever one branch connects with another branch. The boundary surface elevation, temperatures, and constituent concentrations are calculated internally by the model.

Surface Boundary Conditions (required). The model requires the following surface boundary conditions:

1. **Surface heat exchange.** Surface heat exchange is calculated by either of two methods using the input variable [SLHTC] in the control file. The first method uses equilibrium temperatures [ET] and coefficients of surface heat exchange [CSHE] to calculate surface heat exchange (Brady and Edinger, 1975). The second method uses a term-by-term accounting for calculating surface heat exchange. For both methods, latitude [LAT] and longitude [LONG] are specified in the control file and values for air temperature [TAIR], dew point temperature [TDEW], wind speed [WIND] and direction [PHI], and cloud cover [CLOUD] *must* be

- included in the meteorological file (even if short wave solar radiation is read into the model). If available, short wave solar radiation can be input directly into the model.
2. **Solar radiation absorption.** Distribution of solar radiation in the water column is controlled by the fraction of solar radiation absorbed in the surface layer [BETA] and the attenuation rate due to water [EXH2O], inorganic suspended solids [EXINOR], and organic suspended solids [EXORG]. Values for [EXINOR] and [EXORG] affect solar radiation only if constituents are modeled. These values are specified in the control file.
 3. **Wind stress.** Wind speed [WIND] and direction [PHI] must be supplied in the meteorological file [METFN]. Wind stress is an extremely important physical process and should be included in all applications. The model allows the user to specify a wind sheltering coefficient [WSC] which, when multiplied with the wind speed, reduces effects of the wind to take into account differences in terrain from the met station and the prototype site. The sheltering coefficient is specified in the wind sheltering file [WSCFN].
 4. **Gas exchange.** The wind speed [WIND] supplied in the meteorological file is also used for computing gas exchange at the water surface if dissolved oxygen and/or total inorganic carbon are simulated. Gas exchange is also affected by the wind sheltering coefficient [WSC].

Temperature transport cannot be turned off in the model. Temperature can be treated conservatively by turning off heat exchange computations [HEATC].

Hydraulic Parameters

Dispersion/diffusion coefficients. The horizontal dispersion coefficients for momentum [AX] and temperature/constituents [DX] are specified in the control file. They are presently time and space invariant. Sensitivity analyses on numerous applications have shown the model is relatively insensitive to variations in the default values for reservoirs, but can be important in rivers and estuaries.

The vertical diffusion coefficients for momentum [AZ] and temperature/constituents [DZ] vary in space and time and are computed by the model. There are a number of different vertical turbulence algorithms available. The k- ϵ turbulence closure model is applicable to all types of waterbodies and is recommended. Earlier versions of CE-QUAL-W2 successfully used the 'W2' closure scheme for stratified reservoirs.

Bottom friction. The latest version now allows the user the option of specifying longitudinally varying values for the Chezy coefficient or Manning's n for bottom friction. The friction type is specified in the control file [FRICC]. They are used in calculating boundary friction that varies spatially as a function of exposed bottom area and temporally as a function of the flow field. The values are specified in the bathymetry file.

Kinetic Parameters

There are more than 120 coefficients affecting water quality constituent kinetics, although on the order of 10 are normally adjusted during water quality calibration. The values are specified in the control file. If water quality is not simulated, these are not needed.

DATA PREPARATION

Calibration Data

Calibration data are used to provide initial and boundary conditions and assess model performance during calibration. A great deal of thought should go into assessing the amount and type of data necessary to adequately characterize and understand the limnology of a waterbody and to develop the database required to support a water quality modeling effort. Gaugush (1986; 1987; 1993) provides detailed information on sampling design and frequency. ***Determining the availability of adequate calibration data should be done as early in the study as possible.*** If the user determines calibration data are inadequate, then immediate steps should be taken to collect sufficient data. Results will be suspect at best and will not withstand scrutiny at worst if the model is applied with insufficient and/or inadequate calibration data. The following discussion provides an overview of data required for the proper application of CE-QUAL-W2.

In-Pool. Proper application of mechanistic water quality models requires at least one set of in-pool observed data. The preferred method is ***at least*** two sets of data encompassing different extremes in the prototype (i.e., high and low flow years, warm and cold years, spring phytoplankton bloom and no spring phytoplankton bloom, etc.). In-pool data is used to set initial conditions and assess the model's ability to reproduce observed conditions. Given sufficient time and funding, ***all years*** in which sufficient data are available should be included during model calibration.

Time-Varying Boundary Conditions. It cannot be overemphasized that data used to drive the model needs to be as accurate as possible. For temperature calibration, this typically means using continuous inflow temperatures or developing regression relationships for inflow temperatures based on flow and air or equilibrium temperature to generate at least daily inflow temperatures (see Ford & Stein, 1984). Equilibrium temperature is preferred since it includes more of the mechanisms affecting water temperature.

For meteorological data, use the most frequent data available. Previously, daily average values were used to drive the model because earlier 1-D models used daily timesteps. Many modelers still take hourly or three-hourly data and generate daily averages for model input. ***Any time data is averaged, information is lost.*** For most reservoirs, thermocline depth and shape are a function of two physical mechanisms - wind mixing and convective cooling. Using daily average air temperatures eliminates nighttime convective mixing that can be a very important physical process affecting epilimnetic depths and thermocline shapes for reservoirs. As another example, applying a daily average wind speed and direction can generate an artificial water surface slope that incorrectly drives hydrodynamics. Daily averaging of wind speeds can also result in much less energy input into the model since the energy input by wind is a function of the wind speed cubed. Hence, it is good modeling practice to use hourly meteorological data if available.

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. It is a waste of time and effort to collect in-pool data in support of water quality modeling when inflow concentrations/loadings have not been adequately characterized since they often drive the system. As in the development of inflow temperatures, regressions relating concentration/loadings with flow and possibly refined for season should be developed for tributary inflows. Ideally, several storm events should be intensively sampled since this is when loadings are generally highest to a waterbody. Also, point source loadings should be identified and loading estimates obtained. Some estimate of non-point source loadings should also be made. In some cases, meteorological loading estimates should be obtained. A software package, FLUX (Walker, 1986), is useful for generating loadings over time from intermittent samples. [Table 3](#) gives general guidelines for data collection.

DATA PREPARATION

Kinetic Rates. Because water quality modeling is still very much an art with numerous rate coefficients available for adjustment during calibration, it is highly preferable to obtain actual measurements of these coefficients used in the water quality formulations. If all of the rate coefficients have been determined for a waterbody, then any discrepancies between computed and observed data highlight the model's shortcomings, help to identify the bounds of the model's predictive capabilities, and provide direction for efficient use of resources to provide a better understanding of the system's water quality dynamics.

Ideally, a model should be used as a starting point for limnological investigations of a waterbody, with the data and formulations continuously refined to reflect the increased understanding of the system and processes gained over time. Unfortunately, this approach is rarely taken in practice due in large part to the expense involved, but also, even more unfortunately, due to the inability of aquatic biologists/limnologists and engineers to collaborate.

This cooperative approach between experimentalists and theoreticians is the main impetus behind the tremendous advances in physics, chemistry, and, to some extent, biology (e.g., genetic research) during the last century, but is seldom seen in the field of water quality modeling. A notable exception is the Chesapeake Bay Modeling Study (Cerco and Cole, 1994). Researchers in the Chesapeake Bay region, including both biologists and engineers, were actively involved in data acquisition and water quality formulations and provided invaluable knowledge and feedback during the course of the study. This cooperative arrangement is continuing and should be a model for all future water quality model development.

Table 3. General guidelines for in-pool water quality sampling.

Boundary Conditions		
Minimum parameters	Additional parameters	Frequency
inflow/outflow temperature	conductivity dissolved oxygen pH total dissolved solids ¹	daily or continuous
total organic carbon	dissolved and/or particulate organic carbon BOD ²	weekly w/ storm sampling
soluble reactive phosphorous total phosphorous	total dissolved phosphorus total inorganic phosphorus dissolved inorganic phosphorus	weekly w/ storm sampling
nitrate+nitrite nitrogen ammonium nitrogen	total Kjeldahl nitrogen filtered total Kjeldahl nitrogen	weekly w/ storm sampling
	total suspended solids ³ inorganic and/or volatile suspended solids	weekly w/ storm sampling
	chlorophyll <i>a</i> dissolved silica ⁴ alkalinity	weekly w/ storm sampling
In-Pool		
Minimum parameters	Additional parameters	Frequency
Temperature ⁵ Dissolved oxygen ⁵ pH ⁵ Conductivity ⁵	total dissolved solids ¹	monthly ⁶
Chlorophyll <i>a</i> ⁷	phytoplankton biomass and type	monthly

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Total organic carbon ⁷	dissolved and/or particulate organic carbon BOD ²	monthly
Soluble reactive phosphorus Total phosphorus ⁷	total dissolved phosphorus total inorganic phosphorus dissolved inorganic phosphorus	monthly
nitrate + nitrite nitrogen ammonium nitrogen ⁷	total Kjeldahl nitrogen filtered total Kjeldahl nitrogen	monthly
	secchi depth/light transmission	monthly
	total inorganic carbon alkalinity	monthly
	total suspended solids ³ inorganic and/or volatile suspended solids	monthly
	dissolved/total iron ⁸ dissolved/total manganese ⁸ dissolved/total silica ⁸ total dissolved sulfide ⁸ sulfate ⁸ iron sulfide ⁸	monthly
¹ enough samples to correlate to conductivity - important for density effects ² used to characterize decay rates of organic matter ³ suspended solids affect phosphorus partitioning, light penetration, and density ⁴ can be limiting for diatom growth ⁵ preferably bi-weekly - samples should be taken at 1m intervals ⁶ 1m intervals ⁷ minimum number of samples includes one each in epilimnion, metalimnion, and hypolimnion - preferred number of samples (depending on depth) would be at 3m intervals with more frequent metalimnetic sampling ⁸ when concerned about sediment release during anoxic periods		

Since water quality compartments are coupled, calibration of one compartment may affect other compartments making calibration difficult. ***An understanding of the processes modeled as well as knowledge of the system being simulated is an absolute must if the modeling effort is to succeed.*** A complete description of kinetic coefficients along with guidelines for appropriate default and a range of literature values is given in Part 3 of the User's Manual.

Constituents are grouped into four levels ([Table 4](#)). Level I includes constituents that have no interaction with phytoplankton/nutrient/DO dynamics. Level II includes constituents affecting phytoplankton/nutrient/DO dynamics. Level III includes constituents that interact with level II constituents, but that are not transported. In level IV, alkalinity and total inorganic carbon are transported by the model and are thus state variables. They are necessary for computing pH and carbonate species.

Data Analysis. An often overlooked step in model applications is plotting and analyzing observed data for all stations and times for which data are available. Do not plot up just the data chosen for calibration as the additional data may reveal important information about the prototype. Unfortunately, most mechanistic water quality modelers come from an engineering background with only cursory exposure to limnology. If a limnologist is available, they should be consulted during this stage to help in identifying the dominant processes occurring in the system. Once these have been identified, then efforts should be made to ensure the dominant forcing functions are represented as accurately as possible in the model, either as accurate boundary conditions or as additional water quality formulations.

Table 4. Constituent levels and names.

Level	Constituent
I	Total dissolved solids (or salinity)
	Generic constituents
	Inorganic suspended solids (and MFT, mine fine tailings)
II	Dissolved inorganic phosphorus
	Ammonium
	Nitrate-nitrite
	Dissolved silica
	Particulate biogenic silica
	Total Metals (Iron)
	Labile DOM, DOM-N, DOM-P
	Refractory DOM, DOM-N, DOM-P
	Labile POM, POM-N, POM-P
	Refractory POM, POM-N, POM-P
	CBOD, CBOD-N, CBOD-P
	Dissolved oxygen
	Zooplankton
	Phytoplankton
	Mn+2, Fe+2, MnO ₂ (s), FeOOH(s)
	CH ₄ , H ₂ S
III	Epiphyton/periphyton
	Organic sediments, sediment C, N, P, and Fe, Mn, CH ₄ , H ₂ S
	Macrophytes
IV	Total inorganic carbon (sediments and water column)
	Alkalinity (sediments and water column)

For example, phosphorus coprecipitation with calcite is not currently included in the model. If this is known to be an important mechanism for phosphorus removal from the photic zone resulting from pH changes due to phytoplankton primary production, then this mechanism should be included in the kinetic formulations. This is a common mechanism for many freshwater systems located in limestone topography, such as Texas, Tennessee, and Florida. Another example would be the presence of macrophytes that affect hydrodynamics, nutrient uptake rates, phytoplankton primary production, and water column oxygen dynamics. Since macrophytes are not in the current release, then they would have to be included in the hydrodynamic and kinetic formulations.

Another important task in data development and analysis is to analyze the data for reasonableness. Checks for reasonableness should go beyond outlier checks to include checks to see if changes in concentrations over space and time make limnological sense. For example, if reservoir hypolimnetic nitrate concentrations increase during anoxic conditions and inflow temperatures are warmer than epilimnetic temperatures and/or inflow nitrate concentrations are less than the hypolimnetic concentrations, then there is no way for nitrate concentrations to increase during this time in either the prototype or in the model. So, there is no use wasting time during calibration trying to reproduce this behavior and the failure of the model to reproduce this behavior should not be viewed as a shortcoming of the model. Another example would be

observed reservoir hypolimnetic release temperatures that were greater than the hypolimnetic temperatures. It would be impossible for the model to match these temperatures during calibration.

4. Model Download Files

All files on the CE-QUAL-W2 web site (<http://www.ce.pdx.edu/w2>) are in a compressed zip file. The download compressed file is organized in directories that contain the source code, executables, user manual, and example applications. Model downloads over the last 15 years have averaged over 3 model downloads/day, and in 2018 the website averaged between 500 and 1000 unique visitors/month.

After downloading the model package, you will end up with a directory structure as shown below:

- Examples
- Excel macro utility for writing files in W2 format from Excel
- Executables
- Sediment diagenesis documentation
- Source
- User Manual
- USGS documentation for using USGS Auto Port Selection Algorithm
- USGS Examples for using USGS Auto Port Selection Algorithm
- W2ControlGUI
- W2tools post-processor integrated with W2control preprocessor
- Waterbalance utility

These are descriptions of the subdirectories and files:

1. **Examples** – Model application examples include DeGray Reservoir, Spokane River, Spokane River (input files in csv format), Columbia Slough estuary, a reservoir model illustrating the sediment diagenesis model of Version 4.0, a multiple cascade reservoir example, a SYSTDG example, and several reservoirs that illustrate the USGS auto-port selection algorithm (introduced in Version 3.72). DeGray Reservoir is a reservoir with a single branch and a complete water quality application. The Spokane River is an example of a river system with multiple river sections. The Columbia Slough is a fresh-water estuary example.
2. **Excel macro utility for writing files in W2 format from Excel** - This directory contains an Excel macro that aids in writing our CE-QUAL-W2 compatible files from within Excel. There is a short user manual describing how to use the macro. This macro was developed by Jeffrey Gregory, Civil Engineer, USACE, Nashville District.
3. **Executables** – The executables for the preprocessor and the model in this directory were compiled using the latest Intel Fortran compiler and have both 32- and 64-bit versions. These executables must be placed into the directories of the model input files or be used with the command-line option for setting the default directory where the model files reside.
4. **Sediment diagenesis documentation** – reports and documents explaining the sediment diagenesis model in Version 4.

5. **Source** – This directory contains the source code for the preprocessor and model written in Fortran90+. The compiler settings and files necessary to compile using the Intel compiler are also included using the Intel Fortran compiler. Generally, we use the following compiler settings for the Windows application: /O2 [maximum speed in Intel] and default real is double precision. Also, for the following subroutines we had to use /O1 optimization: init-cond.f90 and init-u-elws.f90. For the preprocessor, the windows source code is compiled using a QuickWin application. We use the debug version for the released executable.
6. **User Manual** - User Manual Parts 1-5.
7. **USGS Documentation for the Auto Port Selection Algorithm** – Technical report for the new USGS algorithm for auto port selection.
8. **USGS Model examples for the Auto Port Selection** – 4 example problems using the USGS algorithm for auto port selection
9. **W2ControlGUI** - The W2Control GUI was compiled using Visual Basic 6. The GUI directory also has an installation routine for W2Control. There is a “setup.exe” routine that installs the Visual Basic W2 V3.7 Model Preprocessor called W2CONTROL which is also compatible with the V4 model. Once installed, the GUI preprocessor is able to aid the model user in setting up the Control File and in evaluating and changing the bathymetry of the system. This preprocessor does not automatically set-up the bathymetry of the system, nor does it provide post-processing support. A lot of effort is required to properly set-up the model bathymetry prior to using the Bathymetry editor within W2Control. A user manual in pdf format is included in this directory. Also, a separate executable, W2Control, is provided in case an earlier version has already been installed. Note that this GUI is a part of the install routine for W2Tools now.
10. **W2Tools post-processor** – This is the new W2 post-processor by Dynamic Solutions-International, LLC (www.ds-international.biz). They have provided an installation routine that includes both the post-processor and the W2ControlGUI. When the user selects W2L output (the old VPL output), the resulting post-processing file is used by W2Tool for all post-processing tasks that include contour plots, animations, profile plots and time series plots. A brief user manual is included showing many of the features of this post-processor as well as a directory that shows how to take field data and plot field data and model results in the post-processor. There is a zip file with an example from DeGray reservoir on how to include model predictions versus field data for reservoir profiles.
11. **Waterbalance utility** – This includes the windows waterbalance utility and the more powerful updated console version of the waterbalance utility. Both are described in Part 5 of the User Manual. The purpose of this code is to approximate the waterbalance for a reservoir or lake by computing flows (positive and negative) that will allow the model predicted water level to agree with water level data for a reservoir.

5. How to Run the Model for the First Time

In order to run the DeGray Reservoir example which is included in the Model Download Files, copy the model executables from the executables/w2 model (for example **w2_v4_64.exe**) and **executables/w2**

preprocessor (for example **preW2-v4_64.exe**) from the executables directory to the **examples/DeGray Reservoir** directory.

The Degray Reservoir directory is shown in Figure 8 before copying the preprocessor and model executable into this directory.




















 w2_con.npt	10/3/2017 5:08 PM	NPT File	26 KB
 w2_envirprf.npt	2/16/2017 5:09 PM	NPT File	3 KB
 met.npt	8/7/2012 3:26 PM	NPT File	144 KB
 w2_selective.npt	10/27/2011 9:59 A...	NPT File	2 KB
 dynpump1.npt	3/31/2011 4:31 PM	NPT File	1 KB
 dynselective1.npt	3/31/2011 4:14 PM	NPT File	1 KB
 w2_aerate.npt	10/9/2010 11:09 A...	NPT File	1 KB
 w2_habitat.npt	9/2/2010 12:45 PM	NPT File	1 KB
 graph.npt	5/31/2010 11:12 P...	NPT File	7 KB
 bth.npt	6/17/2006 2:02 PM	NPT File	12 KB
 bth_2m.npt	6/17/2006 2:02 PM	NPT File	12 KB
 shade.npt	9/3/2002 6:34 PM	NPT File	1 KB
 wsc.npt	9/3/2002 6:34 PM	NPT File	1 KB
 cin_br1.npt	8/29/2001 9:32 AM	NPT File	7 KB
 qin_br1.npt	8/29/2001 9:32 AM	NPT File	6 KB
 qot_br1.npt	8/29/2001 9:32 AM	NPT File	7 KB
 tin_br1.npt	8/29/2001 9:32 AM	NPT File	7 KB
 vpr.npt	8/29/2001 9:32 AM	NPT File	2 KB
 prf_dam.npt	8/12/1998 11:59 A...	NPT File	117 KB

Figure 8. DeGray Reservoir model example files.

Double click the preprocessor executable to run the preprocessor. This produces several output files such as a warning file (**pre.wrn**) and an error file (**pre.err**) if there were any errors. If adjustments were made to input files, rerun the preprocessor until there are no more errors. Once this has completed, double click the w2 model executable. The model will run with a dialog box showing the progress of the simulation. Once it completes, you can then evaluate the model results by examining output files for post-processing. How to set up an application is shown in the next section.

6. How to Set-Up and Run a Model Application

1. Construct all boundary condition files

These files include flow rates, temperatures, and concentrations for all inflows, meteorological conditions for each waterbody, water levels for head BCs, shading for each segment, wind sheltering for segments, outflow rates, withdrawal rates, and precipitation files.

All of these files can be developed in Excel. In some of the model examples from the web page, input files may have a 'csv' or 'npt' extension. The file name and file type for most input files can be specified by the model user. Usually you will find that the inflow files use q (for flow), t (for temperature) and c (for concentration). The meteorological file is often named something like **met*.npt** or **met*.csv**.

How do you develop these files? One could use Excel to set up all the input files. For example, open a new Excel worksheet. Let's develop a flow input file for the model. The 1st 3 lines are ignored by the model and are used for descriptors and column headers. Enter a descriptive comment on the 1st line like: 'Inflow #1 2003'. Skip a line or row. On row 3 add the column headers: 1st column type 'JDAY', 2nd column type 'Q(m3/s)'. On row 4 enter a Julian day, like 1.5 (this corresponds to January 1 at 12 noon) and a corresponding flow like 10.0 (enter decimal points). On row 5 enter 365. and 15. The model has the option of linearly interpolating or viewing these as step functions. How do we save this in the correct text format for W2?

The older model input files relied on fixed text format. To save this in the fixed format, select all the worksheet and set the column widths all to 8 characters. Then File/SaveAs, choose a "prn" file, but in the filename enter the desired filename in quotes, such as "**qin_branch1.npt**". Then click OK. This will save a file with an acceptable format. To output this in csv format, there is an output option in Excel for writing it as a csv file or one can use the Excel macro utility, **w2_tools_L.xlam** (provided on the PSU CE-QUAL-W2 website by Jeffrey Gregory) to write out a file in csv format (also see the W2 Tools Excel Macro Utility User Manual). Note that the first character in line 1 for a csv input file must be a '\$'.

Since the model uses Julian days for all calculations and boundary conditions, it is often useful to convert from a real date field to Julian day and vice versa. The Excel formula to convert a Date field is "**=<Cell with Date>-DATEVALUE("1/1/XXXX")+1**" where XXXX is the reference year for the start of Julian days. Then the user must convert the format to a number field.

A full description of model files is shown in Part 3 of the User Manual.

2. **Develop the Model Grid**

This involves developing a bathymetry file for each water body. Use a text editor to open the existing bathymetry file for DeGray Reservoir (**bth.npt**). Now open the GUI Interface (do this by using the file **W2Control4.exe**) and click on CON for the control file and BTH for the bathymetry editor. You can view the bathymetry graphically with views of the side, top and end of the segments by clicking on appropriate buttons.

Note that the model also now uses "csv" file format so that the grid can be viewed and edited directly in Excel rather than the older, more cumbersome bathymetry fixed file format. The csv format is shown in a file named **bth1.csv** in the **Spokane River csv input format** directory. An example of the bathymetry format for a csv file for a reservoir is shown in Part 3 of the User's Manual.

How does one develop the bathymetry file?

- a. Obtain x,y,z topographic data
- b. For reservoirs or rivers one can take DEM data and merge it with x,y,z topographic data of your waterbody in GIS or Surfer
- c. Create centerline and grid spacing in x for each model branch
- d. Draw polygons around each model segment and create a Volume-area-elevation curve for each segment.

- e. After choosing an appropriate vertical layer spacing, compute segment widths for each vertical layer for each segment using $B = [\text{Volume in layer}] / (\Delta x \Delta z)$
- f. Assemble all the layer widths for each segment into the file compatible with the CE-QUAL-W2 model

Note also that using cross-sections directly for computing segment widths at various elevations is also appropriate if the cross-section is representative of the model segment.

3. Edit the Main Control File

The main control file, **w2_con.npt** or **w2_con.csv** (developed in Excel), is the central file for describing how the model will run. This file tells the code when the model starts, ends, where the inflows/outflows are located, names of files, water quality kinetic parameters, output file designations and content, and items you cannot even imagine. The csv file is developed in Excel while the npt file is edited using a text editor.

4. Edit Auxiliary Input Files

If the model user wants to include additional processes, additional auxiliary input files are required. For example, the model user could use sediment diagenesis (**w2_diagenesis.npt**), automatic port selection (**w2_selective.npt**), or particle tracking (**particle.csv**). These and other input files describe how the model will run with these features. Other input files include: **w2_aerate.npt**, **w2_envirp.npt**, **w2_habitat.npt**, **constriction.npt**, **pH_buffering.npt**, **dynselevX.npt**, **dynpumpX.npt**, **dynpipe.npt**, **w2_systdg.npt**, **multiple_WB.npt**, and others.

5. Run the Preprocessor

This file, **preW2-4_64.exe**, checks for model errors in the control file, bathymetry file, and all boundary condition files. Double click on the executable and look at the preprocessor screen. This file writes out between 1 and 3 files: **pre.opt** (an echo of input data and other useful items), **pre.err** (if fatal errors), and **pre.wrn** (if warnings). Make sure you look at **pre.wrn** and **pre.err** files.

6. Run the W2 Model

The file **w2_v4_64.exe** is the W2 model code. Double click on the w2 executable and notice the dialog box and the dynamic animation boxes for the simulation.

7. Evaluate OUTPUT files or Model Results

CE-QUAL-W2 outputs files have an extension 'opt' or 'csv' depending on the user definition of the filetype. Open the file **snp.opt** (a snapshot file) using a text editor. There are other files you can use with Excel for easy plotting, such as TSR files and Spreadsheet files. The CPL output from the model can also be used directly with Tecplot360 from www.tecplot.com for animating the results. Animation of results and contour plots can also be shown using the free **w2_post.exe** post-processor.

7. How to Use Batch Processing and the Command Line with CE-QUAL-W2

The W2 model preprocessor and executable are both command line aware meaning that users can execute the programs from any directory and set the default model directory. This might be especially helpful if one has 2 linked models that one wants to run independently rather than in one large model.

So let's say that you have 2 directories: **c:\w2\LakeA** and **c:\w2\RiverBelowLakeA** that have all the required input files. If you have the W2 model and preprocessor executable in the **c:\w2** directory, you can execute the preprocessor using a batch file, let's say **checkW2.bat**, that contains the following lines of text:

```
prew2-v4_64.exe "c:\w2\LakeA"
prew2-v4_64.exe "c:\w2\RiverBelowLakeA"
```

Executing this batch file would run the preprocessor for both directories. In each case the model user must close the dialog box for the next command to be executed. This is by design since we want you to look at the results of the preprocessor to see if anything is amiss.

Since the outflow from LakeA goes into the RiverBelowLakeA, the following batch file, let's say **runW2.bat**, runs the models and copies files from one directory to the other:

```
w2_v4_64.exe "c:\w2\LakeA"
copy "c:\w2\LakeA\qwd.opt" "c:\w2\RiverBelowLakeA\qin.npt" /Y
copy "c:\w2\LakeA\twd.opt" "c:\w2\RiverBelowLakeA\tin.npt" /Y
copy "c:\w2\LakeA\cwd.opt" "c:\w2\RiverBelowLakeA\cin.npt" /Y
w2_v4_64.exe "c:\w2\RiverBelowLakeA"
```

Note that by setting the parameter **CLOSEC** to **ON** in **w2_con.npt**, the dialog boxes close when a simulation is completed (and no user intervention is required). The quotation marks are there in case you have any spaces in your file names or directories. The **/Y** flag means that the copy command overwrites the file in the target directory without prompting the model user for permission.

8. How to include relative directory paths for input and output files

Instead of having all your model files in one directory, one can organize some of them by subdirectories. You can specify relative paths in the control file **w2_con.npt** for both input and output files. Let's say that your model directory is **c:\w2\LakeA** and you want to create a subdirectory for the input files and some of the output files. We can then create subdirectories such as:

c:\w2\LakeA\Inflows -- the flow, temperature and concentration input files for both the branch inflow, tributaries, and distributed inflow
c:\w2\LakeA\Inputs -- shading file, bathymetry file, wind sheltering file
c:\w2\LakeA\output_tsr -- tsr file outputs
c:\w2\LakeA\output_snp -- snapshot file outputs

In the section of the control file, **w2_con.npt**, where filenames are given, use the **'.'** to specify a file directory starting from the current directory. Hence, for the shading and wind sheltering file, you would specify:

```
WSC FILE.....WSCFN.....
      .\Inputs\wsc.npt
```

```
SHD FILE.....SHDFN.....
.\Inputs\shade.npt
```

And similarly for branch inflows:

```
QIN FILE.....QINFN.....
BR1      .\Inflows\qP88_2012.npt
```

```
TIN FILE.....TINFN.....
BR1      .\Inflows\tin_P88_2012.npt
```

```
CIN FILE.....CINFN.....
BR1      .\Inflows\cP88_2012_updated.npt
```

And similarly for output file paths:

```
SNP FILE.....SNPFN.....
WB 1      .\output_snp\snp_wb1.opt
```

...

```
TSR FILE.....TSRFN.....
.\output_tsr\tsr.csv
```

9. References

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10. Appendix A: Contributors to the development of CE-QUAL-W2

The list of contributors to the release version of CE-QUAL-W2 is long. It is difficult to know all the individuals who have contributed to the model's development, so this list may only be a partial list. The Corps of Engineers Engineering Research and Development Center (ERDC) has been the primary developer of the CE-QUAL-W2 model. This development work was spearheaded by Tom Cole at ERDC moving the model from Version 1 (impossible to use) to Version 2 and 3 (where you can actually use the model!). His efforts to advance the use of the model cannot be overstated. The development work at Portland State University is merely a continuation of that original development. The goal of this development is (1) to create a tool useful for improving water quality and managing water bodies to meet their beneficial uses and (2) to make that tool freely available.

Below are some of the individuals who have made major contributions to the model development: Ed Buchak and John Edinger (Hydrodynamic code development and model support through Version 2), Tom Cole (spearheaded the development of W2 developing Version 2 and working with S. Wells on Version 3; worked hard to make W2 a workable model and helped countless individuals with their early W2 applications, started W2 modeling workshop in the late 1990's, primary author of 2 major user manuals), Chris Berger (developed the macrophyte model, integrated and revised the sediment diagenesis model, developed the pipe algorithm, and contributed to Version 3.1-4.2), Rob Annear (developed the shading algorithm and contributed to many developments in Version 3.5-3.7), James Martin (worked on Version 1 Water quality algorithms and User Manual), Ray Chapman (developed the coding for Ultimate Quickest and the foundation of the turbulence algorithms that were updated and revised by Gould), Stewart Rounds (added the automatic port algorithm option USGS, non-conservative alkalinity, and many bug fixes and excellent code suggestions such as refining the multiple waterbody algorithms), Annette Sullivan (worked with Stewart on automatic port algorithm option USGS, non-conservative alkalinity, and many bug fixes and excellent code suggestions), and Zhong Zhang who worked hard on the SYSTDG algorithm implementation, made significant improvements in the sediment diagenesis model, and is working on the Hg model).

Others who have contributed code and/or model tools include (not in any particular order): Qinsheng Huang (W2 GUI preprocessor and bathymetry editor), Paul Craig (W2 post-processor development), Jeffrey Gregory (Excel macro utility for file preparation), Andy Goodwin (developed the first particle and fish movement model in W2, parts of the particle model are still in the code), Sam Gould (TKE turbulence closure scheme development), John Tobiason and Lillian Jeznach (generic constituent photo-degradation), S. Prakash and J. A. Vandenberg (first developers of the sediment diagenesis model with CEMA), Ray Walton (model suggestions over the years), Gary Hauser (many model suggestions and W2 GUI preprocessor developer), John Harrison (worked on a bacterial model for W2 for the Snake River, which in the end was not put in the release version), Yoav Bornstein (QGIS bathymetry generator), Dottie Tillman (worked on integration of W2 and HEC-RESSIM models, as well as many W2 applications), and others.

Also, the list of professors and graduate students at many Universities (including Portland State University) who have used the model and suggested improvements and have helped further its applicability include Dan McGinnis, Michael McKillip, Jun Ma, Daobin Ji, Hussein Al-Zubaidi (worked on a 3D version of W2 and compared to W2), Holly Juza, Muhanned Almurib, Sarah Van Glubt, Tim Kraft, Michael Posovich, Nasim Shojai, Ken Lawler, Seth Stevens, Andrew McCulloch, Amory Ceravich, Michelle Henry, Sarah Burnett, Corina Overman, Sher-Jamal Khan, Tel Jensen, Bernadel Garstecki and others. There is also a long list of

individuals who have researched the code finding model bugs. Besides those already mentioned that list also includes Lindsey Bearup from USBR and others.

11. Appendix B: Selected List of CE-QUAL-W2 Publications

Below is a list of CE-QUAL-W2 publications first put together by Tom Cole. This list has been updated, but it is still incomplete. Nevertheless, it provides some background into who is using the model and what papers are being disseminated or presentations being made using the CE-QUAL-W2 model.

Peer Reviewed Publications and Proceedings

Annear, R. L., and Wells, S. A. 2007. A comparison of five models for estimating clear-sky solar radiation, *Water Resources Research*, 43, W10415, doi:10.1029/2006WR005055.

Al-Murib, M. and Wells, S. A. 2016. "Application of CE-QUAL-W2 on the Tigris River in Iraq," Proceedings ASCE World Environmental and Water Congress, <http://dx.doi.org/10.1061/9780784479858.052#sthash.TVasrBU0.dpuf>.

Al-Murib, M., Wells, S., and Talke, S. 2017. "Estimation of Surface Water Temperature of the Tigris River System in Iraq," Proceedings ASCE EWRI Congress, Sacramento, May 21-25, DOI: <http://dx.doi.org/10.1061/9780784480632.016>.

Al Murib, M. D., Wells, S., Talke, S. A. 2019. "Use of Landsat TM/ETM+ to Estimate Water Temperature in the Tigris River in Iraq for Numerical Modeling Using CE-QUAL-W2," *Water*, 11, 892; doi:10.3390/w11050892.

Al Murib, M. D. and Wells, S. 2019. "Hydrodynamics and Total Dissolved Solids Model of the Tigris River Using CE-QUAL-W2," *Environmental Processes*, DOI: 10.1007/s40710-019-00381-y

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