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AQUATOX (RELEASE 3.1)

MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS

TECHNICAL NOTE 3: MODELING WATER FLOWS WITH AQUATOX RELEASE 3.1

Technical Note 3: Modeling Water Flows with AQUATOX Release 3.1

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Horsley Witten Group

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August 2012

Technical Note 3: Modeling Water Flows with AQUATOX Release 3.1

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Disclaimer

This document was designed to help users properly characterize water flows within the AQUATOX model. Anticipated users of this document include persons who are interested in using the model for various purposes, including but not limited to researchers and regulators. The model described in this document is not required, and the document does not change any legal requirements or impose legally binding requirements on EPA, states, tribes or the regulated community. This document has been approved for publication by the Office of Science and Technology, Office of Water, U.S. Environmental Protection Agency. Mention of trade names, commercial products or organizations does not imply endorsement or recommendation for use.

Background

Modeling water flows within AQUATOX is an important part of setting up an ecological simulation and can also be the cause of confusion to a model user. This document attempts to clarify how to specify water flows into and out of an AQUATOX simulation in both single-segment and linked-segment modes.

Each time AQUATOX has been applied to a linked system (Lower Boise River, ID; Tenkiller Lake, OK; and DeGray Reservoir, AR) the nature and quality of available hydrodynamic data has necessitated a different approach to obtaining and managing the input data. Given these technical complexities, this document summarizes the different approaches taken so that similar methods can be utilized in new model applications.

Single Segment Overview

When modeling water flows in a single segment, there are four basic options that are available by double clicking on “Water Volume” at the bottom of the state variables list (Figure 1). Note also that for single-segment simulations, water volumes can also be entered via the AQUATOX Wizard interface.

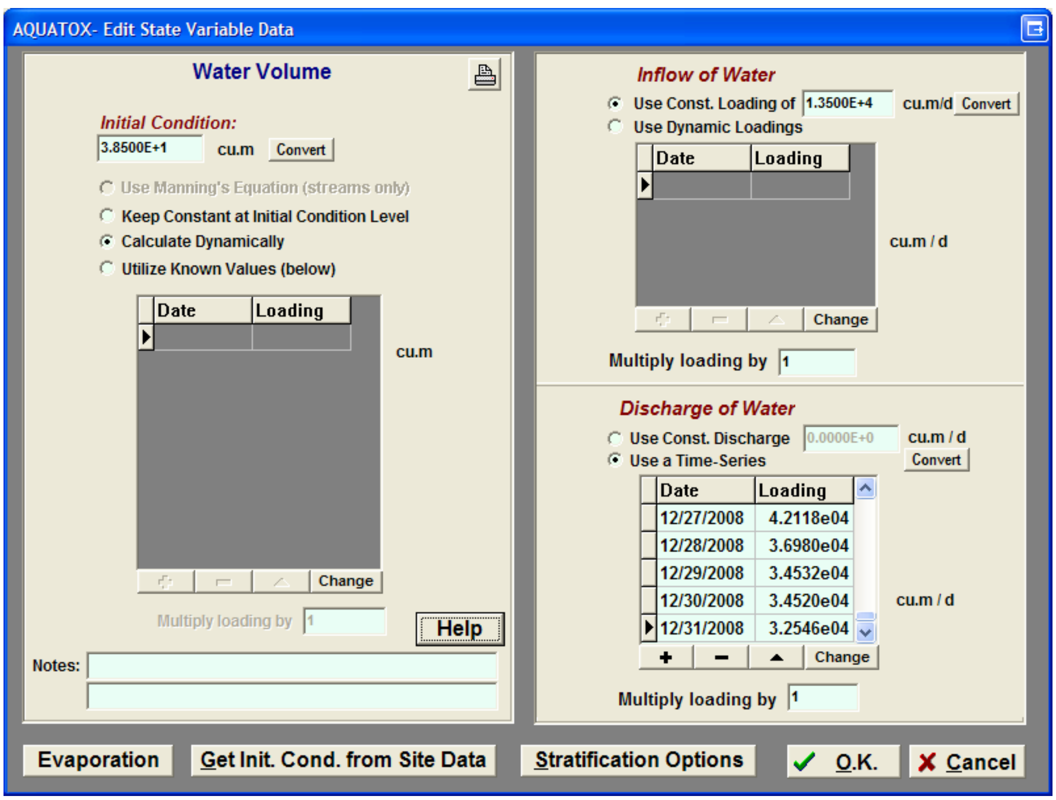

Figure 1: Water Volume Entry Screen in AQUATOX

Four Options for Modeling Water Volume in Single-Segment Mode

- The **Manning's Equation** Method (streams only): This method requires discharge data, often available from USGS stream gages. The site's volume at each time step is then estimated using Manning's Equation and the length of the stream segment. The inflows required to maintain these volumes are also automatically calculated. Careful attention should be given to the "Channel Slope" and "Manning's Coefficient" parameters entered in the "Stream Data" screen (within the site underlying data screen.)
- The **Keep Constant at Initial Condition Level** approach: This method requires inflow data. Discharge is calculated based on inflow and evaporation.
- **Calculate Dynamically**: In this case, volume is calculated based on time series of inflow, outflow and evaporation.
- **Utilize Known Values:** This method requires a time series of known volumes and inflow data. Outflow is calculated taking evaporation into account.

At each time step, segment volume is increased by the inflow coming into the system, and reduced by the outflow and evaporation. Site volumes, inflows and discharges may be entered using the time-series inputs available on the left and the right of the "Water Volume" entry screen (Figure 1). Inputs that are not relevant to the water volume choice selected are colored a dark grey and unavailable for user entry.

As a simplification, in single-segment mode, inflows of water due to direct precipitation are ignored[1]. However, nutrient and organic toxicant loadings associated with direct precipitation may be specified by clicking on any of the nutrients (or toxicants) in the state-variable list, moving to the "direct precipitation" entry box, and adding the mass loaded to the system in units of "g/m^2 d."

Evaporation

New to Release 3.1, a user may also specify time-varying evaporation. Evaporation time-series and constant values are not located on the water-volume screen, but instead are available in the "Site Data" entry screen (Figure 2). For convenience, an "Evaporation" button is available at the lower left of the water-volume screen for the user to quickly jump to the relevant entry screen.

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[1] If water volume added due to direct precipitation is a critical component of the water balance of a single-segment model, this water volume may be added to the inflow waters. However, note that concentrations of nutrients or toxicants associated with the inflow waters will also be added to your direct-precipitation water loadings. Another possibility is to model your segment using the multi-segment interface and adding a tributary input that represents precipitation of water. This method is discussed in *Water Flows in Multi-Segment Mode* below.

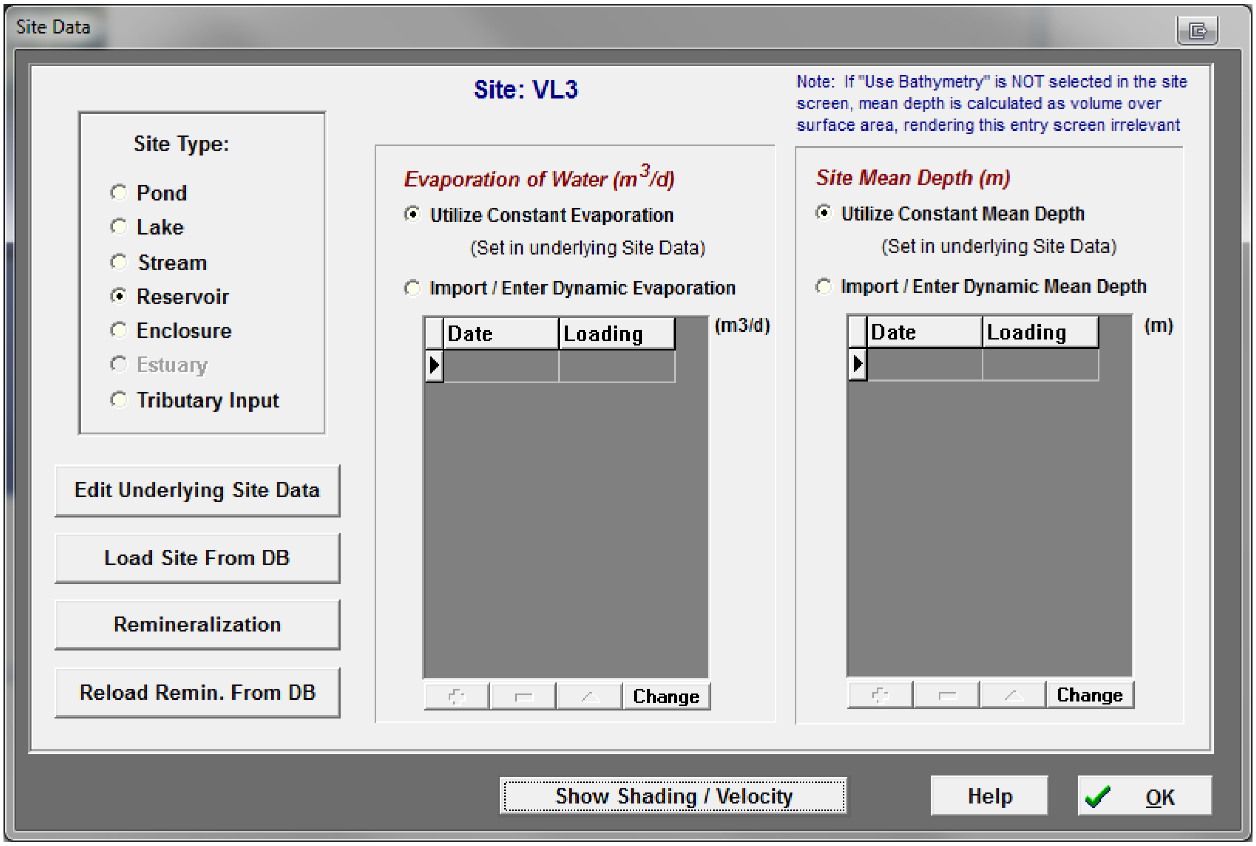

Figure 2: Site Data Entry Screen, including Time-Varying Evaporation

Evaporation may be specified in daily cubic meters lost or, alternatively, the mean evaporation from the site database may be used. The entry in the database is given in inches per year and is converted to cubic meters per day. This entry is part of the "underlying site data."

Stratification Considerations

The "Stratification Options" button allows a user to modify default model behavior regarding stratification by specifying dates of stratification, thermocline depth, or flow routing options. (Default model behavior is to initiate stratification when the mean water temperature exceeds 4 deg C. and the difference in temperature between the epilimnion and hypolimnion exceeds 3 deg C. Overturn occurs when the temperature of the epilimnion is less than 3 deg. C, usually in the fall.)

In single-segment mode, when a system becomes “stratified,” the number of biotic and nutrient state variables are doubled; one set of state variables represents the upper epilimnion layer and one represents the lower hypolimnion layer.   Water can mix between the upper and lower layers due to turbulent diffusion and again when the system is completely mixed due to “overturn.” However, the overall water volume of the system is not changed because of stratification. The water volume inputs represent the entire modeled segment and are not specific to either the upper or lower segment. Water volume outputs also represent the water volume of the entire segment.

Within the “Stratification Options” menu, options to route water into and out of the epilimnion and hypolimnion segments are available (Figure 3). Again, this does not affect the overall water volume of the system, only how water is flowing through the system.

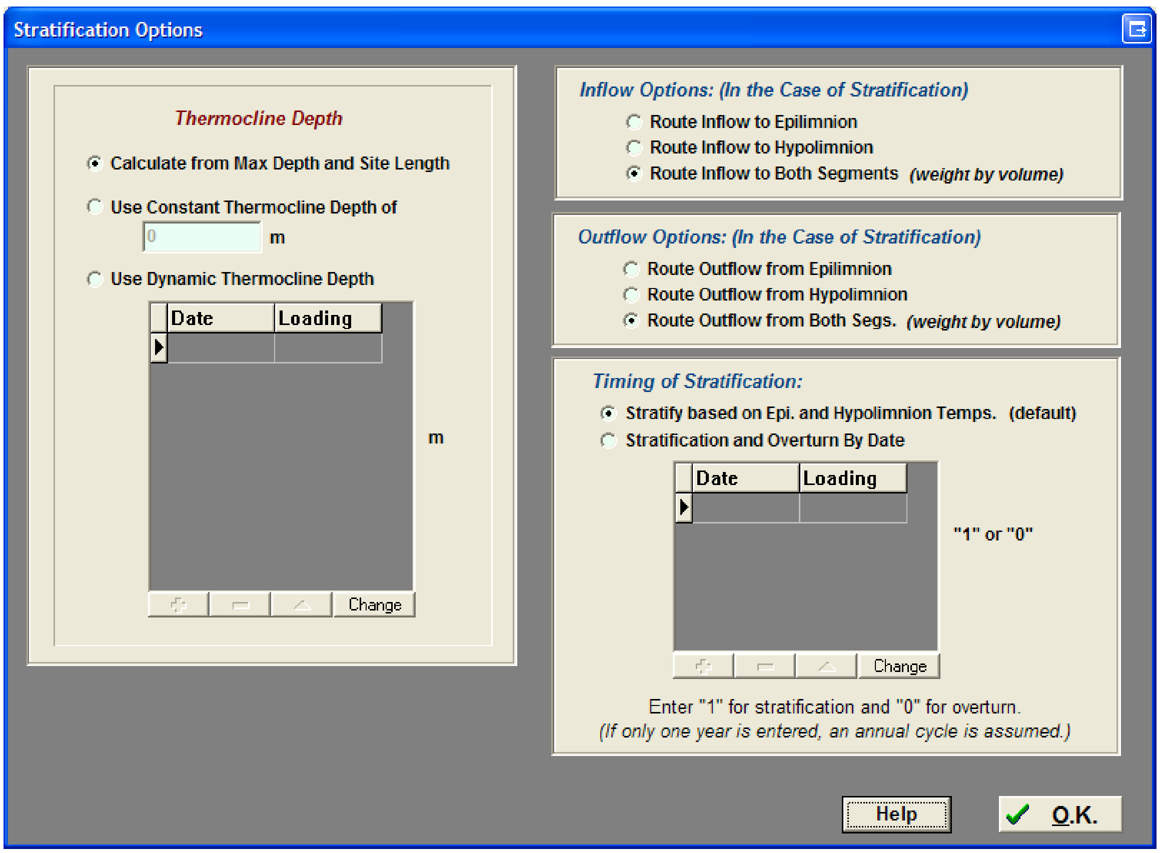

Figure 3: Stratification Options Including Flow Routing Options

Water Flows in Multi-Segment Mode

In the multi-segment model, each segment has multiple potential sources of water inputs as shown in Figure 4. When a system is linked together, AQUATOX requires that the water volume be solved using the "Calculate Dynamically" method described above (on pg. 4). In other words, the user specifies all inflows to and outflows from each segment, including evaporation, precipitation, and groundwater (if important) and AQUATOX calculates the resultant volume of each segment.

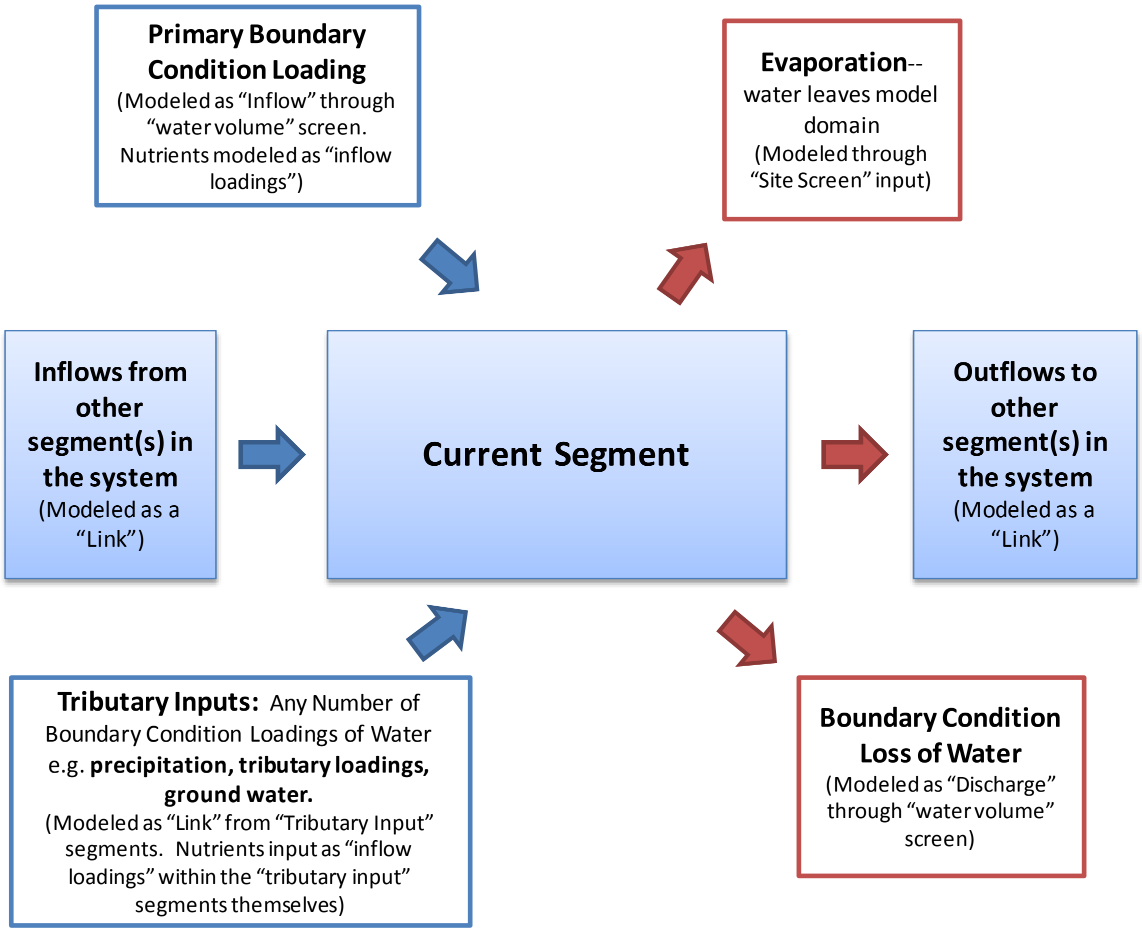

Figure 4: Diagram of potential water inputs and losses from each segment within a linked system

Water Inflows

There are three primary sources of water inflows into an AQUATOX segment:

- **Primary boundary condition loading:** This usually represents the primary source of water coming into the segment that is not part of the modeled spatial domain. Inflows of water are specified as "inflow loadings" through the water volume screen within the segment. (First double click on the relevant segment to access its state variable list and then double click on "water volume" in the segment's state variable list, as shown in Figure 5.) Nutrients, gases, toxicants, organic and inorganic sediments, and biotic loadings within this water may be specified by double-clicking on the relevant state variable and specifying the concentration of that loading within inflow water.

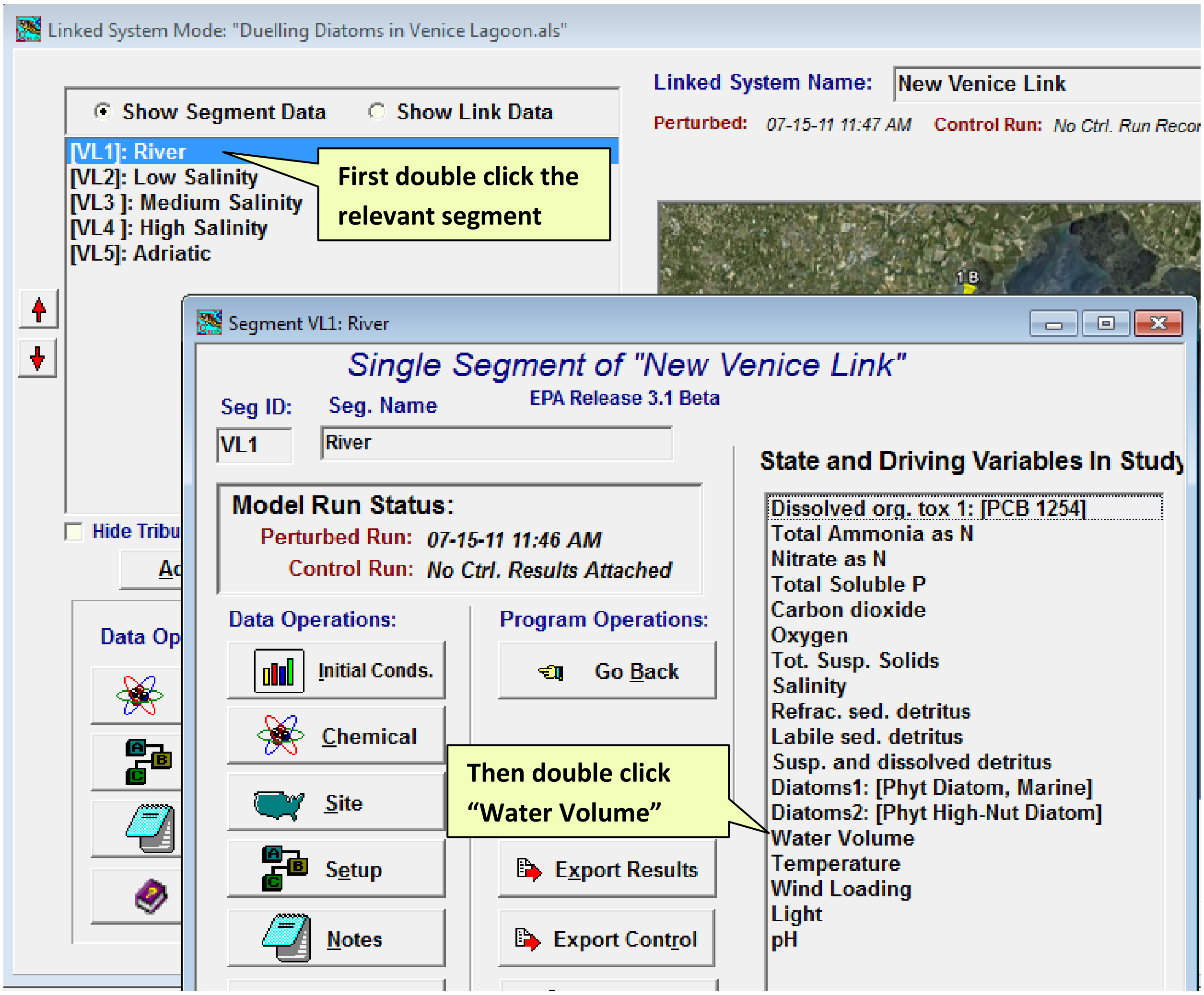

Figure 5: Manner of accessing water volume loadings in linked-segment mode

- **Inflows from other modeled segments:** These loadings can either be unidirectional "cascade" water loadings, or bi-directional "feedback" water loadings. To specify such a loading, first a "link" between the two modeled segments must be created ("Show Link Data" check-box then "Add"). When the link is then edited, the user may specify water flows from one segment to the next. Note that nutrients, toxicants, organic matter, biotic, and inorganic-sediment loadings do not need to be specified as they are being calculated by AQUATOX within the other modeled segment.

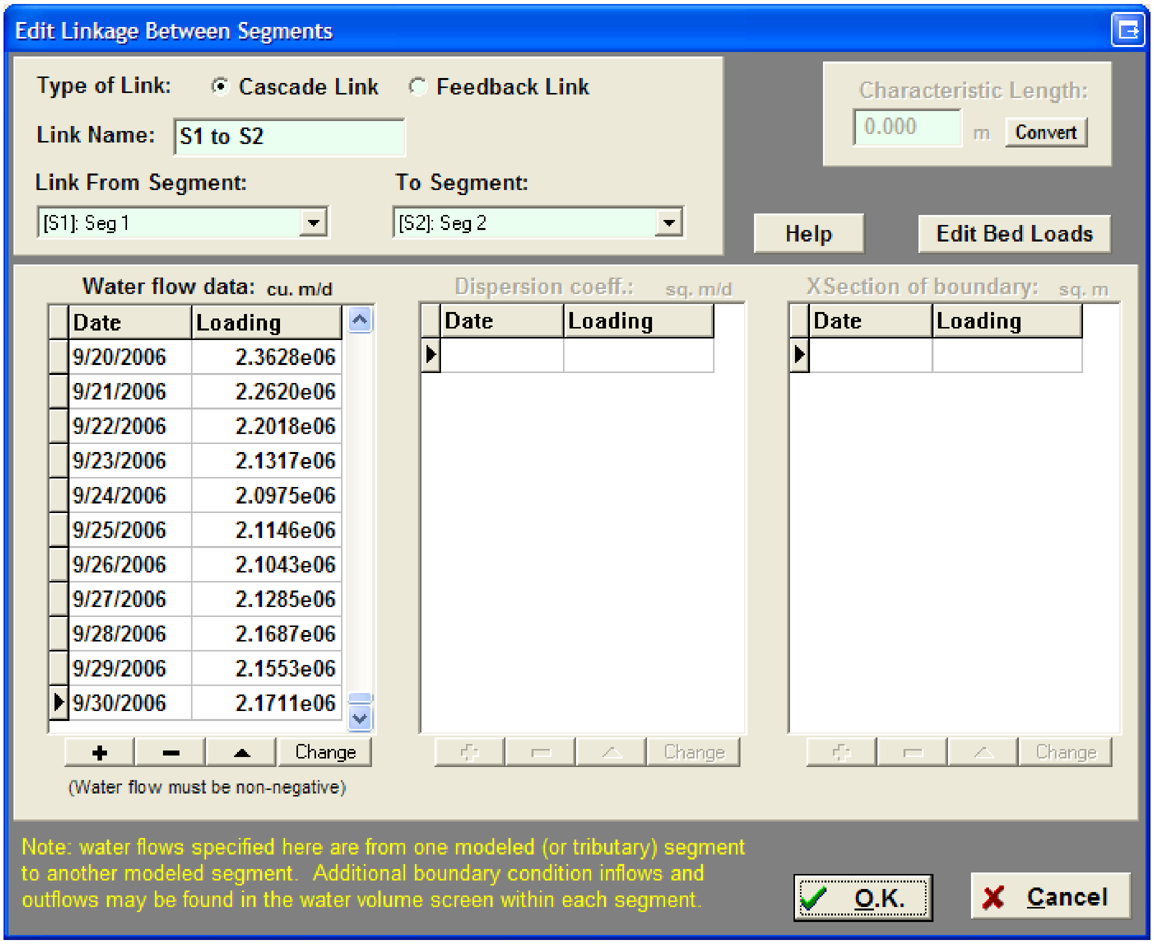

Figure 6: Entry screen to edit water flows between segments

- **Tributary inputs:** Any number of additional boundary-condition loadings of water may be specified including point sources, non-point sources, direct precipitation, tributary loadings, and ground water. First, an additional segment is added and designated as a "tributary input" type in the site data-entry screen (Figure 2). The new tributary input must then be linked to the segment in question by adding a "link" and specifying water flows from the tributary input into the segment (Figure 6).

  In order to specify nutrients, organic and inorganic sediments, toxicants, and biotic loadings that are associated with the inflow water from the tributary input, these items are specified as part of the inflow loadings to the tributary input itself. The tributary input segment is not part of the model domain, but water flows and state variables associated with them are loaded into the spatial domain of the model.

  Using "tributary inputs" to break boundary-condition inflows of water into their components, rather than aggregating all flows and dissolved and suspended state variables, has several benefits. First, AQUATOX can determine the total loads of dissolved and suspended state variables and water to the modeled system rather than requiring the user to sum water flows and to perform a complex weighted-average of nutrients, toxicants, gasses, and sediments. Secondly, setting up scenarios that pertain to a single input then becomes much more straightforward (e.g. "what would be the ecological effect if nutrients and organic matter from a given wastewater treatment plant were to be reduced?"). The Lower Boise River example discussed below made extensive use of tributary inputs to model dozens of tributaries, groundwater, and point-source inputs to the model domain.

Water Losses

- **Primary boundary-condition loss:** This represents the sum of non-evaporative water losses from the segment. Because each segment is assumed to be well mixed, specifying different locations for water losses is not required. This could represent withdrawal (to a location outside the model domain) or the main-stem outflow for the stream segment furthest downstream (with no linked segments below it). These outflows or withdrawals are specified as "discharge of water" through the water-volume screen within the segment. (Figure 5.)
- **Outflows to other modeled segments:** As was the case with inflows from modeled segments, outflows to and from other segments can either be unidirectional or bi-directional. To specify such an outflow, a "link" must be created and water flows added as specified above.
- **Evaporation:** New to Release 3.1, a user may also specify time-varying evaporation for each segment using the "Site Data" entry screen (Figure 2). Evaporative water losses can be separated from the primary boundary-condition losses so that the state variable concentration is properly computed.

Flow Balance Considerations

As discussed above, the entire water balance of the linked system must be externally specified by the user, including both internal and external water flows. As we will discuss within this document, there are many ways to set up such a water balance model ranging from simple spreadsheet models to complex hydrodynamic modeling systems.

When a complex water balance is set up, it may prove to be overly time-consuming to enter all of the flows and nutrient concentrations into the AQUATOX interface by importing many dozens of individual time-series. For this reason, the "Excel Template Import Capability" was designed and implemented. This allows a user to maintain all water and nutrient loadings in a single auditable Microsoft Excel® template (Figure 7) that can then communicate directly with the AQUATOX interface. Using Excel spreadsheets a user can both set up a new linked-mode simulation and also modify such a simulation for scenario analysis. For more information about this capability, please see the section on "Excel Template Import Capability" within the *AQUATOX Help and Users Manual.*

	A	B	C	D	E	F	G
1	**Addition Type**	NewSeg	NewSeg	Inflow	<--------	NewLink	<--------
2	**Addition Name (ND Flag?)**	Seg 1	Seg 2	FALSE		S1 to S2	
3	**Seg/Link ID (seg ID from)**	S1	S2	S1		S1	
4	**Length km** *(seg ID to) (comment1)*	4.50	13.03	*Upstream Boundary*		S2	
5	**Vol IC m^3** *(link type) (comment2)*	113,231	243,304	*Boundary Condition*		Cascade	
6	**SARA m^2 (time series header)**	289,620	456,152	Date:	Flow (m3/d)	Date:	Flow (m3/d)
7	**Mean Depth m (time series)**	2.558	1.875	1/1/1998	604,304	1/1/1998	605,408
8	**Max Depth m**	3.837	2.812	1/2/1998	594,518	1/2/1998	594,241
9	**Slope m/m <or blank>**	0.0023	0.0024	1/3/1998	596,964	1/3/1998	597,518
10	**Manning's N <or blank>**	0.043	0.043	1/4/1998	592,071	1/4/1998	591,794
11				1/5/1998	594,518	1/5/1998	593,965
12	**(set inflow, disch to zero)**			1/6/1998	599,411	1/6/1998	598,860
13	**(calc dynamic)**			1/7/1998	604,304	1/7/1998	605,131
14				1/8/1998	596,964	1/8/1998	596,413
15							

Figure 7. Example spreadsheet used for flow data import

Stratification Considerations

Unlike single-segment mode, in linked-mode AQUATOX handles stratification by modeling each vertically-stratified layer as a unique model segment. When segments are vertically stratified, they must be linked together with a bi-directional "feedback" linkage. A stratification screen within each segment's main interface allows a user to specify whether a segment is part of a vertically stratified pair and, if so, whether it is the epilimnion or the hypolimnion segment. For more information see "Stratification in a Linked System" within the AQUATOX *Users' Manual.*

Also unlike the single-segment model, water flows must be specified between the two segments. Overturn may be specified by a high degree of mixing between the two segments whereas periods of stratification will have considerably lower flow. One possible source of inputs for vertical water flows would be a 3D hydrodynamic model, though vertical stratification must be well calibrated within that model and that model's output would likely need to be spatially and temporally aggregated before being input to AQUATOX.

The specification of vertical water flows may be estimated as a function of temperature or oxygen data. Methods used to derive these flows are documented in the reservoir case-studies presented below.

Case Study: Modeling a River, Lower Boise River ID

Overview

The Lower Boise River in Idaho is an example in which AQUATOX was used to model a long river span of over 60 river miles (Figure 8). This site has considerable spatial variability with respect to water quality and river flows and was characterized using 13 main-stem segments. Some characteristics of the project included

- 26 "tributary inputs"
- Groundwater inputs
- Wastewater treatment facilities
- Input drains and tributaries
- Extensive agricultural water withdrawals

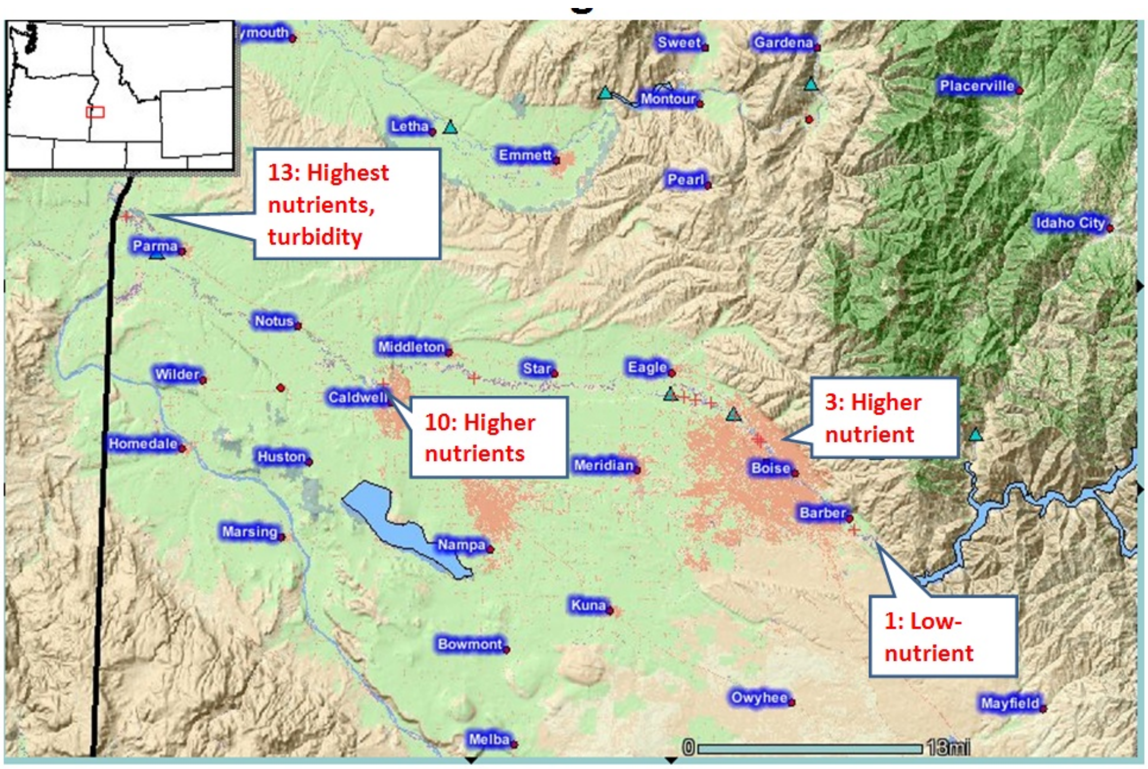

Figure 8: Overview of segments in Lower Boise River AQUATOX implementation

Water-flow Model

To model the Lower Boise River (LBR), a complex water-flow accounting was created for this site with the assistance of the City of Boise. Given all of the tributary inputs and withdrawals of water, nutrients and organic matter were then integrated within the main-stem of the model.

The basic steps taken to implement the LBR model were to:

1. Create a continuous accounting of water inputs and withdrawals from all of the wastewater treatment plants and agricultural drains[2].
2. Gather main-stem flow data from all relevant USGS gages.
3. Estimate groundwater flow contributions to each segment given available estimates from City of Boise[3].
4. Estimate flow rates for each segment using the simple equation presented here, all units being in cubic meters per day *(tributary inputs include groundwater contributions, agricultural drains, and wastewater treatment plants):*

$$Outputs_{Seg\ N} = Outputs_{Seg\ N-1} + \sum Trib.Inputs - \sum Withdrawals$$

5. When gage data downstream were available these were used preferentially and were also used to check the assumptions of the equation shown above.
6. The average daily flow for each river segment was then calculated, as the average of water flows coming into the reach and water flows leaving the reach each day.

Water-volume Model

To estimate the water volume of each segment, the flows were used along with the river length and Manning's equation. This was done within a spreadsheet, combining equations **(4)** and **(5)** from the AQUATOX *Technical Documentation*:

$$Volume = \left(\frac{Q \times Manning}{\sqrt{Slope} \times Width}\right)^{3/5} \times CLength \times Width$$

where:

Volume	=	volume of segment (m^3);
Q	=	(average daily) flow rate (m^3/s) as derived from water-flow model;
Manning	=	Manning's roughness coefficient ($s/m^{1/3}$);
Slope	=	slope of channel (m/m);
Width	=	channel width (m); and
CLength	=	length of reach (m);

[2] These data were primarily based on USGS water chemistry data and monitoring reports from National Pollutant Discharge Elimination System (NPDES) permittees.

[3] Groundwater flows derived from R.D. Schmidt's 2006 document, *A Distributed Parameter Water Budget Data Base for the Boise Valley*.

This equation provided a daily estimate of segment volume for each segment in the simulation.

Water-balance Model

To complete the process a “closed system” water-balance spreadsheet model was produced that accounts for changes in volume as well as changes in inflows and outflows for each segment. The inflow of each river segment was defined by its boundary condition loadings as well as any modeled water inputs from the upstream reach. Then the outflow of each river segment was calculated as follows:

$$Outflow = Inflow + Inputs - Withdrawals - \Delta Volume$$

where:

Outflow	=	flow rate over downstream boundary (m^3/d);
Inflow	=	inflow from upstream boundary (m^3/d);
Inputs, Withdrawals	=	boundary conditions used in the water flow model (m^3/d);
ΔVolume	=	increase in volume from previous day derived from water volume model (m^3/d), can be negative.

In the main stem of the Lower Boise River, evaporation was assumed to be negligible and was set to zero.

There were some complications to this approach, however, since in some cases, due to the influence of the calculated volume for each segment, negative flows were derived, indicating a water flow from a downstream to an upstream segment. Water flowing up the main stem did not match our conceptual model for the site (i.e. did not seem realistic) and also adds complexity to the modeling. Negative flows require bi-directional “feedback” which can cause model runtimes to increase. This problem primarily occurred in the smaller upper reaches during low-flow conditions, probably due to uncertainty in the water volume estimation based on Manning’s equation.

To avoid this occurrence, any negative flows were added to the boundary condition inflow at the top of the main stem. This process ensured that water flows could remain unidirectional and that the water-volume model would be maintained throughout the study area.

Model Verification

The results of the “water balance” model provided us with a second estimate of water flows, compared with the “water flow” analysis above. In the “water flow” analysis water flows were estimated based on inflows and outflows for each segment or gage data where available. In the water “balance” analysis, the water volume for each segment was calculated using Manning’s equation and outflows were calculated as a function of changes in water volume combined with inflows. Because the latter analysis balances the mass of water in the entire system and also takes into account segment volumes, flows from one segment to another could differ somewhat from the water “flow” analysis.

To assess the importance of this difference, the average percent “error” was calculated for each segment, comparing the “closed-system” flows with the flows derived using USGS data and the estimated flow discussed above. In general, average errors were below 10% and highest at the boundary of segments 11 and 12 (Figure 9). This percent error was deemed acceptable given the modeling objectives at this site.

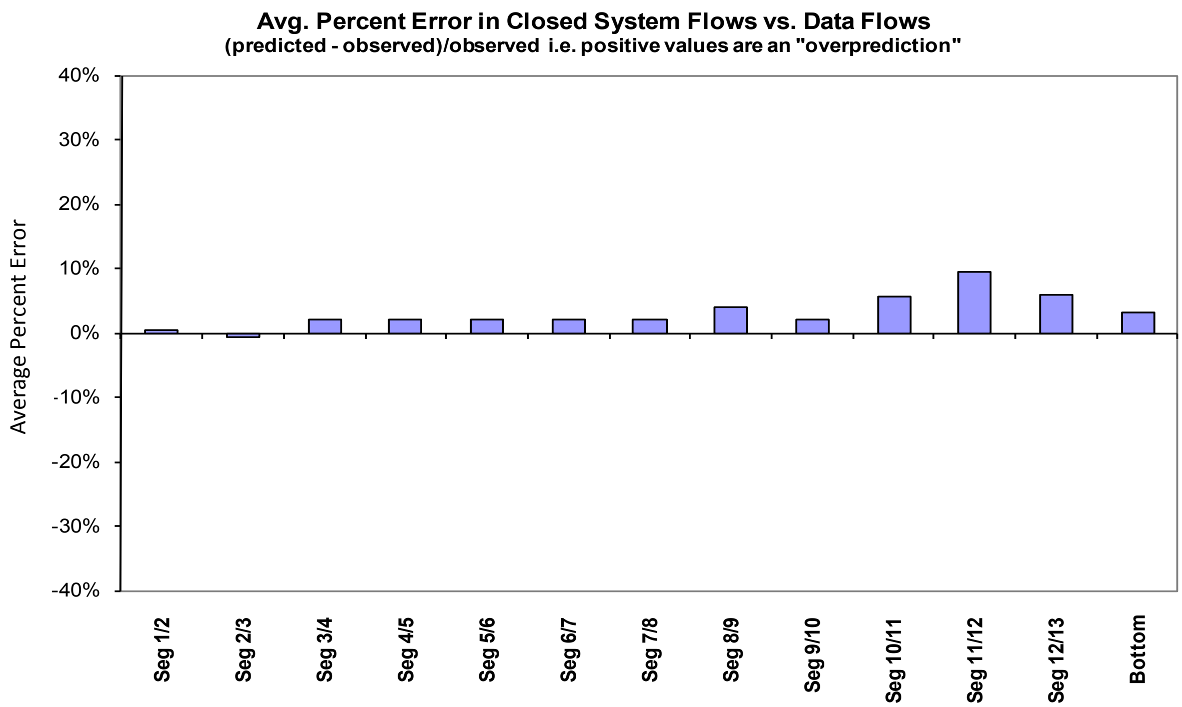

Figure 9: Percent Error Calculation for Alternative Flow Derivations

Finally, a continuous accounting of nutrient, algae, and organic-matter data for all tributary, groundwater, and wastewater sources was associated with each water input when importing these into the model (including point sources). The final main-stem results were compared to water column observed data with generally favorable results (Figure 9).

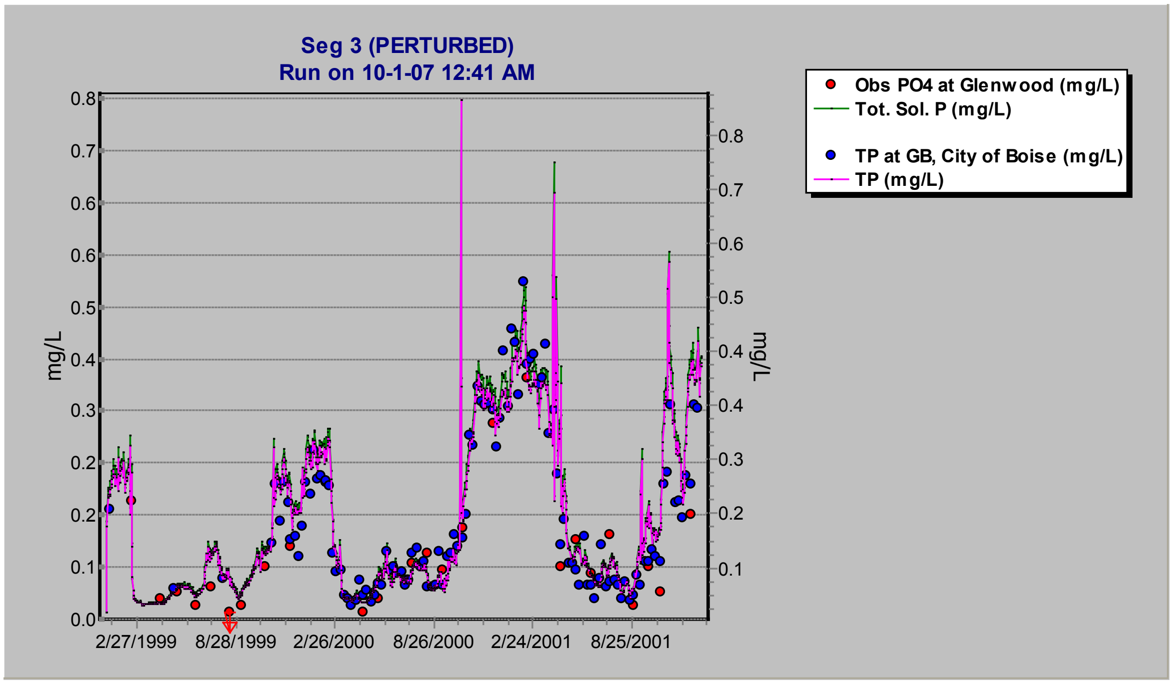

Figure 10. Simulated and observed total phosphorus at Veteran's

Case Study: Modeling a Reservoir with Linked Hydrodynamics, Tenkiller Lake, OK

Overview

In 2008-2009, Tenkiller Ferry Lake in Oklahoma was selected as the location for a nutrient criteria modeling case study. The AQUATOX model domain comprised approximately 43 million square meters, modeled with five horizontal segments (Figure 11). All segments other than the riverine segment were assumed to undergo vertical stratification. Therefore, a total of nine segments were utilized within AQUATOX:

- Riverine
- Transitional Epilimnion
- Transitional Hypolimnion
- Lacustrine A to Lacustrine B to Lacustrine C Epilimnion (3 segments)
- Lacustrine A to Lacustrine B to Lacustrine C Hypolimnion (3 segments)

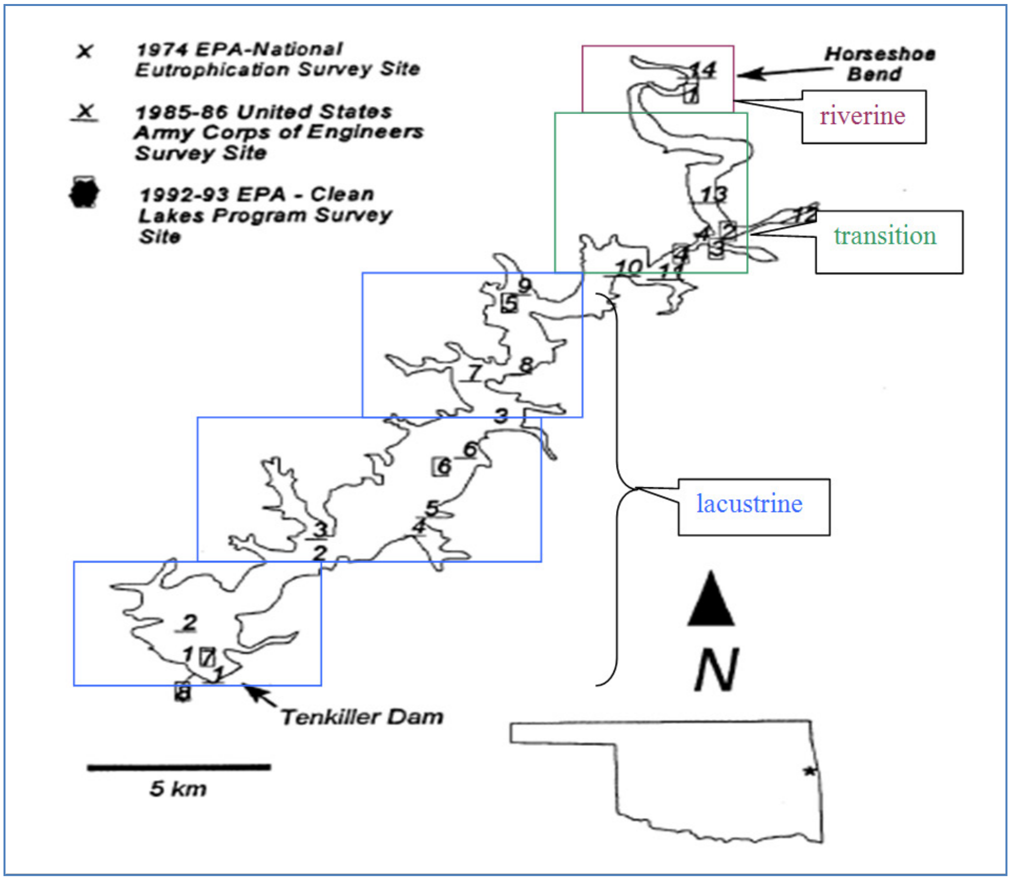

Figure 11: Longitudinal segments and sampling stations on Tenkiller Ferry Lake, Oklahoma. Base map from (Oklahoma State University 1996)

Boundary-condition water flows for this study area were available from a linked HSPF and EFDC model simulation calibrated for the years 1992-1993 (Figure 12). The original intention was to model horizontal and vertical water flows between AQUATOX segments using EFDC results. This proved to be possible with horizontal flows, but not vertical flows, as detailed below.

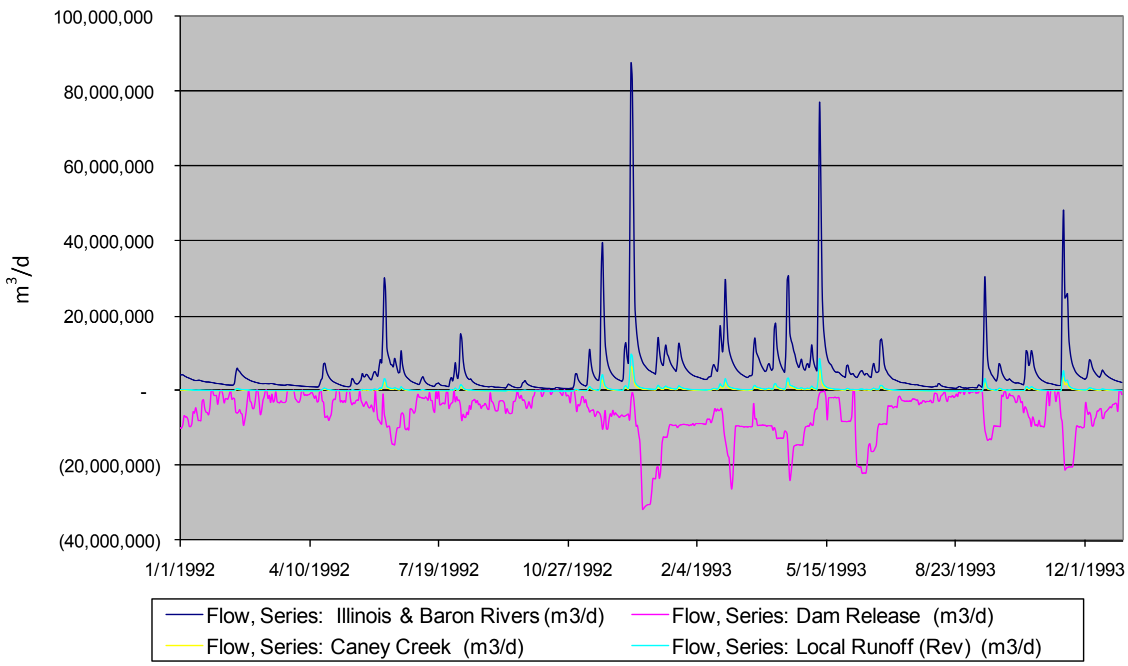

Figure 12: Boundary condition water flows from EFDC and HSPF

Data from Model Linkage

The EFDC modeling team provided a water balance for the entire site that did not precisely match the river flow input data from HSPF. To solve this problem, the flows for the Illinois and Baron rivers were calculated using the EFDC total boundary condition inputs and subtracting the water inputs from Caney Creek. In this manner, a model was produced in which the boundary-condition inputs plus the change in system volume are equal to boundary-condition outputs for each day of the simulation[4]. Similarly, EFDC-derived outflows over the Tenkiller Dam were used preferentially to alternative data sources.

EFDC model runs were also used to derive horizontal water flows from Riverine to Transitional, from Transitional to Lacustrine A, and throughout the three lacustrine segments.

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[4] Initial modeling by the EFDC team used “cell-center” velocities to estimate water flows over AQUATOX boundaries. This resulted in a model that would not balance the mass of water in a reasonable manner. “Cell edge” velocities were then utilized, which resulted in a much better fit. This illustrates the importance of precision and difficulty of setting up linkages between models.

Water-balance Model

The volume of the river segment was estimated using EFDC inflows and Manning's equation as shown on page 12 of this document. Outflow from the river segment could then be calculated as a function of boundary condition river inflow minus any gain in river volume.

Initial condition water volumes for non-riverine segments were derived using information from EFDC regarding the total volume of the site and then distributing this using the surface area and mean depth of each segment. Multiplying the estimated surface area by the mean depth provides mean-volume estimates for each segment. For each segment, percentages of the whole-site mean volume can be derived. Multiplying these percentages by the initial condition water volume for the entire study area provides an estimate of initial-condition water volume for each segment.

Using the derived data discussed above, a spreadsheet was used to solve the water volume for each segment on each day as follows:

$$Vol_{Seg} = Vol_{Seg\ T-1} + Inflows_{Upper\ Segment} + Runoff_{EFDC} - Outflow_{\ EFDC}$$

where:

Vol	=	Segment volume in cubic meters;
Inflows	=	inflow from upstream segment or boundary condition (m^3/d);
$Runoff_{EFDC}$	=	runoff water from EFDC water balance (m^3/d);
$Outflow_{EFDC}$	=	horizontal movement of water from EFDC (m^3/d).

The resulting predicted water volumes by horizontal segment (m^3) are shown in Figure 13.

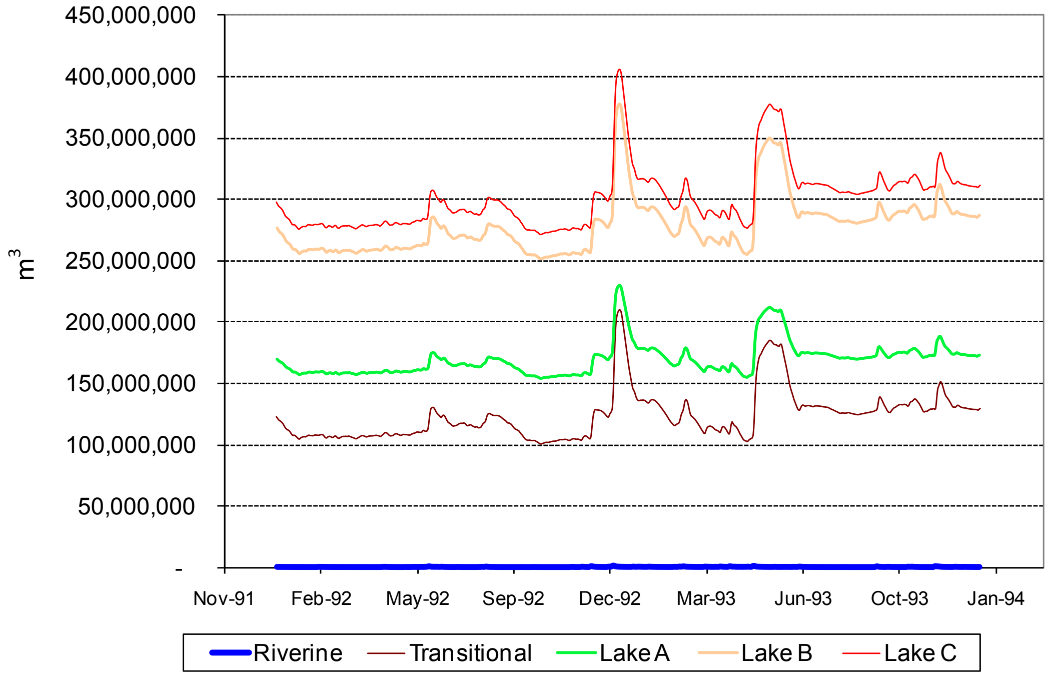

Figure 13: Predicted Tenkiller water volumes in each horizontal AQUATOX segment

Vertical Mixing

The original intention was to use vertical flows as specified from the EFDC linkage to specify site stratification and overturn. However, vertical flow fields between segments based on EFDC predicted an unrealistically high mixing rate of at least 20% per day and were essentially linear over time for each segment. This did not match site data that showed significant temperature and oxygen stratification by depth and strong seasonal differences in stratification regime[5].

Because of this, vertical mixing was computed offline from observed temperature data and, for the Transition segment, from dissolved oxygen data. An example is provided here from the Lacustrine C segment.

1. Based on mean temperatures and temperature ranges for the epilimnion and hypolimnion segments, a temperature time-series was synthesized for both segments using equation **(24)** from the AQUATOX *Technical Documentation* (Figure 14).

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[5] This mis-match could have been a function of how EFDC defined thermocline depth. Due to variable water depth in each cell a certain degree of "churning" between segments might have been predicted simply due to water volume changes in the overall system. Whatever the cause, this problem again highlights the potential complexities in linking fine-resolution spatial models with models of a coarser spatial resolution.

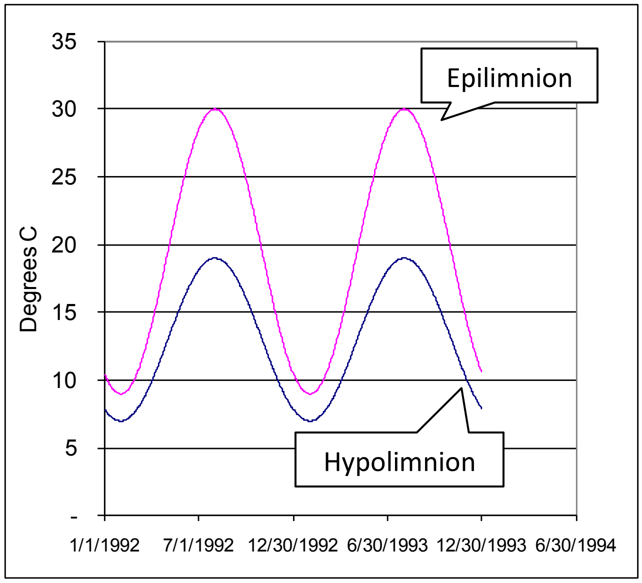


Figure 14: Estimated Temperatures differences between Vertical Segments for Lacustrine C

2. Within the spreadsheet, vertical dispersion is calculated in square meters per day, using equation **(18)** from the AQUATOX *Technical Documentation:*

$$VertDispersion = Thick \cdot \left(\frac{HypVolume}{ThermoclArea \cdot Deltat} \cdot \frac{T_{hypo}^{t-1} - T_{hypo}^{t+1}}{T_{epi}^{t} - T_{hypo}^{t}} \right)$$

where:

VertDispersion	=	vertical dispersion coefficient (m^2/d);
Thick	=	distance between the centroid of the epilimnion and the centroid of the hypolimnion, effectively the mean depth (m);
HypVolume	=	volume of the hypolimnion (m^3);
ThermoclArea	=	area of the thermocline (m^2);
Deltat	=	time step (d);
T_{hypo}^{t-1}, T_{hypo}^{t+1}	=	temperature of hypolimnion one time step before and one time step after present time (deg. C); and
T_{epi}^{t}, T_{hypo}^{t}	=	temperature of epilimnion and hypolimnion at present time step (deg.C).

3. Percent mixing per day is then estimated as follows:

$$Percent\ Mixing = \frac{VertDisp \times ThermoclArea}{\frac{1}{2}(ZMean) \times Volume}$$

where:

VertDisp	=	vertical dispersion coefficient (m^2/d);
ThermoclArea	=	area of the thermocline (m^2);
ZMean	=	mean depth (m);
Volume	=	Segment Volume (m^3).

4. In this modeling exercise, the entire system was assumed to undergo overturn at the same time. Therefore, if the temperature difference between vertical segments in the Lacustrine C segment was less than 3 degrees centigrade, the entire system was assumed to be well-mixed. In this case, percent mixing for all segments was estimated at 25% per day.
5. Offsetting upward and downward flows were then estimated as the percent mixing each day multiplied by the volume of the entire horizontal segment on that day. These time series were then entered as flows associated with upward and downward links between vertical segments.

Within the transitional segment, available temperature data at depth were quite limited. However, oxygen data were available (Figure 15). In this case, we calculated vertical dispersion in square meters per day, using equation **(18)** from the AQUATOX *Technical Documentation,* but substituting oxygen differences for temperature differences.

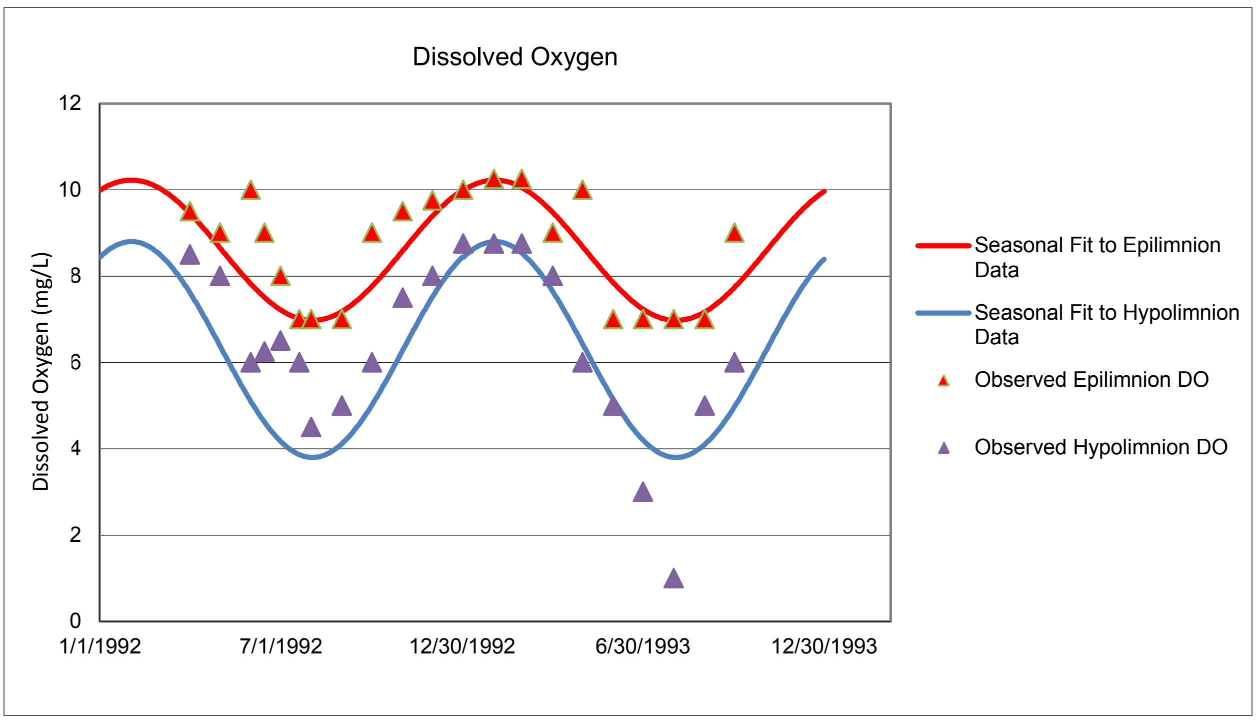


Figure 15: Oxygen differences between transitional epilimnion and hypolimnion layers

The above example shows how vertical mixing can be derived based on either oxygen or temperature data, if only one or the other is available. Vertical differences in concentrations for both oxygen and temperature can provide a strong indication of how well-mixed a segment is. However, if high-resolution temperature data are available, they are generally better to use in such an analysis as temperature is a more "conservative" variable. In other words, oxygen concentrations are subject to effects from sediment oxygen demand and microbial degradation (among other effects) and these effects have the potential to complicate the analysis.

Withdrawal and Entrainment

The final complexity addressed within this water-balance model pertains to the withdrawal of water from the reservoir. All withdrawals over the Tenkiller Lake dam were assumed to come from the upper (epilimnion) segment. For this reason, some water needed to be routed from hypolimnion to epilimnion segments to prevent epilimnion segments from becoming "water-volume zero."

Our model application assumed that entrainment from the hypolimnion was spread equally between the three lacustrine segments. To manage this within the spreadsheet the quantity of outflow that would have come from the hypolimnion if the water withdrawals were weighted by volume was calculated.

$$Entrainment\ Required = Dam\ Withdrawal\left(\frac{Volume_{Hypolimnion}}{Volume_{Epilimnion+Hypolimnion}}\right)$$

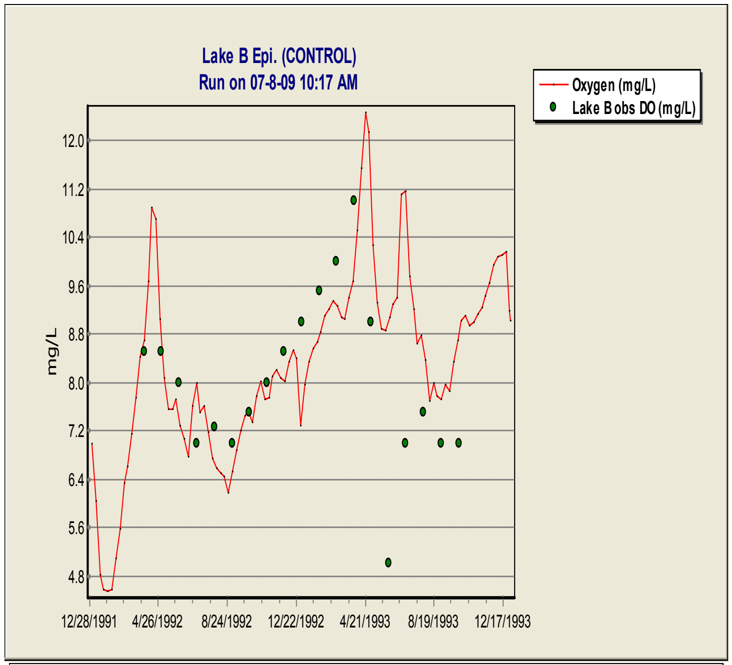
This quantity was then divided by three and added to the upward flux of water from the hypolimnion to the epilimnion for each of the three lacustrine segments.

This procedure also required some specification of additional horizontal flows in the upper layer after water had been entrained. The horizontal flows from Lacustrine A to Lacustrine B and from Lacustrine B to Lacustrine C within the epilimnion were also increased to allow the entrained water to exit the system at the top of the Lacustrine C segment. Horizontal flows within the hypolimnion segments were reduced by this entrainment quantity because the water that would be flowing through the hypolimnion had been entrained in the epilimnion layer.

Model Verification

There are no specific flow or water-volume data available to verify this particular water balance model, however, using this set of horizontal and vertical flows, AQUATOX does a nice job of estimating oxygen concentrations including seasonality and vertical differences. For example,

Figure 16 shows good correspondence between predicted and observed oxygen concentrations in segment Lacustrine B.



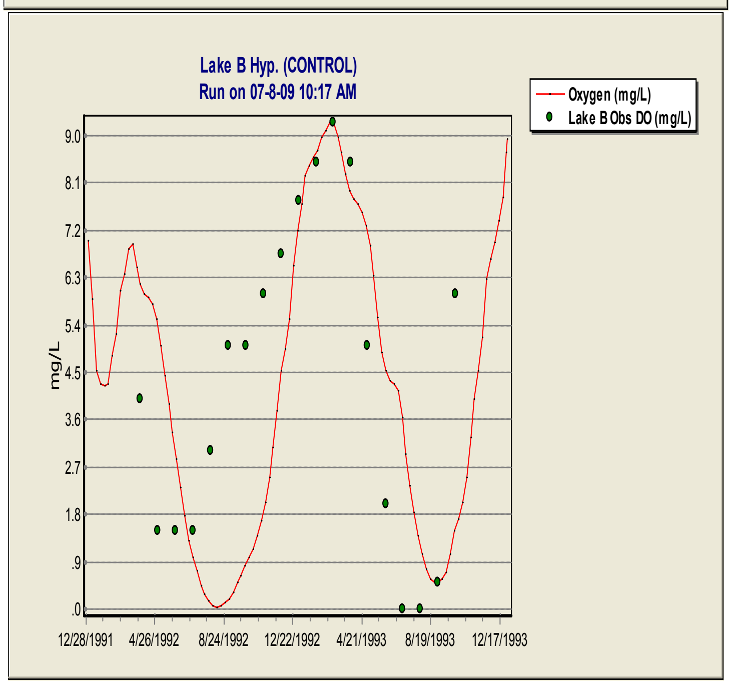


Figure 16: Comparison of Oxygen Simulations in Lacustrine B Hypolimnion vs. Epilimnion

Case Study: Modeling a Reservoir without Linked Hydrodynamics, DeGray Lake, AR

In 2010 and 2011, the AQUATOX model was used in a proof-of-concept analysis of the environmental relationships of a representative reservoir, DeGray Lake, Arkansas. Calibration and verification over an eight-year period were based on hypolimnetic dissolved oxygen, nutrients, overall phytoplankton biomass, chlorophyll a, and biomass of algal groups and fish species.

The model spatial domain was represented by three horizontal segments (Figure 17) and six segments overall due to vertical stratification (Figure 18).

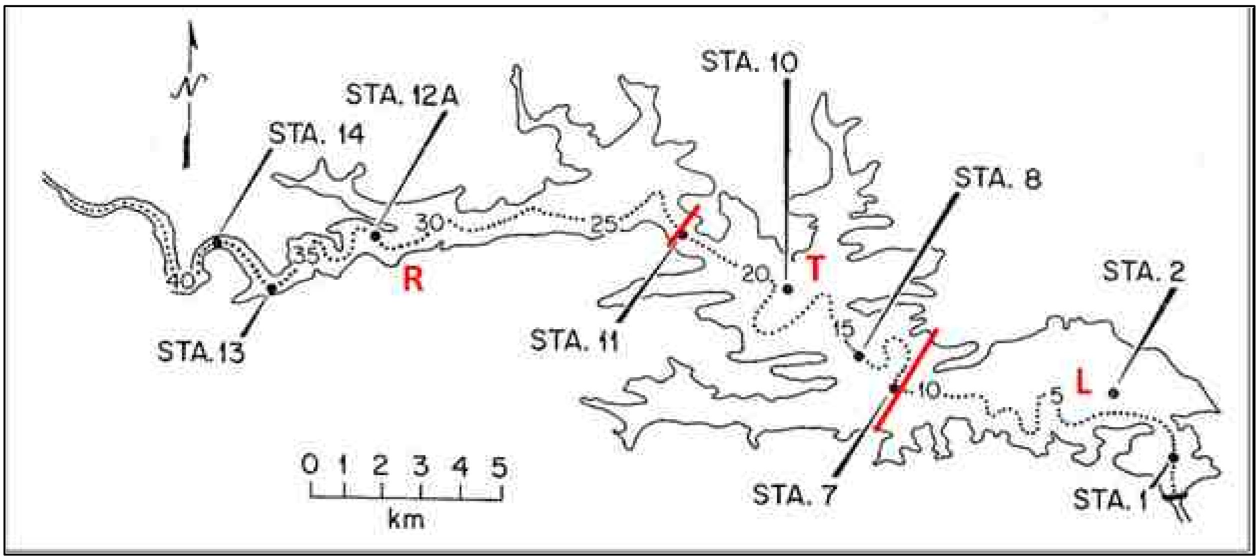


Figure 17. Riverine, transition, and lacustrine zones modeled for DeGray Lake (R, T, and L), respectively (Groeger and Kimmel 1987)

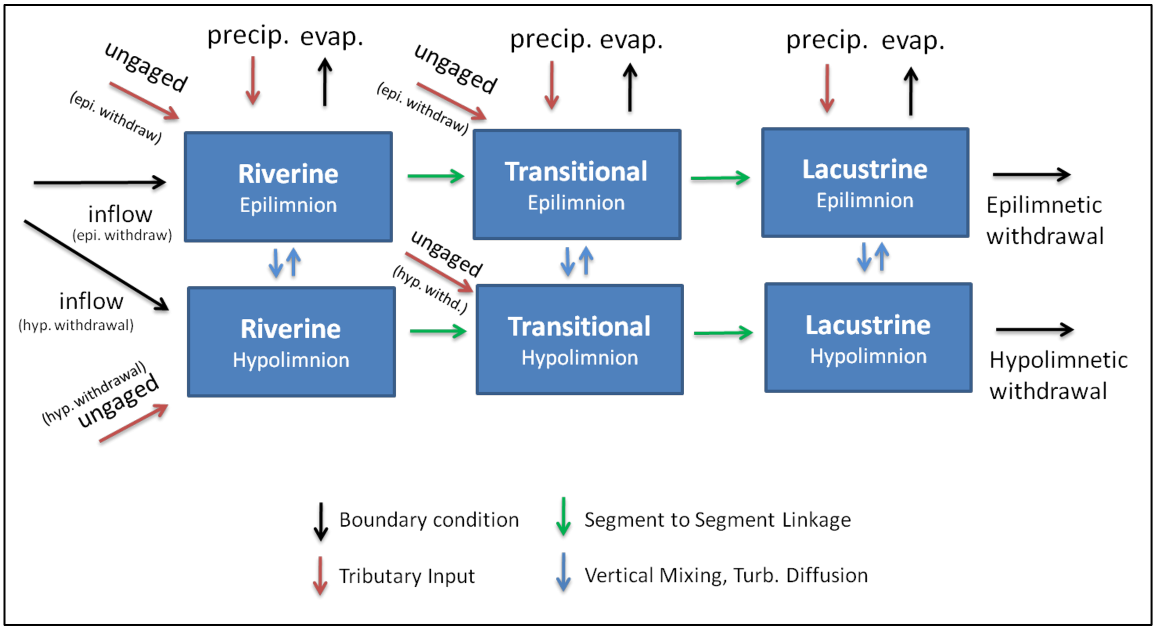


Figure 18: DeGray Reservoir Water Flows within AQUATOX

Water Balance Model

While a hydrodynamic model of water flows was not available for DeGray lake, a very useful resource was available for the calibration period: a table that estimates the water balance for the entire calibration period of 1974-1980 (Table 1), including adjustments for ungaged flow into the lake (Table 2) (Ford and Stein 1984).

Table 1. Water balance for DeGray Lake in 1974, 10^6 m^3 (Ford and Stein 1984)

Month	Direct Precipi-tation	Highway 84 Inflow	Ungaged Inflow	Outflow	Evaporation	Error	Volume Change
Jan	7.32	55.69	26.18	106.29	1.78	18.15	-0.73
Feb	2.90	18.32	8.61	54.70	2.23	11.42	-15.68
Mar	4.13	29.98	14.09	50.28	3.03	8.53	3.43
Apr	7.72	92.68	43.56	7.35	4.88	-7.93	123.80
May	9.15	36.65	17.23	145.23	5.32	12.41	-75.11
Jun	16.71	187.11	87.94	260.82	6.32	-27.78	-3.16
Jul	3.27	4.95	2.33	31.78	6.73	-3.84	-31.81
Aug	11.45	8.38	3.94	14.34	5.53	-1.21	2.69
Sep	9.09	31.04	14.59	59.27	3.33	2.74	-5.13
Oct	5.81	19.15	9.00	70.70	2.73	-0.64	-40.10
Nov	11.19	128.74	60.51	150.58	1.98	-20.25	27.65
Dec	5.79	47.60	22.37	152.62	1.52	6.21	-72.17
Year	94.53	660.29	310.35	1103.96	45.38	-2.19	-86.36

Table 2. Factors for adjusting the ungaged inflow into DeGray Lake to eliminate water imbalances (Ford and Stein 1984)

Year	F
1974	0.47
1975	0.42
1976	0.16
1977	0.21
1978	0.39
1979	0.53
1980	0.68

* Corrected ungaged inflow = factor F × Highway 84 inflow.

As in other studies, an Excel spreadsheet was developed to account for water flows. An example of this spreadsheet is shown in Figure 19. The first step required was to build a boundary condition model for the reservoir in which “what goes in” minus “what is retained in the reservoir” precisely matches “what comes out.” The water balance tables from Ford and Stein nearly solve this problem but there is an “error” column in which their estimates do not balance the volume of water precisely.

Month	Direct Precipi-tation	Highway 84 Inflow	Ungaged Inflow	Outflow	Evap.	Error	Volume Change	Checksum	Difference
Jan	7.32	55.69	26.18	106.29	1.78	18.15	-0.73	-0.73	0.00
Feb	2.9	18.32	8.61	54.7	2.23	11.42	-15.68	-15.68	0.00
Mar	4.13	29.98	14.09	50.28	3.03	8.53	3.43	3.42	0.01
Apr	7.72	92.68	43.56	7.35	4.88	-7.93	123.8	123.8	0.00
May	9.15	36.65	17.23	145.23	5.32	12.41	-75.11	-75.11	0.00
Jun	16.71	187.11	87.94	260.82	6.32	-27.78	-3.16	-3.16	0.00
Jul	3.27	4.95	2.33	31.78	6.73	-3.84	-31.81	-31.8	-0.01
Aug	11.45	8.38	3.94	14.34	5.53	-1.21	2.69	2.69	0.00
Sep	9.09	31.04	14.59	59.27	3.33	2.74	-5.13	-5.14	0.01
Oct	5.81	19.15	9	70.7	2.73	-0.64	-40.1	-40.11	0.01
Nov	11.19	128.74	60.51	150.58	1.98	-20.25	27.65	27.63	0.02
Dec	5.79	47.6	22.37	152.62	1.52	6.21	-72.17	-72.17	0.00
Year	94.53	660.29	310.35	1103.96	45.38	-2.19	-86.36	-86.36	0.00
Checksum	*94.53*	*660.29*	*310.35*	*1103.96*	*45.38*	*-2.19*	*-86.32*	*-86.36*	0.04

Figure 19. Excerpt from DeGray Lake Water Flows Spreadsheet

To account for these error terms, adjustments were made to the most uncertain columns within the table, starting with “ungaged inflow.” If too much error exists, the corrected ungaged inflows could become negative, so the next choice for an adjustment was using “direct precipitation.” Finally, outflow was determined to be the third most uncertain term for any remaining error in the water balance. By adjusting these three factors, a water-volume mass balance could be produced.

An additional complication to the water-volume mass balance was the difference between daily water flows and monthly water-balance estimates. Any discrepancy between daily outflow totals and monthly water-balance outflow estimates was corrected by modifying the monthly water-balance outflows and also the monthly water-balance error term. This procedure assumed that the sum of daily values is a more accurate total than the estimated monthly totals.

Inter-segment Flows

Initial-condition volumes for the three zones were taken from Nix and coworkers (1975). Areas were estimated from the Esri® shape file for the reservoir using ArcView®. Volumes and areas were apportioned among the three zones (Table 3) using the relationships of Junge (1966) described in the AQUATOX *Technical Documentation*, where:

$$AreaFrac = (1 - P)\cdot\frac{Z}{ZMax} + P\cdot\left(\frac{Z}{ZMax}\right)^2$$

$$VolFrac = \frac{6.0\cdot\frac{Z}{ZMax} - 3.0\cdot(1.0 - P)\cdot\left(\frac{Z}{ZMax}\right)^2 - 2.0\cdot P\cdot\left(\frac{Z}{ZMax}\right)^3}{3.0 + P}$$

where:

AreaFrac	=	fraction of area of site above given depth (unitless);
VolFrac	=	fraction of volume of site above given depth (unitless);
ZMax	=	maximum depth (m);
Z	=	depth of interest (m); and
P	=	characterizing parameter for shape (unitless); P is between -1.0 and 1.0.

Table 3. Estimated volume (m^3), and area (m^2) for each of the segments

Segment	Tot Vol	ZMean	ZMax	P	VolFrac	Vol(Epi)	Vol(Hyp)	AreaFrac	Area(Epi)	Area(Hyp)
Riverine	9.40E+07	5	15	-1	0.704	6.61E+07	2.79E+07	0.56	1.08E+07	6.00E+06
Transition	3.01E+08	5	25	-1	0.488	1.47E+08	1.54E+08	0.36	2.13E+07	7.68E+06
Lacustrine	3.78E+08	5	47	-1	0.286	1.08E+08	2.70E+08	0.20	1.45E+07	2.93E+06

After this procedure, precipitation and evaporation could be distributed as a function of surface area. In addition, the fraction of total water volume that each segment represented could be calculated and was estimated as follows:

- Riverine volume fraction: 12% of the total
- Transition volume fraction: 39% of the total
- Lacustrine volume fraction: 49% of the total

The fractions of total volume for each segment were assumed to remain constant throughout the model simulation.

Having an accounting of the water volume for each day of the simulation from the water balance calculations, and an accounting of the volume fraction for each segment, the volume for each segment for each day could be calculated.

The next step was to account for all flows into each segment which, along with the change in volume for each day, could be used to calculate outflows from each segment. Inflows to each segment included boundary condition loadings, ungaged water loadings, and precipitation. Losses included evaporation and boundary condition withdrawals (Figure 18).

As was the case in other model applications, occasional adjustments needed to be made for negative flows. For example, during a low-flow period of 1974 dam withdrawals were calculated to be small negative values (when accounting for inflows minus losses). During these periods, dam withdrawals were simply set to zero; the water volume of the entire system was then slightly lower than would be suggested by the water volume balance derived above, but the differences were negligible.

Stratification Considerations

Vertical stratification added some additional complexity to the modeling of DeGray Lake. The model was assumed to go through periods of stratification and overturn as a function of calendar date. For all three zones stratification was assumed to occur on March 7 of each year, and overturn on December 1, based on data from James and Kennedy (1987). Within this paper, there was a suggestion that stratification progresses downstream through each reservoir with time (i.e. stratification occurs up-reservoir first), but given the available data, the simpler case was used.

Vertical mixing was set to 50% per day during well-mixed periods. Otherwise, vertical mixing was calculated as a function of through-flow as shown in Equations (19) and (20) of the AQUATOX *Technical Documentation*:

$$VertDispersion = 1.37 \times 10^{4} \times Retention^{-2.269}$$

and

$$Retention = \frac{Volume}{TotDischarge}$$

where:

VertDispersion	=	vertical dispersion coefficient (m^2/d);
Retention	=	retention time (d);
Volume	=	segment volume (m^3).
TotDischarge	=	discharge from segment (m^3/d).

Several additional assumptions were utilized when specifying vertical water flows:

- Hypolimnetic withdrawal was assumed to start on March 15, 1979, prior to that there was epilimnetic withdrawal (Wlosinski and Collins 1985a, Dewey and Moen 1987)
- Inflow was assumed to be directed to the hypolimnion during stratification and to the epilimnion during well-mixed periods. (Actually, inflow was to the metalimnion, but that layer was combined with the hypolimnion. As a simplification within AQUATOX, the metalimnion is never explicitly modeled.)
- Ungaged inflow was assumed to be routed directly to the epilimnion and was equally distributed between riverine and transition segments.
- Due to imbalance in precipitation, evaporation, and water loadings, the volume of epilimnetic segments could get bigger as simulations progress. These imbalances were reset to the original epilimnetic and hypolimnetic proportions during turnover or storms, whenever mixing exceeded 25%.

The final segment-by-segment water balance is presented below, in Figure 20.

As with other multi-segment applications, all water inflows, links between segments, nutrient, toxicant and organic matter concentrations could have been entered manually into the interface as specified in the section on *Water Flows in Multi-Segment Mode* above. It was more convenient, however, to utilize the "Excel Template Import Capability." This allowed us to maintain all water and nutrient loadings in a single Excel template that could then communicate directly with the AQUATOX interface both for initial model setup and for editing model assumptions. For more information about this capability, please see the section on "Excel Template Import Capability" within the *AQUATOX Help and Users Manual.*

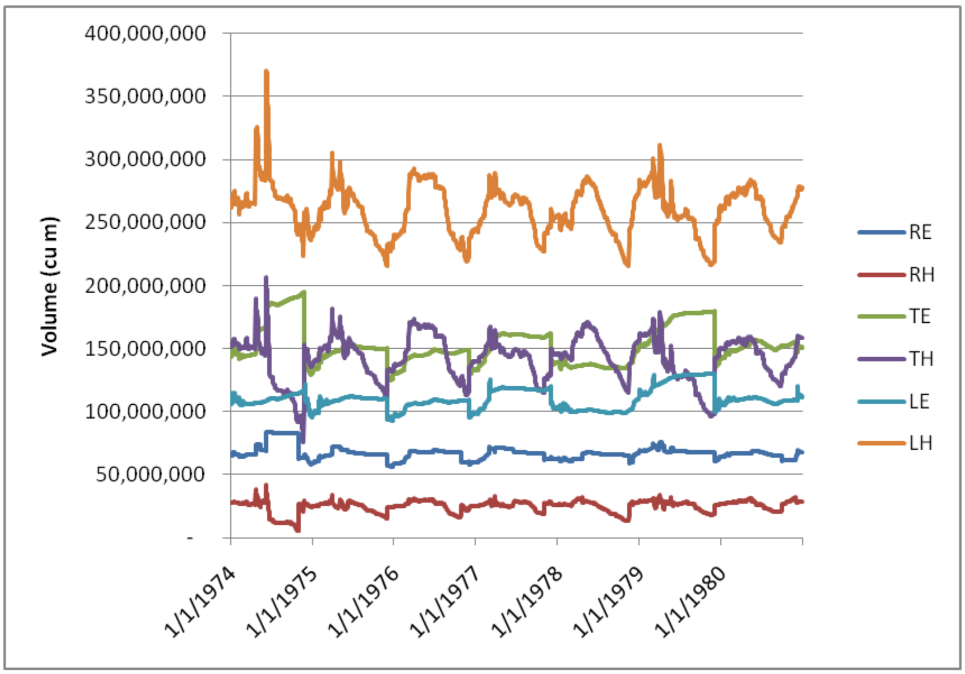
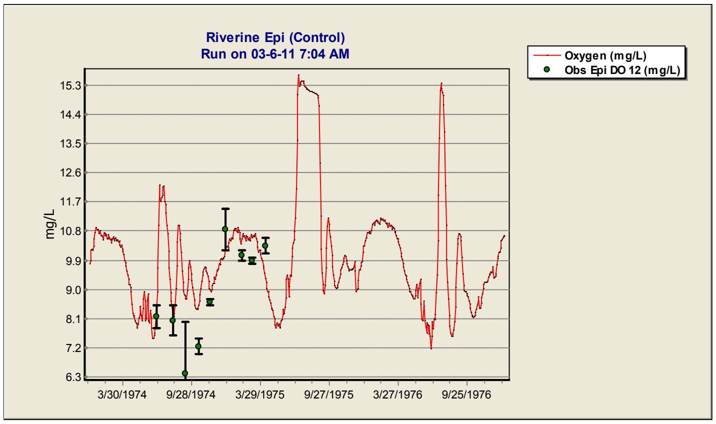


Figure 20. Calculated change in volume of segments in the spreadsheet input to AQUATOX for simulating DeGray Lake

Model Verification

As was the case with Tenkiller lake, no definitive verification of water flows exists for DeGray Lake, otherwise it would have been used in the modeling analysis. However, an examination of oxygen concentrations within stratified segments indicates that overall horizontal and vertical mixing rates were reasonable (Figure 21). Observed and predicted oxygen concentrations in the epilimnion, transitional, and lacustrine segments matched observed data closely. This outcome would not be possible if vertical mixing was too great or seasonal effects in vertical mixing were misrepresented.



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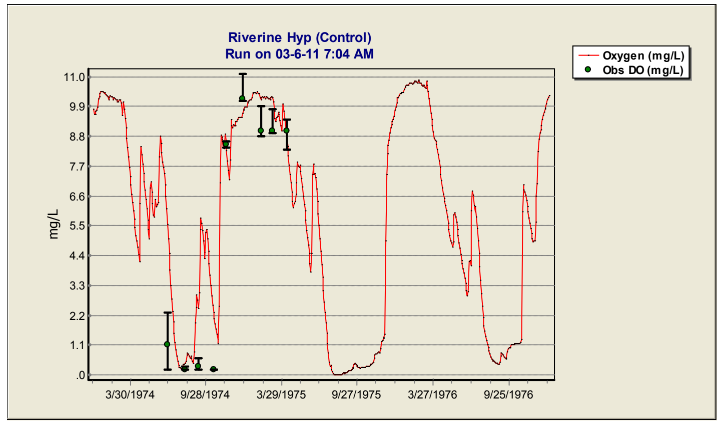

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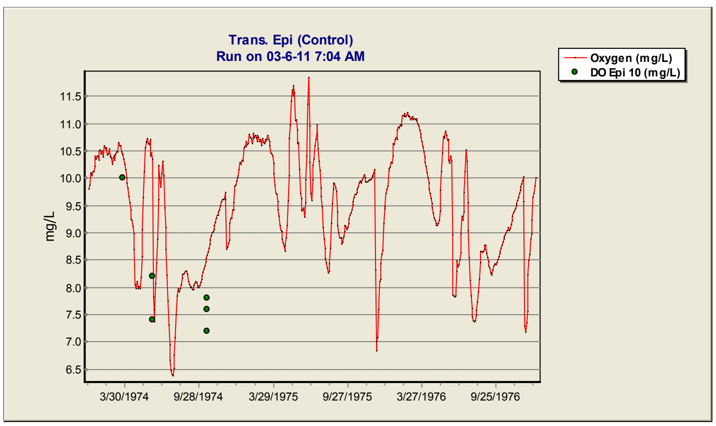

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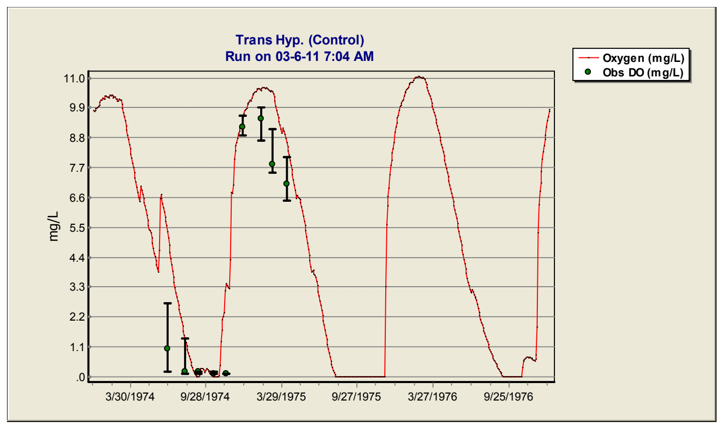

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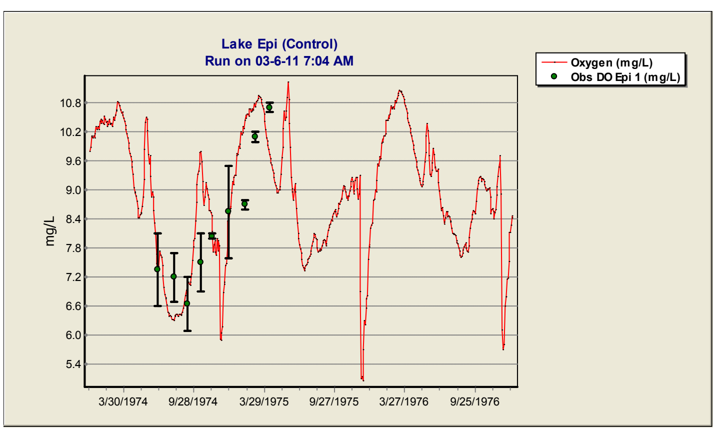

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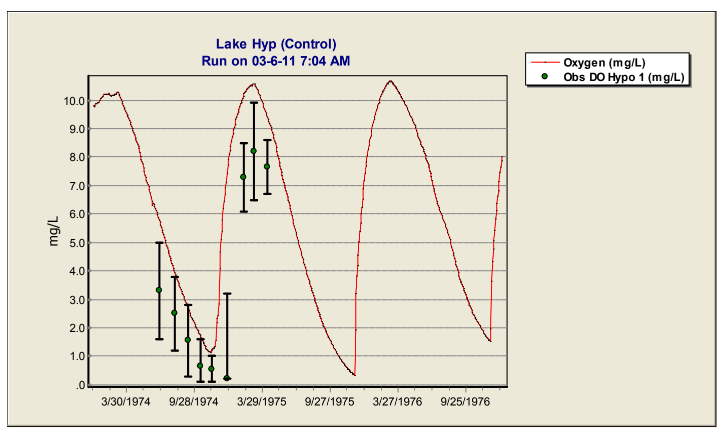

F

Figure 21. Simulated and observed dissolved oxygen in epilimnion and hypolimnion of riverine (A, B), transition (C, D), and lacustrine (E, F) segments

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