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AQUATOX (RELEASE 2)

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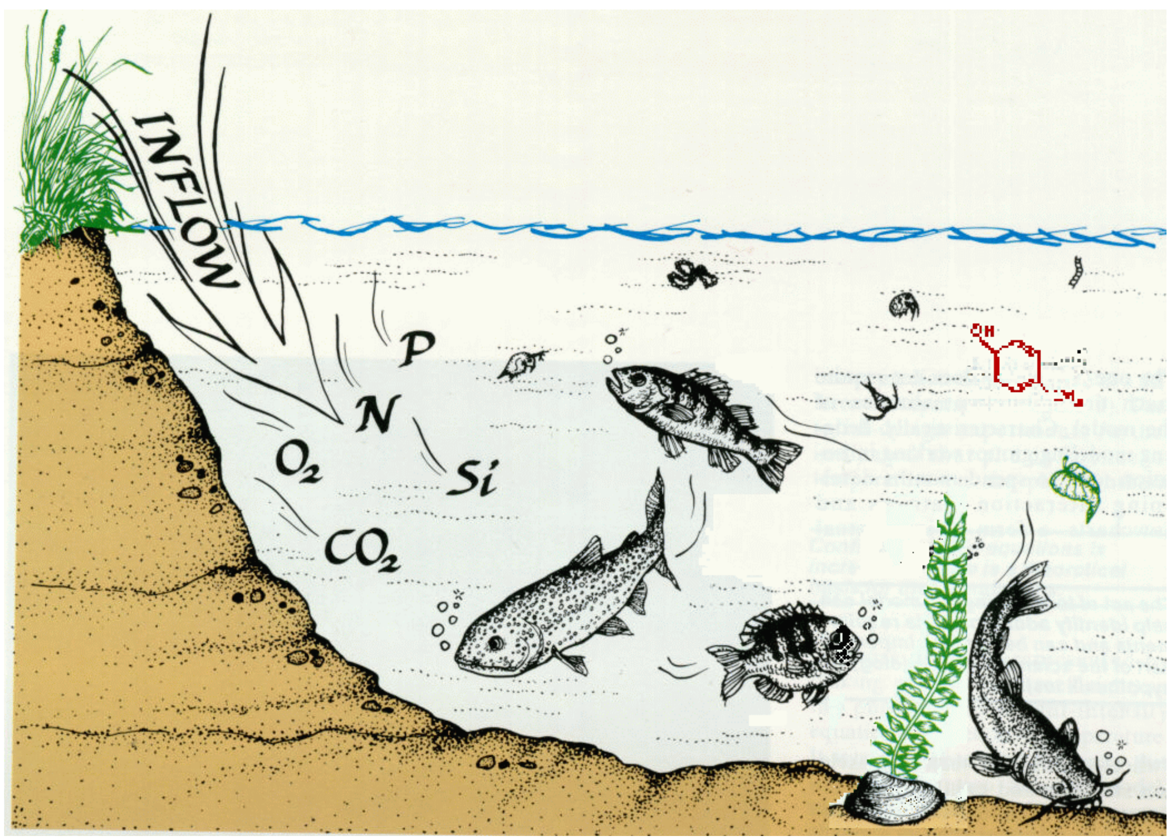
VOLUME 2: TECHNICAL DOCUMENTATION



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MODELING ENVIRONMENTAL FATE
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VOLUME 2: TECHNICAL DOCUMENTATION

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U.S. ENVIRONMENTAL PROTECTION AGENCY
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This document describes an aquatic ecosystem simulation model. It is not intended to serve as guidance or regulation, nor is the use of this model in any way required. This document cannot impose legally binding requirements on EPA, States, Tribes, or the regulated community.

ACKNOWLEDGMENTS

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The assistance, advice, and comments of the EPA work assignment manager, Marjorie Coombs Wellman of the Health Protection and Modeling Branch, Office of Science and Technology have been of great value in developing this model and preparing this report. Further technical and financial support from Donald Rodier of the Office of Pollution Prevention and Toxics and David A. Mauriello, and Rufus Morison formerly of that Office, is gratefully acknowledged. Marietta Echeverría, Office of Pesticide Program, contributed to the integrity of the model through her careful analysis and comparison with EXAMS. The model underwent independent peer review by Donald DeAngelis, Robert Pastorok, and Frieda Taub, whose diligence is greatly appreciated.

TABLE OF CONTENTS

PREFACE

The Clean Water Act— formally the Federal Water Pollution Control Act Amendments of 1972 (Public Law 92-50), and subsequent amendments in 1977, 1979, 1980, 1981, 1983, and 1987—calls for the identification, control, and prevention of pollution of the nation's waters. In the National Water Quality Inventory: 2000 Report (US EPA, 2002), 40 percent of assessed river lengths and 45 percent of assessed lake areas were impaired for one or more of their designated uses. The most commonly reported causes of impairment in rivers and streams were pathogens, siltation, habitat alterations, oxygen-depleting substances, nutrients, thermal modifications, metals (primarily mercury), and flow alterations; in lakes and reservoirs the primary causes included nutrients, metals, siltation, total dissolved solids, oxygen-depleting substances, excess algal growth and pesticides. The most commonly reported sources of impairment were agriculture, hydrologic modifications, habitat modification, urban runoff/storm sewers, forestry, nonpoint sources, municipal point sources, atmospheric deposition, resource extraction and land disposal. There were 2838 fish consumption advisories, which may include outright bans, in 48 States, the District of Columbia and American Samoa. Of these 2838 advisories, 2242 were due to mercury, with the rest due to PCBs, chlordane, dioxin, and DDT (US EPA, 2002). States are not required to report fish kills for the National Inventory; however, available information for 1992 indicated 1620 incidents in 43 States, of which 930 were attributed to pollution, particularly oxygen-depleting substances, pesticides, manure, oil and gas, chlorine, and ammonia.

New approaches and tools, including appropriate technical guidance documents, are needed to facilitate ecosystem analyses of watersheds as required by the Clean Water Act. In particular, there is a pressing need for refinement and release of an ecological risk methodology that addresses the direct, indirect, and synergistic effects of nutrients, metals, toxic organic chemicals, and non-chemical stressors on aquatic ecosystems, including streams, rivers, lakes, and estuaries.

The ecosystem model AQUATOX is one of the few general ecological risk models that represents the combined environmental fate and effects of toxic organic chemicals. The model also represents conventional pollutants, such as nutrients and sediments, and considers several trophic levels, including attached and planktonic algae, submerged aquatic vegetation, several types of invertebrates, and several types of fish. It has been implemented for streams, small rivers, ponds, lakes, and reservoirs.

AQUATOX Release 2 is described in these documents. Volume 1: User’s Manual describes the usage of the model. Because the model is menu-driven and runs under Microsoft Windows on microcomputers, it is user-friendly and little guidance is required. Volume 2: Technical Documentation provides detailed documentation of the concepts and constructs of the model so that its suitability for given applications can be determined. Volume 3: BASINS AQUATOX Extension Documentation describes how AQUATOX can be run with site characteristics and loadings input directly from the BASINS data layers or from the HSPF and SWAT watershed models.

1 INTRODUCTION

1.1 Overview

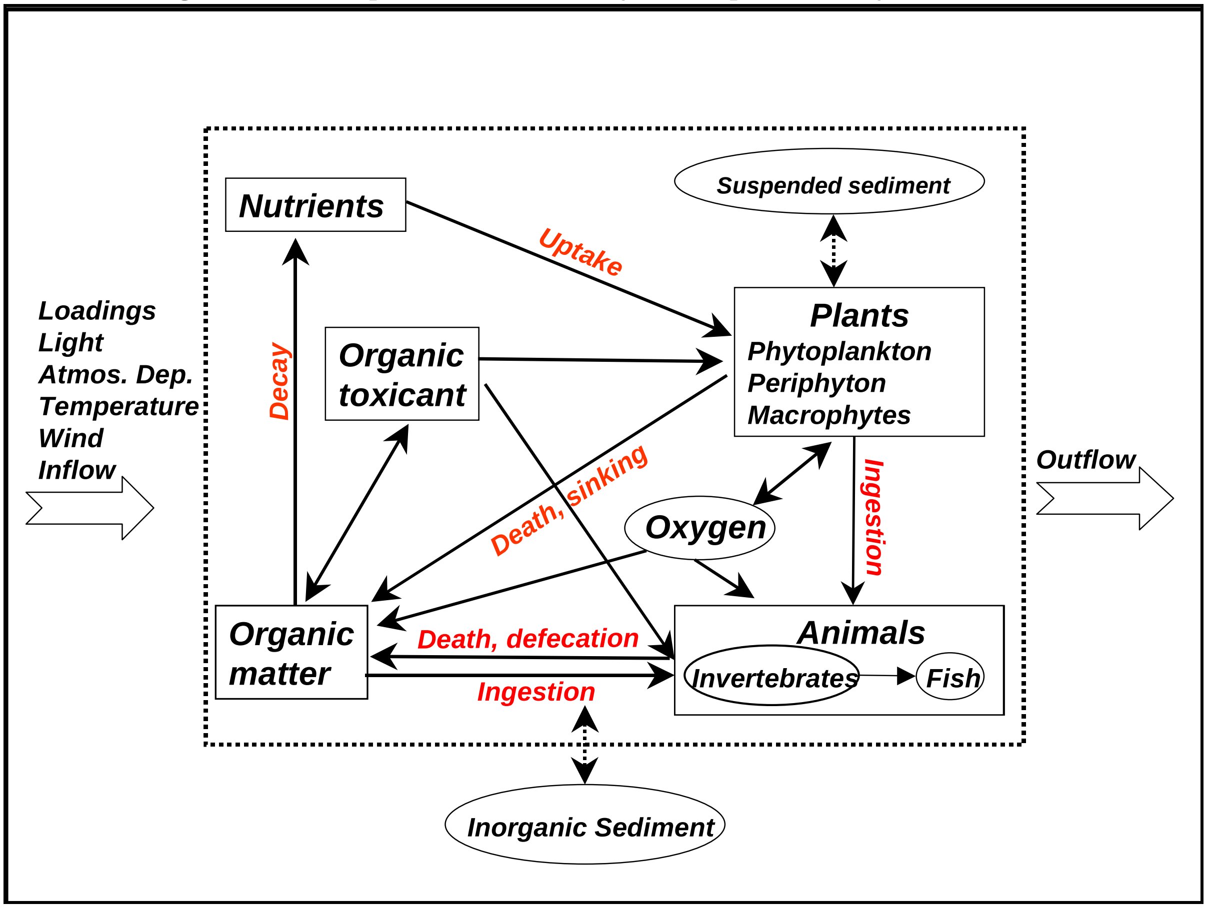
The AQUATOX model is a general ecological risk assessment model that represents the combined environmental fate and effects of conventional pollutants, such as nutrients and sediments, and toxic chemicals in aquatic ecosystems. It considers several trophic levels, including attached and planktonic algae and submerged aquatic vegetation, invertebrates, and forage, bottom-feeding, and game fish; it also represents associated organic toxicants. It can be implemented as a simple model (indeed, it has been used to simulate an abiotic flask) or as a truly complex food-web model. Often it is desirable to model a food web rather than a food chain, for example to examine the possibility of less tolerant organisms being replaced by more tolerant organisms as environmental perturbations occur. "Food web models provide a means for validation because they mechanistically describe the bioaccumulation process and ascribe causality to observed relationships between biota and sediment or water" (Connolly and Glaser 1998). The best way to accurately assess bioaccumulation is to use more complex models, but only if the data needs of the models can be met and there is sufficient time (Pelka 1998).

The model has been implemented for streams, small rivers, ponds, lakes, and reservoirs. The model is intended to be used to evaluate the likelihood of past, present, and future adverse effects from various stressors including potentially toxic organic chemicals, nutrients, organic wastes, sediments, and temperature. The stressors may be considered individually or together.

The fate portion of the model, which is applicable especially to organic toxicants, includes: partitioning among organisms, suspended and sedimented detritus, suspended and sedimented inorganic sediments, and water; volatilization; hydrolysis; photolysis; ionization; and microbial degradation. The effects portion of the model includes: chronic and acute toxicity to the various organisms modeled; and indirect effects such as release of grazing and predation pressure, increase in detritus and recycling of nutrients from killed organisms, dissolved oxygen sag due to increased decomposition, and loss of food base for animals.

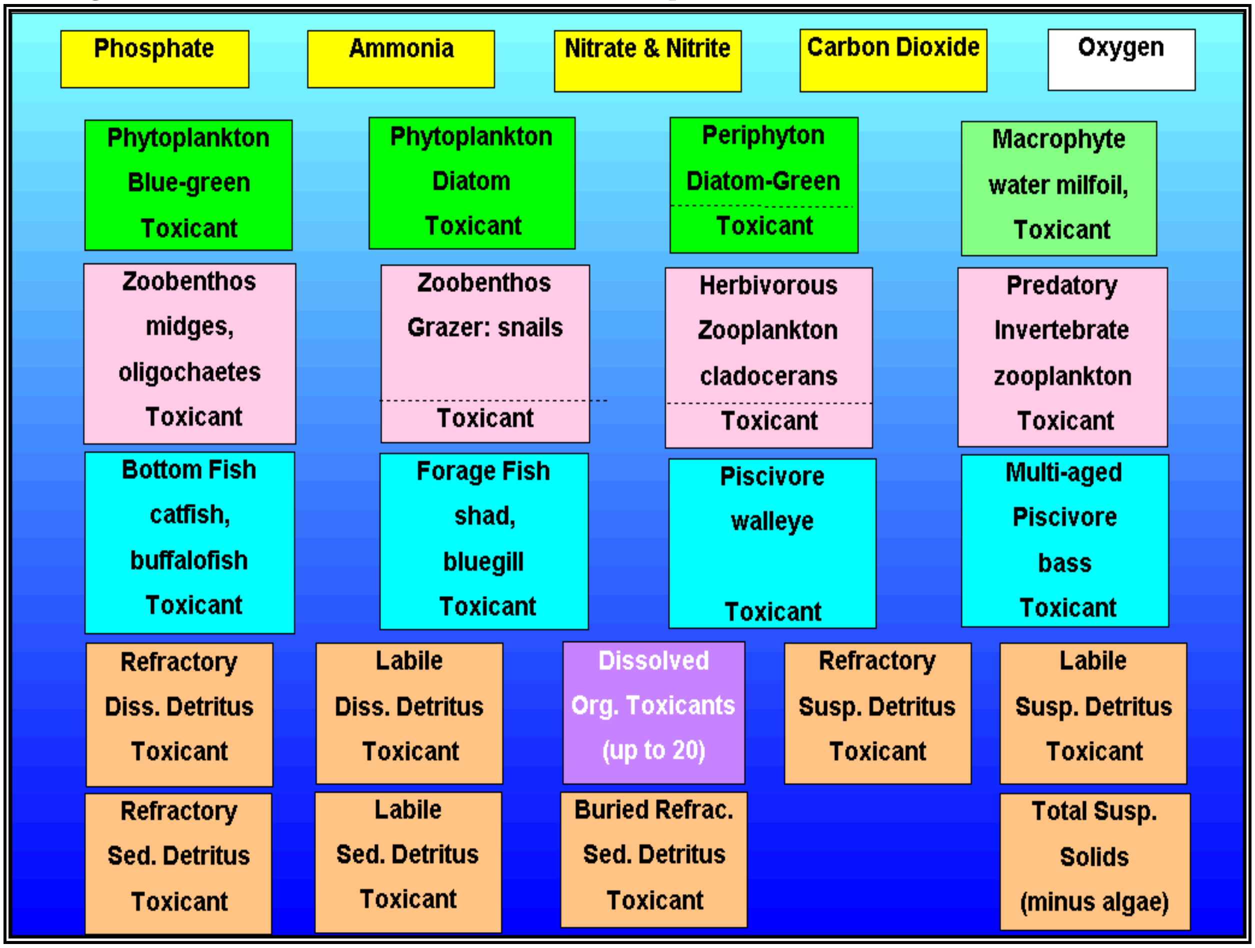
AQUATOX represents the aquatic ecosystem by simulating the changing concentrations (in mg/L or g/m^3) of organisms, nutrients, chemicals, and sediments in a unit volume of water (**Figure 1**). As such, it differs from population models, which represent the changes in numbers of individuals. As O'Neill et al. (1986) stated, ecosystem models and population models are complementary; one cannot take the place of the other. Population models excel at modeling individual species at risk and modeling fishing pressure and other age/size-specific aspects; but recycling of nutrients, the combined fate and effects of toxic chemicals, and other interdependencies in the aquatic ecosystem are important aspects that AQUATOX represents and that cannot be addressed by a population model.

Figure 1. Conceptual model of ecosystem represented by AQUATOX



Any ecosystem model consists of multiple components requiring input data. These are the abiotic and biotic **state variables** or compartments being simulated (**Figure 2**). In AQUATOX the biotic state variables may represent trophic levels, guilds, and/or species. The model can represent a food web with both detrital- and algal-based trophic linkages. Closely related are **driving variables**, such as temperature, light, and nutrient loadings, which force the system to behave in certain ways. In AQUATOX state variables and driving variables are treated similarly in the code. This provides flexibility because external loadings of state variables, such as phytoplankton carried into a reach from upstream, may function as driving variables; and driving variables, such as pH and temperature, could be treated as dynamic state variables in a future implementation. Constant, dynamic, and multiplicative loadings can be specified for atmospheric, point- and nonpoint sources. Loadings of pollutants can be turned off at the click of a button to obtain a **control** simulation for comparison with the **perturbed** simulation.

Figure 2. State Variables in AQUATOX as implemented for Coralville Reservoir, Iowa.



The model is written in object-oriented Pascal using the Delphi programming system for Windows. An object is a unit of computer code that can be duplicated; its characteristics and methods also can be inherited by higher-level objects. For example, the organism object, including variables such as the *LC50* (lethal concentration of a toxicant) and process functions such as respiration, is inherited by the plant object; that is enhanced by plant-specific variables and functions and is duplicated for three kinds of algae; and the plant object is inherited and modified slightly for macrophytes. This modularity forms the basis for the remarkable flexibility of the model, including the ability to add and delete given state variables interactively.

AQUATOX utilizes **differential equations** to represent changing values of state variables, normally with a reporting time step of one day. These equations require starting values or **initial conditions** for the beginning of the simulation. If the first day of a simulation is changed, then the initial conditions may need to be changed. A simulation can begin with any date and may be for any length of time from a few days, corresponding to a microcosm experiment, to several years, corresponding to an extreme event followed by long-term recovery.

The **process equations** contain another class of input variables: the **parameters** or **coefficients** that allow the user to specify key process characteristics. For example, the maximum consumption rate is a critical parameter characterizing various consumers. AQUATOX is a mechanistic model with many parameters; however, default values are available so that the analyst only has to be concerned with those parameters necessary for a specific risk analysis, such as characterization of a new chemical. In the pages that follow, differential equations for the state variables will be followed by process equations and parameter definitions.

Finally, the system being modeled is characterized by **site constants**, such as mean and maximum depths. At present one can model small lakes, reservoirs, streams, small rivers, and ponds—and even enclosures and tanks. The generalized parameter screen is used for all these site types, although the hypolimnion entries obviously are not applicable to all. The temperature and light constants are used for simple forcing functions, blurring the distinctions between site constants and driving variables.

1.2 Background

AQUATOX is the latest in a long series of models, starting with the aquatic ecosystem model CLEAN (Park et al., 1974) and subsequently improved in consultation with numerous researchers at various European hydrobiological laboratories, resulting in the CLEANER series (Park et al., 1975, 1979, 1980; Park, 1978; Scavia and Park, 1976) and LAKETRACE (Collins and Park, 1989). The MACROPHYTE model, developed for the U.S. Army Corps of Engineers (Collins et al., 1985), provided additional capability for representing submersed aquatic vegetation. Another series started with the toxic fate model PEST, developed to complement CLEANER (Park et al., 1980, 1982), and continued with the TOXTRACE model (Park, 1984) and the spreadsheet equilibrium fugacity PART model. AQUATOX combined algorithms from these models with ecotoxicological constructs; and additional code was written as required for a truly integrative fate and effects model (Park, 1990, 1993). The model was then restructured and linked to Microsoft Windows interfaces to provide greater flexibility, capacity for additional compartments, and user friendliness (Park et al., 1995). Release 1 from the U.S. Environmental Protection Agency (US EPA) was improved with the addition of constructs for chronic effects and uncertainty analysis, making it a powerful tool for probabilistic risk assessment (US EPA, 2000a, b, c). Release 1.1 (US EPA 2001a, b) provided a much enhanced periphyton submodel and minor enhancements for macrophytes, fish, and dissolved oxygen. This technical documentation describes Release 2, which has a number of major enhancements (see **1.3 What's New**).

This document is intended to provide verification of individual constructs or mathematical and formulations programming algorithms used in AQUATOX. The scientific basis of the constructs reflects empirical and theoretical support; and precedence in the open literature and in widely used models is noted. Units are given to confirm the dimensional analysis. The mathematical formulations have been programmed and graphed in spreadsheets and the results have been evaluated in terms of behavior consistent with our understanding of ecosystem response; many of those graphs are given in the following documentation. The variable names in the documentation correspond to those used in the program so that the mathematical formulations and code can be compared, and the computer code has been checked for consistency with those formulations. Much of this has been done as part of the continuing process of internal review. The model and documentation also have undergone successful peer review by an external panel convened by the U.S. Environmental Protection Agency.

1.3 What's New

AQUATOX Release 2 has numerous enhancements and a few corrections from Release 1. Some of these appeared in Release 1.1 and were documented in an Addendum, and some have occurred since the Release 2 Beta Test version was posted on the developers' Web site. The changes fall in three categories.

Enhanced Scientific Capabilities

The model is much more powerful and can better represent a variety of environments, especially streams and rivers compared to Release 1. Specific enhancements include:

- a large increase in the number of biotic state variables, with two representatives for each taxonomic group or ecologic guild;
- the addition of bryophytes as a special type of macrophyte;
- a multi-age fish category with up to fifteen age classes for age-dependent bioaccumulation and limited population modeling;
- an increase in the number of toxicants from one to a maximum of twenty, with the capability for modeling daughter products due to biotransformations;
- disaggregation of stream habitats into riffle, run, and pool;
- mechanistic current- and stress-induced sloughing, light extinction, and accumulation of detritus in periphyton;
- macrophyte breakage due to currents;
- computation of chlorophyll *a* for periphyton and bryophytes, as well as for phytoplankton;
- fish biomass is entered and tracked in g/m^2;
- entrainment and washout of animals, including fish, can occur during high flow;
- the options of computing respiration and maximum consumption in fish as functions of mean individual weight using allometric parameters from the Wisconsin Bioenergetics Model;
- respiration in fish is density-dependent;
- fish spawning can occur on user-specified dates as an alternative to temperature-cued spawning;
- elimination of toxicants is more robust;
- settling and erosional velocities for inorganic sediments are user-supplied parameters;

- uncertainty analysis now covers *all* parameters and loadings;
- biotic risk graphs are provided as an alternative means of portraying probabilistic results;
- limitation factors for photosynthesis are output along with the biotic rates; and
- AQUATOX is now an extension to BASINS, providing linkages to geographic information system data, and HSPF and SWAT simulations.

Additional User Interfaces

The model is even more user-friendly, taking full advantage of current Windows capabilities on modern high-speed personal computers. Capabilities include:

- a Wizard to guide the user through the setup for a new study;
- context-sensitive Help screens;
- multiple windows for simultaneous simulations and input and output screens;
- a task bar that can be customized by the user;
- enhanced graphics, including secondary Y axes; and
- a hierarchical tree structure for choosing variables for uncertainty analysis.

Corrected Errors

Several errors were discovered and corrected during the course of continuing model evaluation. Some of these may require recalibration of studies. The example studies provided with the software have been recalibrated, but users may wish to check their own calibrations in upgrading from various versions. The corrections include:

- a change in the bathymetric computations affecting the areas of the thermocline and littoral zone (Release 1);
- removal of an unnecessary conversion from phosphate and nitrate, assuming that all nutrient input is in terms of N and P; this could affect nutrient limitations (all versions);
- inclusion of an oxygen to organic matter conversion factor (a factor of 1.5) and inclusion of specific dynamic action in the allometric computation of fish respiration (Release 2 Beta Test only);
- adding a second-to-day conversion factor for inorganic sediment deposition; previously, deposition of suspended sediments was much slower than expected (all versions);
- adding a conversion factor for wind measured at 10 m height to wind occurring at 10 cm above the water surface in the volatilization computations; for some compounds this could result in a two-fold reduction in volatilization (all versions);
- nitrification is formulated to occur only at the sediment-water interface (Release 1); and
- bioaccumulation, and hence toxicity, are constrained by the life span of an animal (all versions).

2 SIMULATION MODELING

2.1 Temporal and Spatial Resolution and Numerical Stability

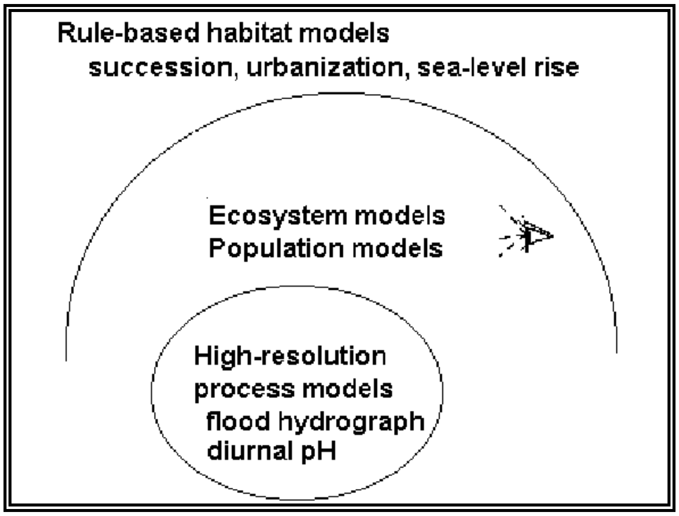
AQUATOX Release 2 is designed to be a general, realistic model of the fate and effects of pollutants in aquatic ecosystems. In order to be fast, easy to use, and verifiable, it has been designed with the simplest spatial and temporal resolutions consistent with this objective. It is designed to represent average daily conditions for a well-mixed aquatic system (in other words, a non-dimensional point model). It also can represent one-dimensional vertical epilimnetic and hypolimnetic conditions for those systems that exhibit stratification on a seasonal basis. Furthermore, the effects of run, riffle, and pool environments can be represented for streams.

According to Ford and Thornton (1979), a one-dimensional model is appropriate for reservoirs that are between 0.5 and 10 km in length; if larger, then a two-dimensional model disaggregated along the long axis is indicated. The one-dimensional assumption is also appropriate for many lakes (Stefan and Fang, 1994). Similarly, one can consider a single reach or stretch of river at a time. A spatially-distributed version of the model (Version 3.00) that is able to simulate linked segments also has been developed, but has not been released.

Usually the reporting time step is one day, but numerical instability is avoided by allowing the step size of the integration to vary to achieve a predetermined accuracy in the solution. This is a numerical approach, and the step size is not directly related to the temporal scale of the ecosystem simulation. AQUATOX uses a very efficient fourth- and fifth-order Runge-Kutta integration routine with adaptive step size to solve the differential equations (Press et al., 1986, 1992). The routine uses the fifth-order solution to determine the error associated with the fourth-order solution; it decreases the step size (often to 15 minutes or less) when rapid changes occur and increases the step size when there are slow changes, such as in winter. However, the step size is constrained to a maximum of one day so that daily pollutant loadings are always detected. The reporting step, on the other hand, can be as long as 99 days or as short as 0.1 day; the results are integrated to obtain the desired reporting time period.

The temporal and spatial resolution is in keeping with the generality and realism of the model (see Park and Collins, 1982). Careful consideration has been given to the hierarchical nature of the system. Hierarchy theory tells us that models should have resolutions appropriate to the objectives; phenomena with temporal and spatial scales that are significantly longer than those of interest should be treated as constants, and phenomena with much smaller temporal and spatial scales should be treated as steady-state properties or parameters (**Figure 3**, O'Neill et al., 1986). The model uses a longer time step than dynamic hydrologic models that are concerned with representing short-term phenomena such as storm hydrographs (and, indeed, it is not intended to capture fully the dynamics of short-term pulses less than once per day), and it uses a shorter time step than fate models that may be concerned only with long-term patterns such as bioaccumulation in large fish.

Figure 3. Position of ecosystem models such as AQUATOX in the spatial-temporal hierarchy of models.



Changing the permissible relative error (the difference between the fourth- and fifth-order solutions) of the simulation can affect the results. The model allows the user to set the relative error, usually between 0.005 and 0.01. Comparison of output shows that up to a point a smaller error can yield a marked improvement in the simulation—although execution time is slightly longer. For example, simulations of two pulsed doses of chlorpyrifos in a pond exhibit a spread in the first pulse of about 0.6 μg/L dissolved toxicant between the simulation with 0.001 relative error and the simulation with 0.05 relative error (**Figure 4**); this is probably due in part to differences in the timing of the reporting step. However, if we examine the dissolved oxygen levels, which combine the effects of photosynthesis, decomposition, and reaeration, we find that there are pronounced differences over the entire simulation period. The simulations with 0.001 and 0.01 relative error give almost exactly the same results, suggesting that the more efficient 0.001 relative error should be used; the simulation with 0.05 relative error exhibits instability in the oxygen simulation; and the simulation with 0.1 error gives quite different values for dissolved oxygen (**Figure 5**). The observed mean daily maximum dissolved oxygen for that period was 9.2 mg/L (US EPA 1988), which corresponds most closely with the results of simulation with 0.001 and 0.01 relative error.

Figure 4. Pond with Chlorpyrifos in Dissolved Phase.

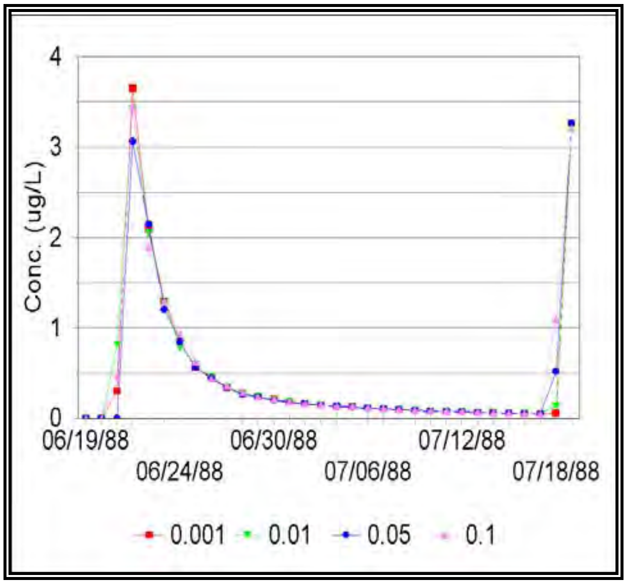
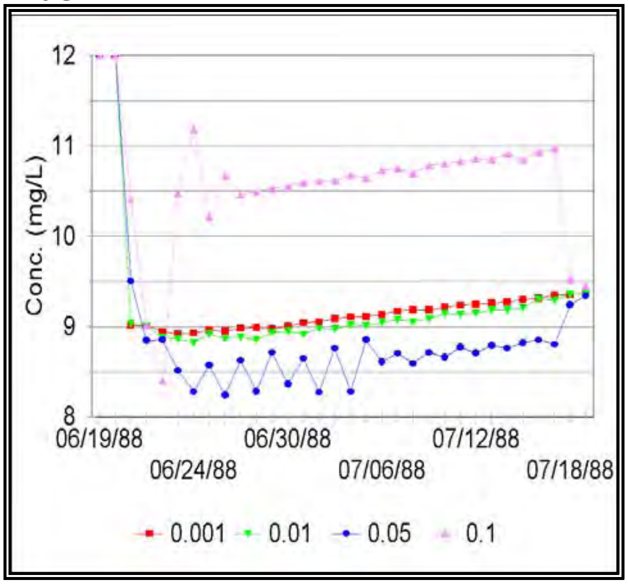


Figure 5. Same as **Figure 4** with Dissolved Oxygen.



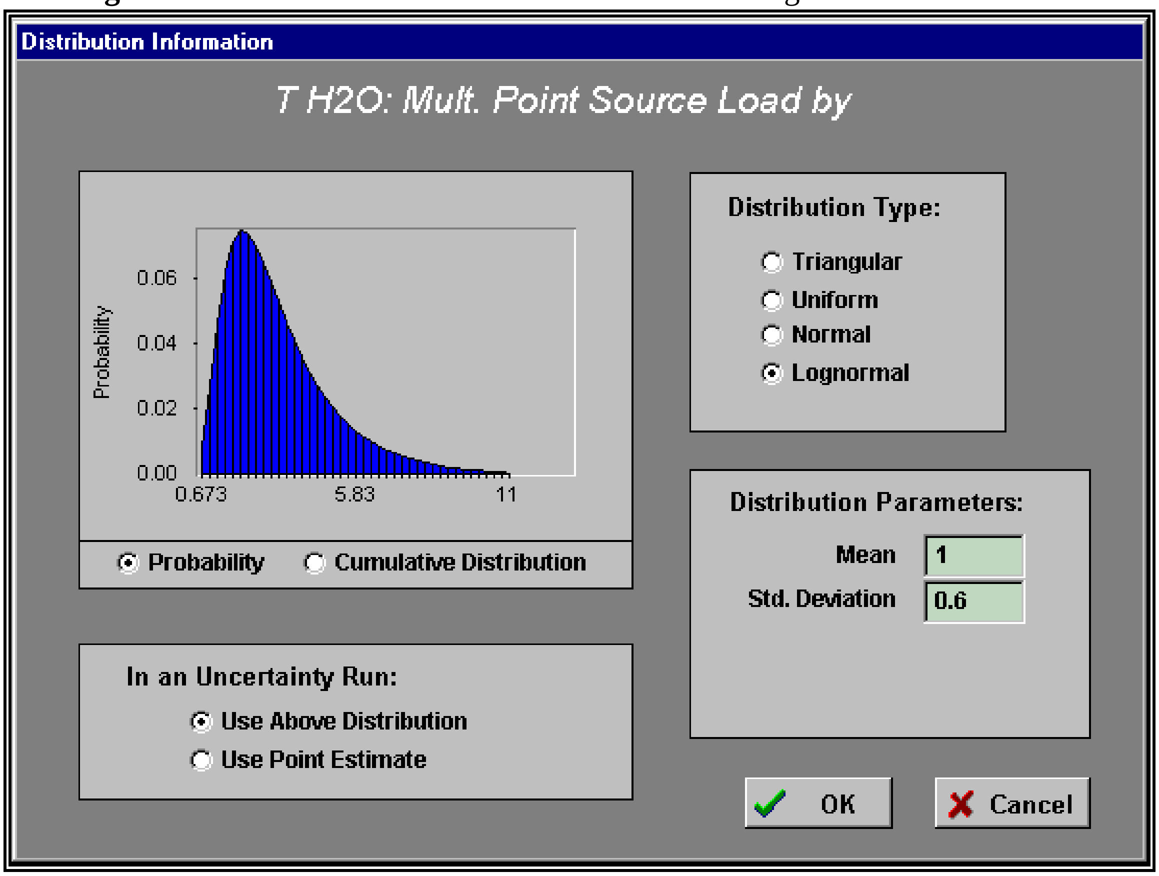
2.2 Uncertainty Analysis

There are numerous sources of uncertainty and variation in natural systems. These include: site characteristics such as water depth, which may vary seasonally and from site to site; environmental loadings such as water flow, temperature, and light, which may have a stochastic component; and critical biotic parameters such as maximum photosynthetic and consumption rates, which vary among experiments and representative organisms.

In addition, there are sources of uncertainty and variation with regard to pollutants, including:
pollutant loadings from runoff, point sources, and atmospheric deposition, which may vary stochastically from day to day and year to year; physico-chemical characteristics such as octanol-water partition coefficients and Henry Law constants that cannot be measured easily; chemodynamic parameters such as microbial degradation, photolysis, and hydrolysis rates, which may be subject to both measurement errors and indeterminate environmental controls.

Increasingly, environmental analysts and decision makers are requiring probabilistic modeling approaches so that they can consider the implications of uncertainty in the analyses. AQUATOX provides this capability by allowing the user to specify the types of distributions and key statistics for any and all input variables. Depending on the specific variable and the amount of available information, any one of several distributions may be most appropriate. A lognormal distribution is the default for environmental and pollutant loadings. In the uncertainty analysis, the distributions for constant loadings are sampled daily, providing day-to-day variation within the limits of the distribution, reflecting the stochastic nature of such loadings. A useful tool in testing scenarios is the multiplicative loading factor, which can be applied to all loads. Distributions for dynamic loadings may employ multiplicative factors that are sampled once each iteration (**Figure 6**). Normally the multiplicative factor for a loading is set to 1, but, as seen in the example, under extreme conditions the loading may be ten times as great. In this way the user could represent unexpected conditions such as pesticides being applied inadvertently just before each large storm of the season. Loadings usually exhibit a lognormal distribution, and that is suggested in these applications, unless there is information to the contrary. **Figure 7** exhibits the result of such a loading distribution.

Figure 6. Distribution Screen for Point-Source Loading of Toxicant in Water.



A sequence of increasingly informative distributions should be considered for most parameters (see **Volume 1: User's Manual**.) If only two values are known and nothing more can be assumed, the two values may be used as minimum and maximum values for a uniform distribution (**Figure 8**); this is often used for parameters where only two values are known. If minimal information is available but there is reason to accept a particular value as most likely, perhaps based on calibration, then a triangular distribution may be most suitable (**Figure 9**). Note that the minimum and maximum values for the distribution are constraints that have zero probability of occurrence. If additional data are available indicating both a central tendency and spread of response, such as parameters for well-studied processes, then a normal distribution may be most appropriate (**Figure 10**). The result of applying such a distribution in a simulation of Onondaga Lake, New York, is shown in **Figure 11**, where simulated benthic feeding affects decomposition and subsequently the predicted hypolimnetic anoxia. All distributions are truncated at zero because negative values would have no meaning.

Figure 7. Sensitivity of bass (g/m^2) to variations in loadings of dieldrin in Coralville Lake, Iowa.

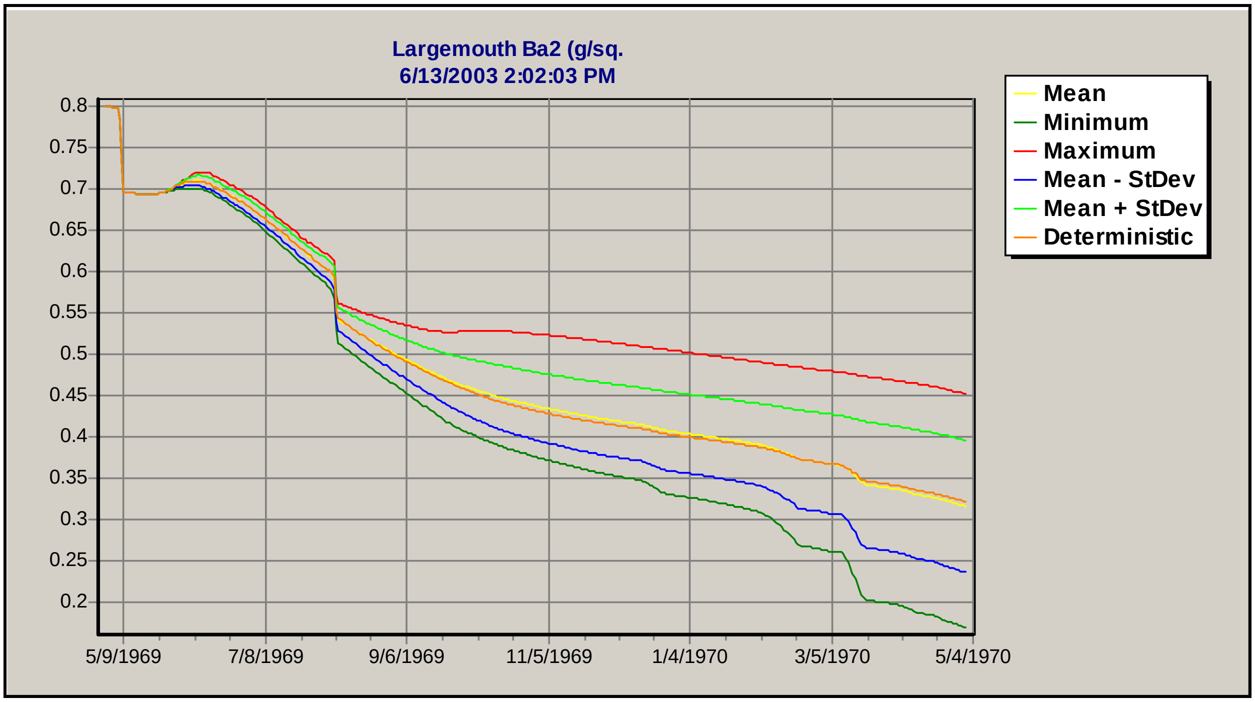


Figure 8. Uniform Distribution for Henry's Law Constant for Esfenvalerate.

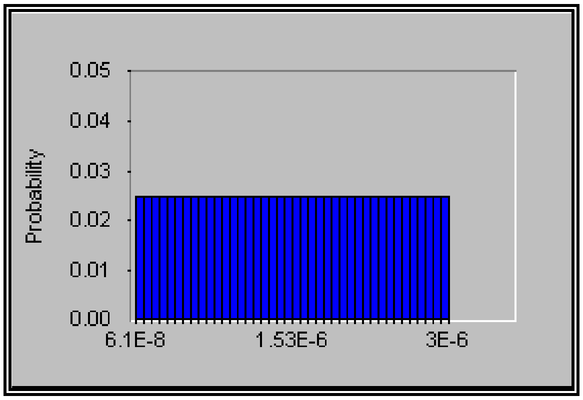


Figure 9. Triangular Distribution for Maximum Consumption Rate for Bass.

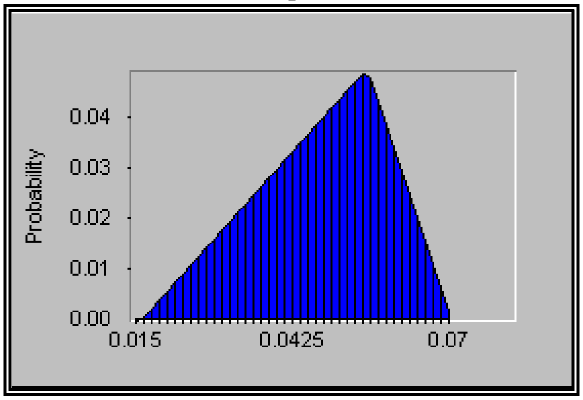


Figure 10. Normal Distribution for Maximum Consumption Rate for the Detritivorous Invertebrate *Tubifex*.

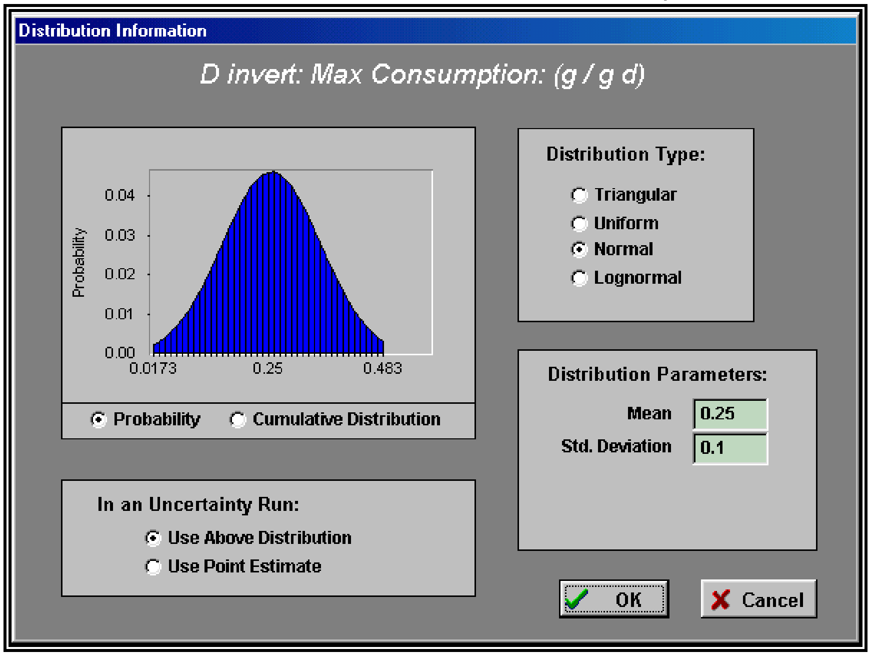
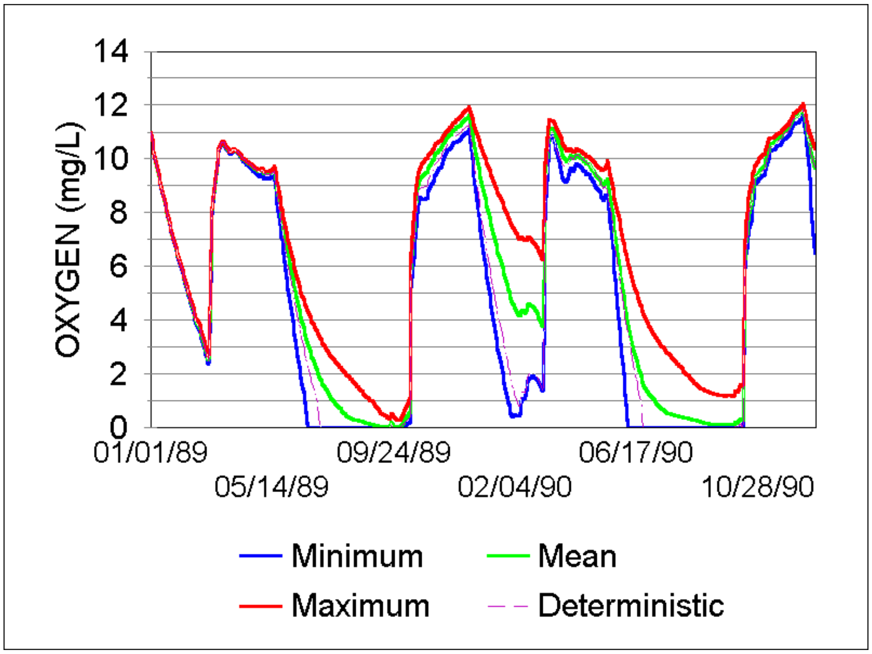
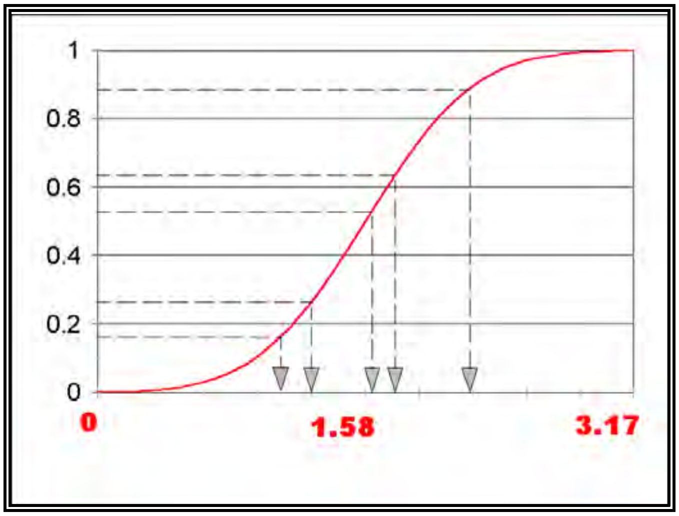


Figure 11. Sensitivity of Hypolimnetic Oxygen in Lake Onondaga to Variations in Maximum Consumption Rates of Detritivores.



Efficient sampling from the distributions is obtained with the Latin hypercube method (McKay et al., 1979; Palisade Corporation, 1991), using algorithms originally written in FORTRAN ((Iman and Shortencarier 1984)Anonymous, 1988). Depending on how many iterations are chosen for the analysis, each cumulative distribution is subdivided into that many equal segments. Then a uniform random value is chosen *within* each segment and used in one of the subsequent simulation runs. For example, the distribution shown in **Figure 10** can be sampled as shown in **Figure 12**. This method is particularly advantageous because all regions of the distribution, including the tails, are sampled. A non-random seed can be used for the random number generator, causing the same sequence of numbers to be picked in successive applications; this is useful if you want to be able to duplicate the results exactly. The default is twenty iterations, meaning that twenty simulations will be performed with sampled input values; this should be considered the minimum number to provide any reliability. The optimal number can be determined experimentally by noting the number required to obtain convergence of mean response values for key state variables; in other words, at what point do additional iterations not result in significant changes in the results? As many variables may be represented by distributions as desired, but the method assumes that they are independently distributed. By varying one parameter at a time the sensitivity of the model to individual parameters can be determined. This is done for key parameters in the following documentation.

Figure 12. Latin Hypercube Sampling of a Cumulative Distribution with a Mean of 25 and Standard Deviation of 8 Divided into 5 Intervals.



An alternate way of presenting uncertainty is by means of a biomass risk graph, which plots the probability that biomass will be reduced by a given percentage by the end of the simulation (Mauriello and Park 2002). In practice, AQUATOX compares the end value with the initial condition for each state variable, expressing the result as a percent decline:

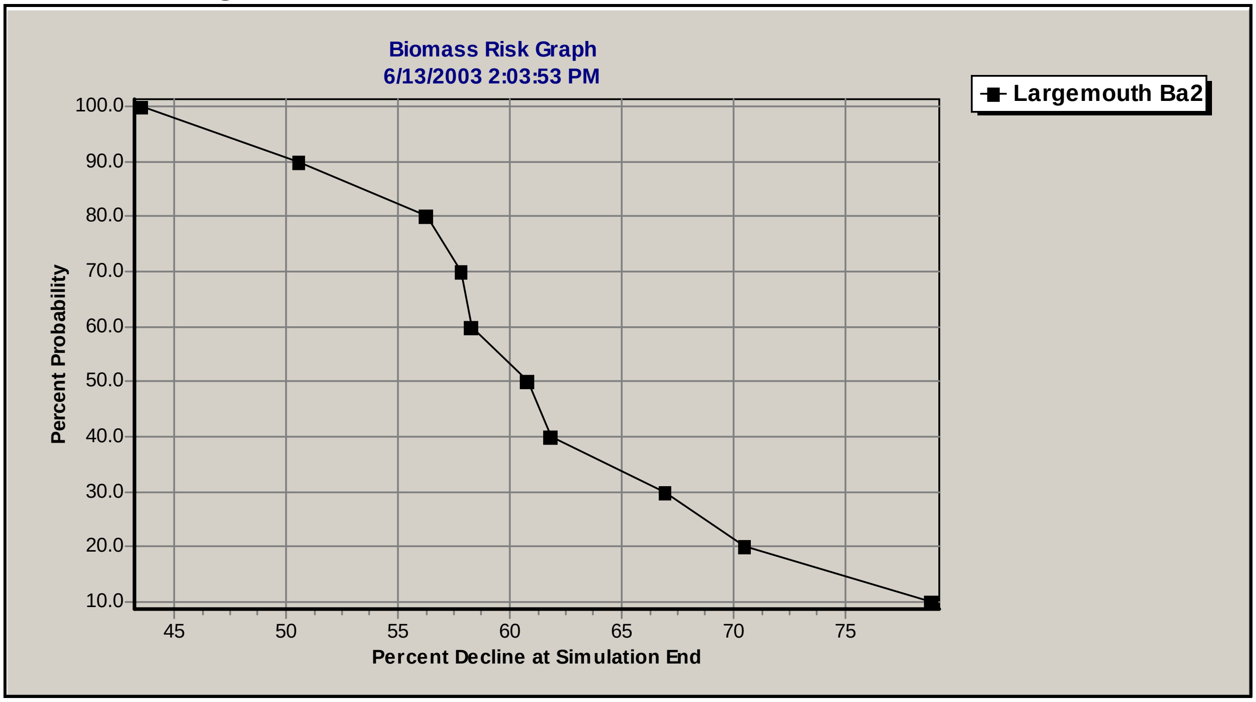
$$Decline = \left(1 - \frac{EndVal}{StartVal}\right) \cdot 100 \qquad \textbf{(1)}$$

where:

Decline	=	percent decline in biomass for a given state variable (%);
EndVal	=	value at the end of the simulation for a given state variable (units depend on state variable);
StartVal	=	initial condition for given state variable.

The results from each iteration are sorted and plotted in a cumulative distribution so that the probability that a particular percent decline will be exceeded can be evaluated (**Figure 13**). Note that there are ten points in this example, one for each iteration as the consecutive segments of the distribution are sampled.

Figure 13. Risk to bass from dieldrin in Coralville Reservoir, Iowa.



3 PHYSICAL CHARACTERISTICS

3.1 Morphometry

Volume

Volume is a state variable and can be computed in several ways depending on availability of data and the site dynamics. It is important for computing the dilution or concentration of pollutants, nutrients, and organisms; it may be constant, but usually it is time varying. In the model, ponds, lakes, and reservoirs are treated differently than streams, especially with respect to computing volumes. The change in volume of ponds, lakes, and reservoirs is computed as:

$$\frac{dVolume}{dt} = Inflow - Discharge - Evap \tag{2}$$

where:

dVolume/dt	=	derivative for volume of water (m^3/d),
Inflow	=	inflow of water into waterbody (m^3/d),
Discharge	=	discharge of water from waterbody (m^3/d), and
Evap	=	evaporation (m^3/d), see (3).

Evaporation is converted from an annual value for the site to a daily value using the simple relationship:

$$Evap = \frac{MeanEvap}{365} \cdot 0.0254 \cdot Area \tag{3}$$

where:

MeanEvap	=	mean annual evaporation (in/yr),
365	=	days per year (d/yr),
0.0254	=	conversion from inches to meters (m/in), and
Area	=	area of the waterbody (m^2).

The user is given several options for computing volume including keeping the volume constant; making the volume a dynamic function of inflow, discharge, and evaporation; using a time series of known values; and, for flowing waters, computing volume as a function of the Manning's equation. Depending on the method, inflow and discharge are varied, as indicated in Table 1. As shown in equation (2), an evaporation term is present in each of these volume calculation options. In order to keep the volume constant, given a known inflow loading, evaporation must be subtracted from discharge. This will reduce the quantity of state variables that wash out of the system. In the dynamic formulation, evaporation is part of the differential equation, but neither inflow nor discharge is a function of evaporation as they are both entered by the user. When setting the volume of a water body to a known value, evaporation must again be subtracted from discharge for the volume solution to be correct. Finally, when using the Manning's volume equation, given a known discharge loading, the effects of evaporation must be added to the inflow loading so that the proper Manning's volume is achieved. (This could increase the amount of inflow loadings of toxicants and sediments to the system, although not significantly.)

Table 1. Computation of Volume, Inflow, and Discharge

Method	Inflow	Discharge
Constant	*InflowLoad*	*InflowLoad - Evap*
Dynamic	*InflowLoad*	*DischargeLoad*
Known values	*InflowLoad*	*InflowLoad - Evap + (State - KnownVals)/dt*
Manning	*ManningVol - State/dt + DischargeLoad + Evap*	*DischargeLoad*

The variables are defined as:

InflowLoad = user-supplied inflow loading (m^3/d);
DischargeLoad = user-supplied discharge loading (m^3/d);
State = computed state variable value for volume (m^3);
KnownVals = time series of known values of volume (m^3);
dt = incremental time in simulation (d); and
ManningVol = volume of stream reach (m^3), see (4).

Figure 14 illustrates time-varying volumes and inflow loadings specified by the user and discharge computed by the model for a run-of-the-river reservoir. Note that significant drops in volume occur with operational releases, usually in the spring, for flood control purposes.

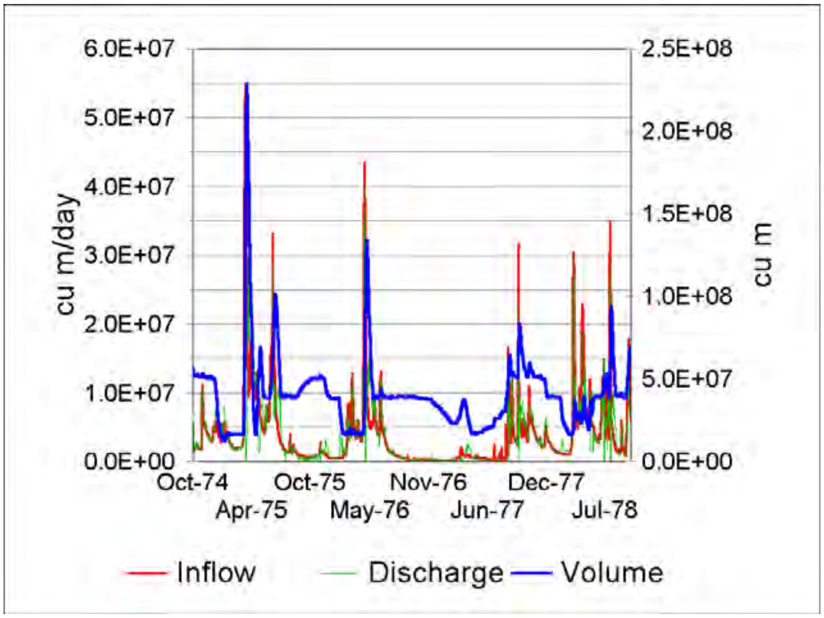
The time-varying volume of water in a stream channel is computed as:

$$ManningVol = Y \cdot CLength \cdot Width \tag{4}$$

where:

Y = dynamic mean depth (m), see (5);
CLength = length of reach (m); and
Width = width of channel (m).

Figure 14. Volume, Inflow, and Discharge for a 4-year Period in Coralville Reservoir, Iowa.



In streams the depth of water and flow rate are key variables in computing the transport, scour, and deposition of sediments. Time-varying water depth is a function of the flow rate, channel roughness, slope, and channel width using Manning's equation ((Gregory and Walling 1973)), which is rearranged to yield:

$$Y = \left(\frac{Q \cdot Manning}{\sqrt{Slope} \cdot Width} \right)^{3/5} \tag{5}$$

where:

Q	=	flow rate (m^3/s);
Manning	=	Manning's roughness coefficient ($s/m^{1/3}$);
Slope	=	slope of channel (m/m); and
Width	=	channel width (m).

The Manning's roughness coefficient is an important parameter representing frictional loss, but it is not subject to direct measurement. The user can enter a value or can choose among the following stream types:

- concrete channel (with a default Manning's coefficient of 0.020);
- dredged channel, such as ditches and channelized streams (default coefficient of 0.030); and
- natural channel (default coefficient of 0.040).

These generalities are based on Chow's (1959) tabulated values as given by Hoggan (1989).

In the absence of inflow data, the flow rate is computed from the initial mean water depth, assuming a rectangular channel and using a rearrangement of Manning's equation:

$$QBase = \frac{IDepth^{5/3} \cdot \sqrt{Slope} \cdot Width}{Manning} \tag{6}$$

where:

QBase	=	base flow (m^3/s); and
Idepth	=	mean depth as given in site record (m).

The dynamic flow rate is calculated from the inflow loading by converting from m^3/d to m^3/s:

$$Q = \frac{Inflow}{86400} \tag{7}$$

where:

Q	=	flow rate (m^3/s); and
Inflow	=	water discharged into channel from upstream (m^3/d).

Bathymetric Approximations

The depth distribution of a water body is important because it determines the areas and volumes subject to mixing and light penetration. The shapes of ponds, lakes, reservoirs, and streams are represented in the model by idealized geometrical approximations, following the topological treatment of Junge (1966; see also Straškraba and Gnauck, 1985). The shape parameter *P* (Junge, 1966) characterizes the site, with a shape that is indicated by the ratio of mean to maximum depth:

$$P = 6.0 \cdot \frac{ZMean}{ZMax} - 3.0 \tag{8}$$

Where:

ZMean	=	mean depth (m);
ZMax	=	maximum depth (m); and
P	=	characterizing parameter for shape (unitless); *P* is constrained between -1.0 and 1.0.

Shallow constructed ponds and ditches may be approximated by an ellipsoid where *Z/ZMax* = 0.6 and *P* = 0.6. Reservoirs and rivers generally are extreme elliptic sinusoids with values of *P* constrained to -1.0. Lakes may be either elliptic sinusoids, with *P* between 0.0 and -1.0, or elliptic hyperboloids with *P* between 0.0 and 1.0. The model requires mean and maximum depth, but if only the maximum depth is known, then the mean depth can be estimated by multiplying *ZMax* by the representative ratio. Not all water bodies fit the elliptic shapes, but the model generally is not sensitive to the deviations.

Based on these relationships, fractions of volumes and areas can be determined for any given depth (**Figure 15**, **Figure 16**; Junge, 1966). The *AreaFrac* function returns the fraction of surface area that is at depth *Z* given *Zmax* and *P*, which defines the morphometry of the water body. For example, if the water body were an inverted cone, when horizontal slices were made through the cone looking down from the top one could see both the surface area and the water/sediment boundary where the slice was made. This would look like a circle within a circle, or a donut (**Figure 17**). *AreaFrac* calculates the fraction that is the donut (not the donut hole). To get the donut hole, 1 - *AreaFrac* is used.

Figure 15
Area as a Function of Depth

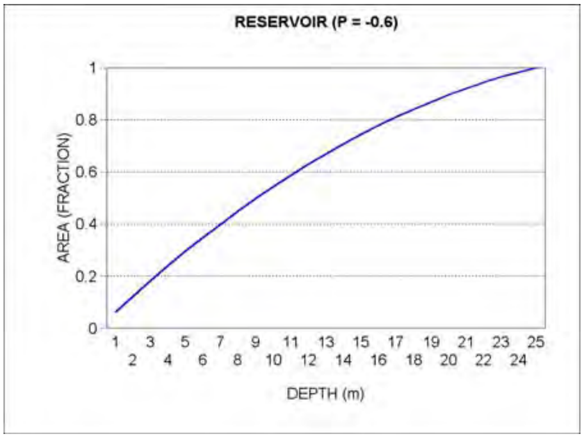
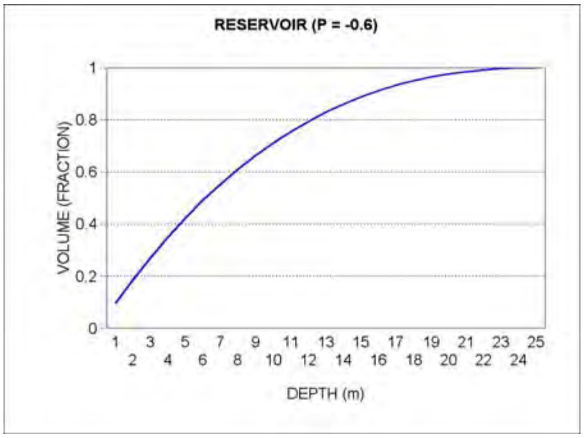


Figure 16
Volume as a Function of Depth



$$AreaFrac = (1 - P) \cdot \frac{Z}{ZMax} + P \cdot \left(\frac{Z}{ZMax}\right)^2 \tag{9}$$

$$VolFrac = \frac{6.0 \cdot \frac{Z}{ZMax} - 3.0 \cdot (1.0 - P) \cdot \left(\frac{Z}{ZMax}\right)^2 - 2.0 \cdot P \cdot \left(\frac{Z}{ZMax}\right)^3}{3.0 + P} \tag{10}$$

where:

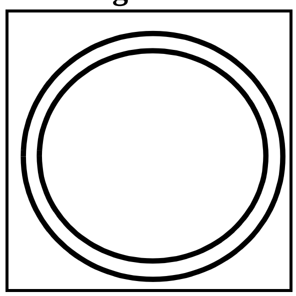
AreaFrac	=	fraction of area of site above given depth (unitless);
VolFrac	=	fraction of volume of site above given depth (unitless); and
Z	=	depth of interest (m).

For example, the fraction of the volume that is epilimnion can be computed by setting depth *Z* to the mixing depth. Furthermore, by setting *Z* to the depth of the euphotic zone, the fraction of the area available for colonization by macrophytes and periphyton can be computed:

$$FracLit = (1 - P) \cdot \frac{ZEuphotic}{ZMax} + P \cdot \left(\frac{ZEuphotic}{ZMax} \right)^2 \qquad \textbf{(11)}$$

A relatively deep, flat-bottomed basin would have a small littoral area and a large sublittoral area (**Figure 17**).

Figure 17



If the site is a limnocorral (an artificial enclosure) then the available area is increased accordingly:

$$FracLittoral = FracLit \cdot \frac{Area + LimnoWallArea}{Area}$$

otherwise **(12)**

$$FracLittoral = FracLit$$

where:

FracLittoral	=	fraction of site area that is within the euphotic zone (unitless);
ZEuphotic	=	depth of the euphotic zone, where primary production exceeds respiration, usually calculated as a function of extinction (m);
Area	=	site area (m^2); and
LimnoWallArea	=	area of limnocorral walls (m^2).

Habitat Disaggregation

Riverine environments are seldom homogeneous. Organisms often exhibit definite preferences for habitats. Therefore, when modeling streams or rivers, animal and plant habitats are broken down into three categories: "riffle," "run," and "pool." The combination of these three habitat categories make up 100% of the available habitat within a riverine simulation. The preferred percentage of each organism that resides within these three habitat types can be set within the animal or plant data. Within the *site* data, the percentage of the river that is composed of each of these three habitat categories also can be set. It should be noted that the habitat percentages are considered constant over time, and thus would not capture significant changes in channel morphology and habitat distribution due to major flooding events.

These habitats affect the simulations in two ways: as limitations on photosynthesis and consumption and as weighting factors for water velocity (see 3.2 Velocity). Each animal and plant is exposed to a weighted average water velocity depending on its location within the three habitats. This weighted velocity affects all velocity-mediated processes including entrainment of invertebrates and fish, breakage of macrophytes and scour of periphyton. The reaeration of the system also is affected by the habitat-weighted velocities.

Limitations on photosynthesis and consumption are calculated depending on a species' preferences for habitats and the available habitats within the water body. If the species preference for a particular habitat is equal to zero then the portion of the water body that contains that particular habitat limits the amount of consumption or photosynthesis accordingly.

$$HabitatLimit = \sum_{Preference_{habitat} > 0} \left(\frac{Percent_{habitat}}{100} \right) \quad \textbf{(13)}$$

where:

$HabitatLimit_{Species}$	=	fraction of site available to organism (unitless), used to limit ingestion, see **(78)**, and photosynthesis, see **(31)**, **(73)**;
$Preference_{habitat}$	=	preference of animal or plant for the habitat in question (percentage); and
$Percent_{habitat}$	=	percentage of site composed of the habitat in question (percentage).

It is important to note that the initial condition for an animal that is entered in g/m^2 is an indication of the total mass of the animal over the total surface area of the river. Because of this, density data for various benthic organisms cannot be used as input to AQUATOX until these values have been converted to represent the entire surface area. This is especially true in modeling habitats; for example, an animal could have a high density within riffles, but riffles might only constitute a small portion of the entire system.

3.2 Velocity

Velocity is calculated as a simple function of flow and cross-sectional area:

$$Velocity = \frac{AvgFlow}{XSecArea} \cdot \frac{1}{86400} \cdot 100 \tag{14}$$

where

Velocity	=	velocity (cm/s),
AvgFlow	=	flow (m^3/d),
XSecArea	=	cross sectional area (m^2),
86400	=	s/d, and
100	=	cm/m.

$$AvgFlow = \frac{Inflow + Discharge}{2} \tag{15}$$

where:

Inflow	=	flow into the reach (m^3/d);
Discharge	=	flow out of the reach (m^3/d).

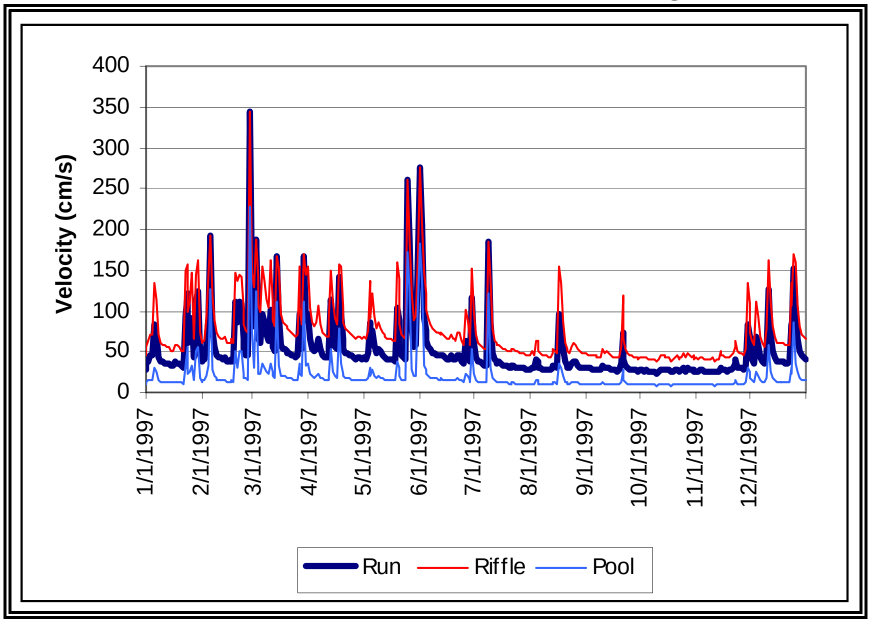
It is assumed that this is the velocity for the run of the stream. No distinction is made in terms of vertical differences in velocity in the stream. Following the approach and values used in the DSAMMt model (Caupp et al. 1995), the riffle velocity is obtained by using a conversion factor that is dependent on the discharge. Unlike the DSAMMt model, pools also are modeled, so a conversion factor is used to obtain the pool velocity as well (Table 2). The consequence of these habitat controls on velocity is shown in **Figure 18**.

Table 2. Factors relating velocities to those of the average reach.

Flows (Q = discharge)	**Run Velocity**	**Riffle Velocity**	**Pool Velocity**
Q < 2.59e5 m^3/d	1.0	1.6	0.36
2.59e5 m^3/d # Q < 5.18e5 m^3/d	1.0	1.3	0.46
5.18e5 m^3/d # Q < 7.77e5 m^3/d	1.0	1.1	0.56
Q $ 7.77e5 m^3/d	1.0	1.0	0.66

Figure 18

Predicted velocities in an Ohio stream according to habitat



3.3 Washout

Transport out of the system, or washout, is an important loss term for nutrients, floating organisms, dissolved toxicants, and suspended detritus and sediments in reservoirs and streams. Although it is considered separately for several state variables, the process is a general function of discharge:

$$Washout = \frac{Discharge}{Volume} \cdot State \tag{16}$$

where:

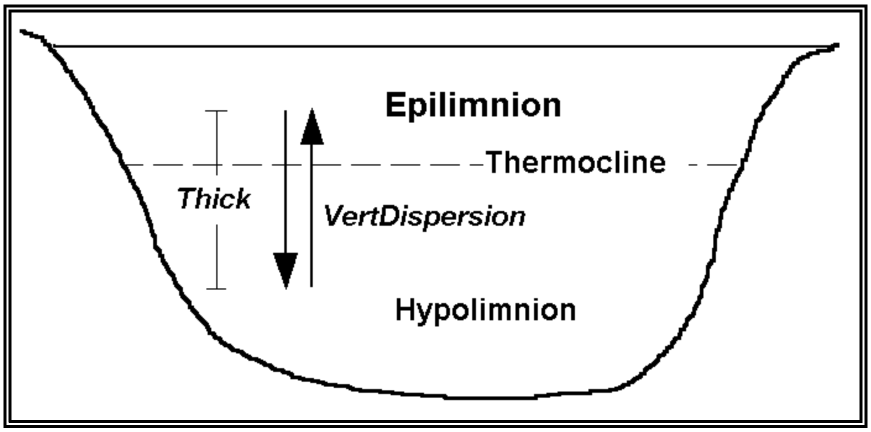
Washout	=	loss due to being carried downstream ($g/m^3 \cdot d$);
Discharge	=	flow out of the reach (m^3/d), see **Table 1**;
Volume	=	volume of stream reach (m^3), see (2); and
State	=	concentration of dissolved or floating state variable (g/m^3).

3.4 Stratification and Mixing

Thermal stratification is handled in the simplest form consistent with the goals of forecasting the effects of nutrients and toxicants. Lakes and reservoirs are considered in the model to have two vertical zones: epilimnion and hypolimnion (**Figure 19**); the metalimnion zone that separates these is ignored. Instead, the thermocline, or plane of maximum temperature change, is taken as the separator; this is also known as the mixing depth (Hanna, 1990). Dividing the lake into two vertical zones follows the treatment of Imboden (1973), Park et al. (1974), and Straškraba and Gnauck (1983). The onset of stratification is considered to occur when the mean water temperature exceeds 4° and the difference in temperature between the epilimnion and hypolimnion exceeds 3°. Overturn occurs when the temperature of the epilimnion is less than 3°, usually in the fall. Winter stratification is not modeled. For simplicity, the thermocline is assumed to occur at a constant depth.

Figure 19

Thermal Stratification in a Lake; Terms Defined in Text



There are numerous empirical models relating thermocline depth to lake characteristics. AQUATOX uses an equation by Hanna (1990), based on the maximum effective length (or fetch). The dataset includes 167 mostly temperate lakes with maximum effective lengths of 172 to 108,000 m and ranging in altitude from 10 to 1897 m. The equation has a coefficient of determination $r^2 = 0.850$, meaning that 85 percent of the sum of squares is explained by the regression. Its curvilinear nature is shown in ?, and it is computed as (Hanna, 1990):

$$\log(MaxZMix) = 0.336 \cdot \log(Length) - 0.245 \tag{17}$$

where:

MaxZMix	=	maximum mixing depth for lake (m); and
Length	=	maximum effective length for wave setup (m, converted from user-supplied km).

Wind action is implicit in this formulation. Wind has been modeled explicitly by Baca and Arnett (1976, quoted by Bowie et al., 1985), but their approach requires calibration to individual sites, and it is not used here.

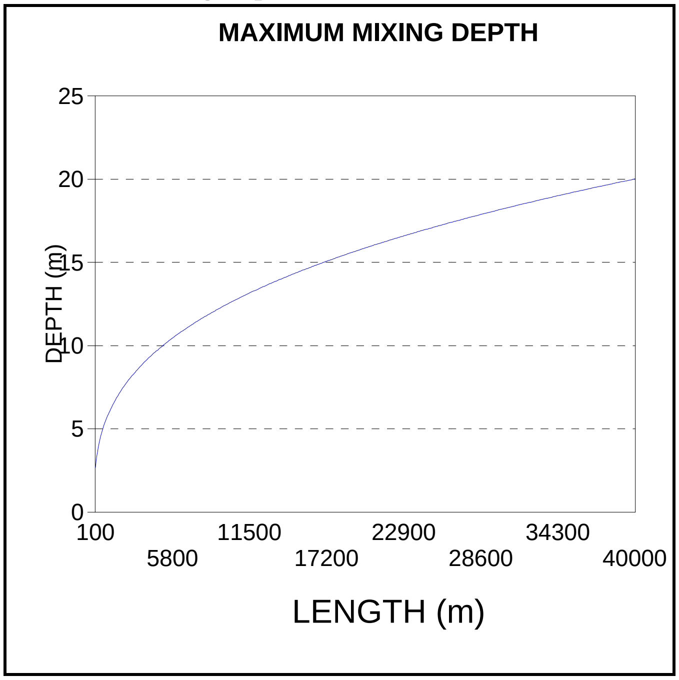
Vertical dispersion for bulk mixing is modeled as a function of the time-varying hypolimnetic and epilimnetic temperatures, following the treatment of Thomann and Mueller (1987, p. 203; see also Chapra and Reckhow, 1983, p. 152; **Figure 21**):

$$VertDispersion = Thick \cdot \left(\frac{HypVolume}{ThermoclArea \cdot Deltat} \cdot \frac{|T_{hypo}^{t-1} - T_{hypo}^{t+1}|}{T_{epi}^{t} - T_{hypo}^{t}} \right) \quad \textbf{(18)}$$

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 (°C); and
T_{epi}^{t}, T_{hypo}^{t}	=	temperature of epilimnion and hypolimnion at present time (°C).

Figure 20
Mixing depth as a function of fetch



Stratification can break down temporarily as a result of high throughflow. This is represented in the model by making the vertical dispersion coefficient between the layers a function of discharge for sites with retention times of less than or equal to 180 days (**Figure 22**), rather than temperature differences as in equation 11, based on observations by Straškraba (1973) for a Czech reservoir:

$$VertDispersion = 1.37 \cdot 10^4 \cdot Retention^{-2.269} \tag{19}$$

and:

$$Retention = \frac{Volume}{TotDischarge} \tag{20}$$

where:

Retention	=	retention time (d);
Volume	=	volume of site (m^3); and
TotDischarge	=	combined discharge of epilimnion and hypolimnion (m^3/d); see **Table 1**.

Figure 21
Vertical dispersion as a function of temperature differences

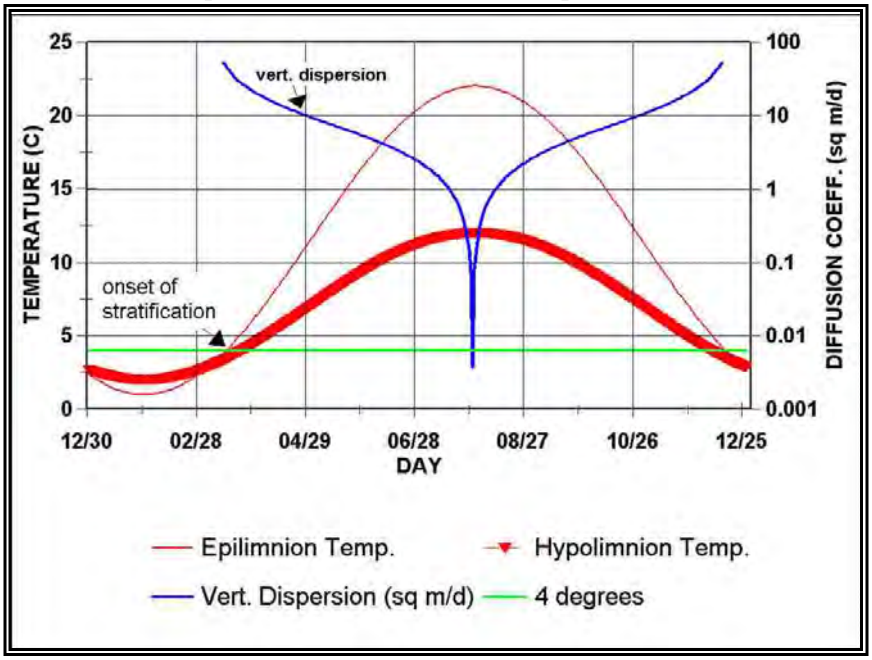
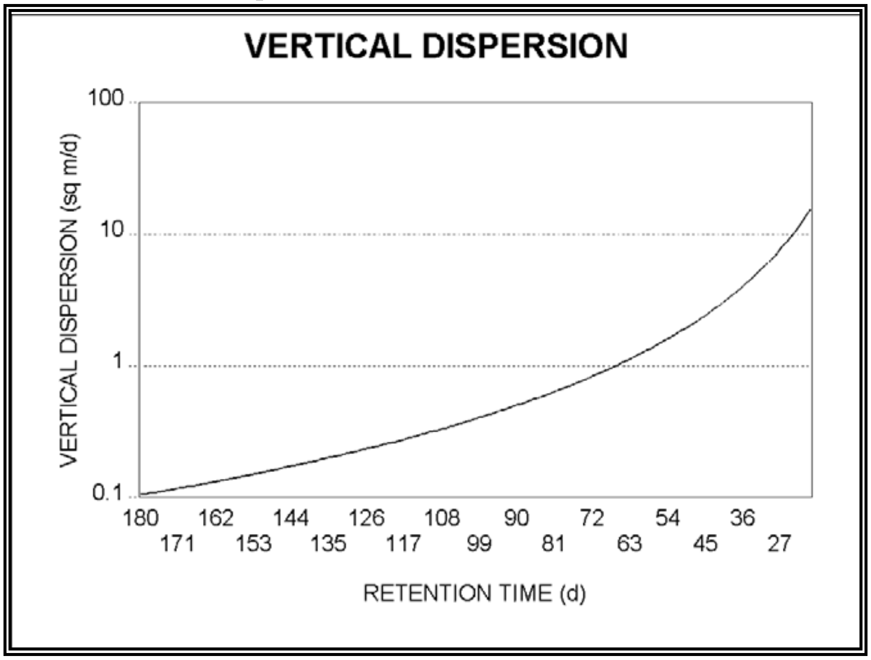


Figure 22
Vertical Dispersion as a Function of Retention Time



The bulk vertical mixing coefficient is computed using site characteristics and the time-varying vertical dispersion (Thomann and Mueller, 1987):

$$BulkMixCoeff = \frac{VertDispersion \cdot ThermoclArea}{Thick} \tag{21}$$

where:

BulkMixCoeff = bulk vertical mixing coefficient (m^3/d),
ThermoclArea = area of thermocline (m^2).

Turbulent diffusion of biota and other material between epilimnion and hypolimnion is computed separately for each segment for each time step while there is stratification:

$$TurbDiff_{epi} = \frac{BulkMixCoeff}{Volume_{epi}} \cdot (Conc_{compartment,\ hypo} - Conc_{compartment,\ epi}) \tag{22}$$

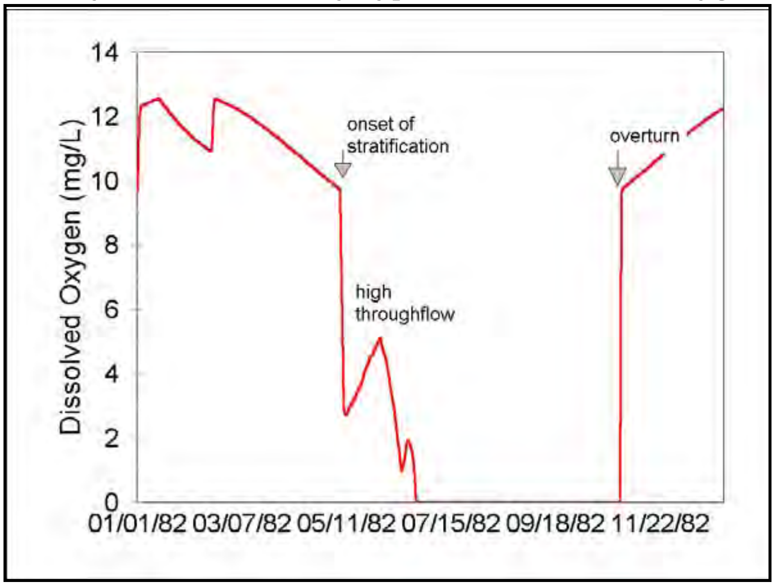
$$TurbDiff_{hypo} = \frac{BulkMixCoeff}{Volume_{hypo}} \cdot (Conc_{compartment,\ epi} - Conc_{compartment,\ hypo}) \tag{23}$$

where:

TurbDiff	=	turbulent diffusion for a given zone ($g/m^{3}\cdot d$) see **(22)** and **(23)**;
Volume	=	volume of given segment (m^3); and
Conc	=	concentration of given compartment in given zone (g/m^3).

The effects of stratification, mixing due to high throughflow, and overturn are well illustrated by the pattern of dissolved oxygen levels in the hypolimnion of Lake Nockamixon, a eutrophic reservoir in Pennsylvania (**Figure 23**).

Figure 23
Stratification and mixing in Lake Nockamixon,
Pennsylvania as shown by hypolimnetic dissolved oxygen



3.5 Temperature

Temperature is an important controlling factor in the model. Virtually all processes are temperature-dependent. These include stratification; biotic processes such as decomposition, photosynthesis, consumption, respiration, reproduction, and mortality; and chemical fate processes such as microbial degradation, volatilization, hydrolysis, and bioaccumulation. On the other hand, temperature rarely fluctuates rapidly in aquatic systems. Default water temperature loadings for the epilimnion and hypolimnion are represented through a simple sine approximation for seasonal variations (Ward, 1963) based on user-supplied observed means and ranges (**Figure 24**):

$$Temperature = TempMean + (-1.0 \cdot \frac{TempRange}{2} \cdot (\sin(0.0174533 \cdot (0.987 \cdot (Day + PhaseShift) - 30))))] \qquad \textbf{(24)}$$

where:

Temperature	=	average daily water temperature (°C);
TempMean	=	mean annual temperature (°C);
TempRange	=	annual temperature range (°C),
Day	=	Julian date (d); and
PhaseShift	=	time lag in heating (= 90 d).

Observed temperature loadings should be entered if responses to short-term variations are of interest. This is especially important if the timing of the onset of stratification is critical, because stratification is a function of the difference in hypolimnetic and epilimnetic temperatures (see **Figure 22**). It also is important in streams subject to releases from reservoirs and other point-source temperature impacts.

3.6 Light

Light is important as the controlling factor for photosynthesis and photolysis. The default incident light function was formulated for AQUATOX and is a variation on the temperature equation, but without the lag term:

$$Solar = LightMean + \frac{LightRange}{2} \cdot \sin(0.0174533 \cdot Day - 1.76) \qquad \textbf{(25)}$$

where:

Solar	=	average daily incident light intensity (ly/d);
LightMean	=	mean annual light intensity (ly/d);
LightRange	=	annual range in light intensity (ly/d); and
Day	=	Julian date (d, adjusted for hemisphere).

The derived values are given as average light intensity in Langleys per day (Ly/d = 10 $kcal/m^2 \cdot d$). An observed time-series of light also can be supplied by the user; this is especially important if the effects of daily climatic conditions are of interest. If the average water temperature drops below 3°C, the model assumes the presence of ice cover and decreases light to 33% of incident radiation. This reduction, due to the reflectivity and transmissivity of ice and snow, is an average of widely varying values summarized by Wetzel (1975; also see LeCren and Lowe-McConnell, 1980). The model does not automatically adjust for shading by riparian vegetation, so a times-series should probably be supplied if modeling a narrow stream.

Photoperiod is an integral part of the photosynthesis formulation. It is approximated using the Julian date following the approach of (Stewart 1975) (**Figure 25**):

$$Photoperiod = \frac{12 + A \cdot \cos(380 \cdot \frac{Day}{365} + 248)}{24} \quad \textbf{(26)}$$

where:

Photoperiod	=	fraction of the day with daylight (unitless); converted from hours by dividing by 24;
A	=	hours of daylight minus 12 (hr); and
Day	=	Julian date (d, converted to radians).

A is the difference between the number of hours of daylight at the summer solstice at a given latitude and the vernal equinox, and is given by a linear regression developed by Groden (1977):

$$A = 0.1414 \cdot Latitude - Sign \cdot 2.413 \quad \textbf{(27)}$$

where:

Latitude	=	latitude (°, decimal), negative in southern hemisphere; and
Sign	=	1.0 in northern hemisphere, -1.0 in southern hemisphere.

Figure 24
Annual Temperature

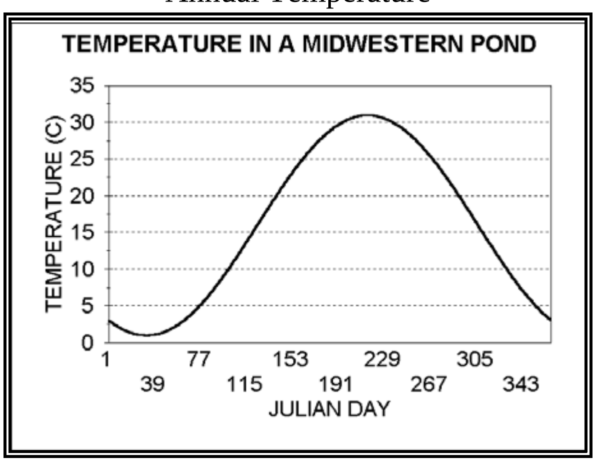
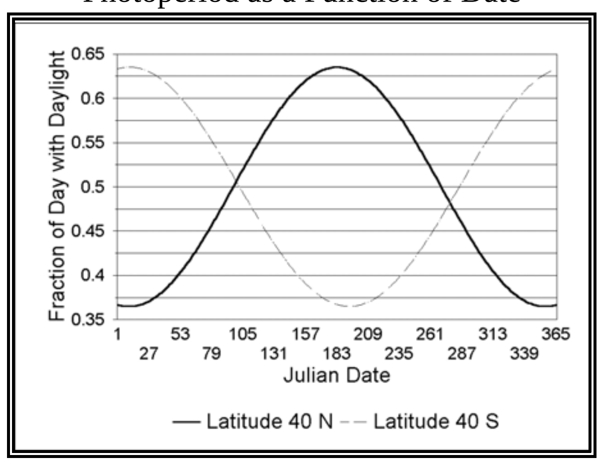


Figure 25
Photoperiod as a Function of Date



3.7 Wind

Wind is an important driving variable because it determines the stability of blue-green algal blooms, affects reaeration or oxygen exchange, and controls volatilization of some organic chemicals. Wind is usually measured at meteorological stations at a height of 10 m and is expressed as m/s. If site data are not available, default variable wind speeds are represented through a Fourier series of sine and cosine terms; the mean and first ten harmonics seem to capture the variation adequately (**Figure 26**):

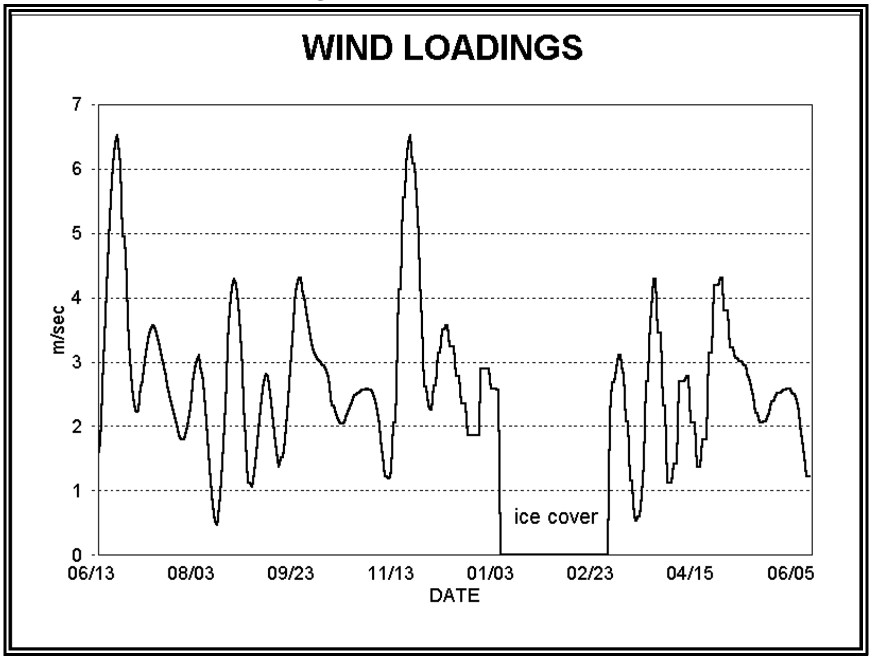
$$Wind = CosCoeff_0 + \sum \left(CosCoeff_n \cdot \mathrm{Cos}\left(\frac{2 \cdot \pi \cdot Day}{WaveLength}\right) + SinCoeff_0 \cdot \mathrm{Sin}\left(\frac{2 \cdot \pi \cdot Day}{WaveLength}\right)\right) \quad \textbf{(28)}$$

where:

Wind	=	wind speed; amplitude of the Fourier series (m/s);
$CosCoeff_0$	=	cosine coefficient for the 0-order harmonic, which is the mean wind speed (default = 3 m/s);
$CosCoeff_n$	=	cosine coefficient for the n^{th}-order harmonic;
Day	=	Julian date (d);
WaveLength	=	wave length (= 5); and
$SinCoeff_n$	=	sine coefficient for the n^{th}-order harmonic.

This default loading is based on an unpublished 140-day record (May 20 to October 12) from Columbia, Missouri; therefore, it has a 140-day repeat, representative of the Midwest during the growing season. This approach is quite useful because the mean can be specified by the user and the variability will be imposed by the function. If ice cover is predicted, wind is set to 0. A user also may input a site-specific time series, which may be important where the timing of a blue-green algal bloom or reaeration is of interest.

Figure 26
Default Wind Loadings for Missouri Pond with Mean = 3 m/s



4 BIOTA

The biota consists of two main groups, plants and animals; each is represented by a set of process-level equations. In turn, plants are differentiated into algae and macrophytes, represented by slight variations in the differential equations. Algae may be either phytoplankton or periphyton. Phytoplankton are subject to sinking and washout, while periphyton are subject to substrate limitation and scour by currents. Bryophytes are modeled as a special class of macrophytes, limited by nutrients in the water column. These differences are treated at the process level in the equations (Table 3). All are subject to habitat availability, but to differing degrees. Plants also are characterized by taxonomic group, which is primarily a way of organizing preferences for grazing and to identify blue-green phytoplankton as floating.

Table 3. Significant Differentiating Processes for Plants

Plant Type	Nutrient Lim.	Current Lim.	Sinking	Washout	Sloughing	Breakage	Habitat
Phytoplankton	[		[	[			[
Periphyton	[	[			[		[
Macrophytes						[	[
Bryophytes	[					[	[

Animals are subdivided into invertebrates and fish; the invertebrates may be pelagic invertebrates, benthic insects or other benthic invertebrates. These groups are represented by different parameter values and by variations in the equations. Insects are subject to emergence and therefore are lost from the system, but benthic invertebrates are not. Any fish may be represented by both juveniles and adults, which are connected by promotion. One fish species can be designated as multi-year with up to 15 age classes connected by promotion. Differences are shown in Table 4. Feeding preferences are very flexible and can accommodate combinations of grazing on plants, detritus feeding, and predation ("predation" is used in the following pages to refer to any type of feeding by animals). Animals also are characterized by taxonomic type or guild, primarily as a way of organizing feeding preferences; these types can be overridden.

Table 4. Significant Differentiating Processes for Animals

Animal Type	Washout	Drift	Entrainment	Emergence	Promotion	Multi-year
Pelagic Invert.	[					
Benthic Invert.		[	[			
Benthic Insect		[	[	[		
Fish			[		[	[

4.1 Algae

The change in algal biomass—expressed as ash-free dry weight in g/m^3 for phytoplankton, but as g/m^2 for periphyton—is a function of the loading (especially phytoplankton from upstream), photosynthesis, respiration, excretion or photorespiration, nonpredatory mortality, grazing or predatory mortality, sloughing, and washout; as noted above, phytoplankton also are subject to sinking. If the system is stratified, turbulent diffusion from one layer to the other also affects the biomass of phytoplankton:

$$\frac{dBiomass_{phyto}}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation \pm Sinking - Washout \pm TurbDiff \quad \textbf{(29)}$$

$$\frac{dBiomass_{peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation - Slough \quad \textbf{(30)}$$

where:

dBiomass/dt	=	change in biomass of phytoplankton and periphyton with respect to time ($g/m^3 \cdot d$ and $g/m^2 \cdot d$);
Loading	=	loading of algal group ($g/m^3 \cdot d$ and $g/m^2 \cdot d$);
Photosynthesis	=	rate of photosynthesis ($g/m^3 \cdot d$ and $g/m^2 \cdot d$), see **(31)**;
Respiration	=	respiratory loss ($g/m^3 \cdot d$ and $g/m^2 \cdot d$), see **(55)**;
Excretion	=	excretion or photorespiration ($g/m^3 \cdot d$ and $g/m^2 \cdot d$), see **(56)**;
Mortality	=	nonpredatory mortality ($g/m^3 \cdot d$ and $g/m^2 \cdot d$), see **(58)**;
Predation	=	herbivory ($g/m^3 \cdot d$ and $g/m^2 \cdot d$), see **(85)**;
Washout	=	loss due to being carried downstream ($g/m^3 \cdot d$), see **(63)**;
Sinking	=	loss or gain due to sinking between layers and sedimentation to bottom ($g/m^3 \cdot d$), see **(61)**;
TurbDiff	=	turbulent diffusion ($g/m^3 \cdot d$), see **(22)** and **(23)**; and
Slough	=	loss due to sloughing ($g/m^2 \cdot d$), see **(67)**.

Figure 27 and **Figure 28** are examples of the predicted changes in biomass and the processes that contribute to these changes in a eutrophic lake. In this and following examples, rates are plotted as a percentage of biomass in an area graph (**Figure 28**). The thickness of the band at any particular date is an indication of the magnitude of a given rate. Because both positive and negative rates are plotted as positive areas, the percentage on a particular date may exceed 100%. Discontinuities in rates may indicate stratification, turnover, anoxia, or high turbidity and washout due to storms.

Figure 27. Predicted Algal Biomass in Lake Onondaga, New York

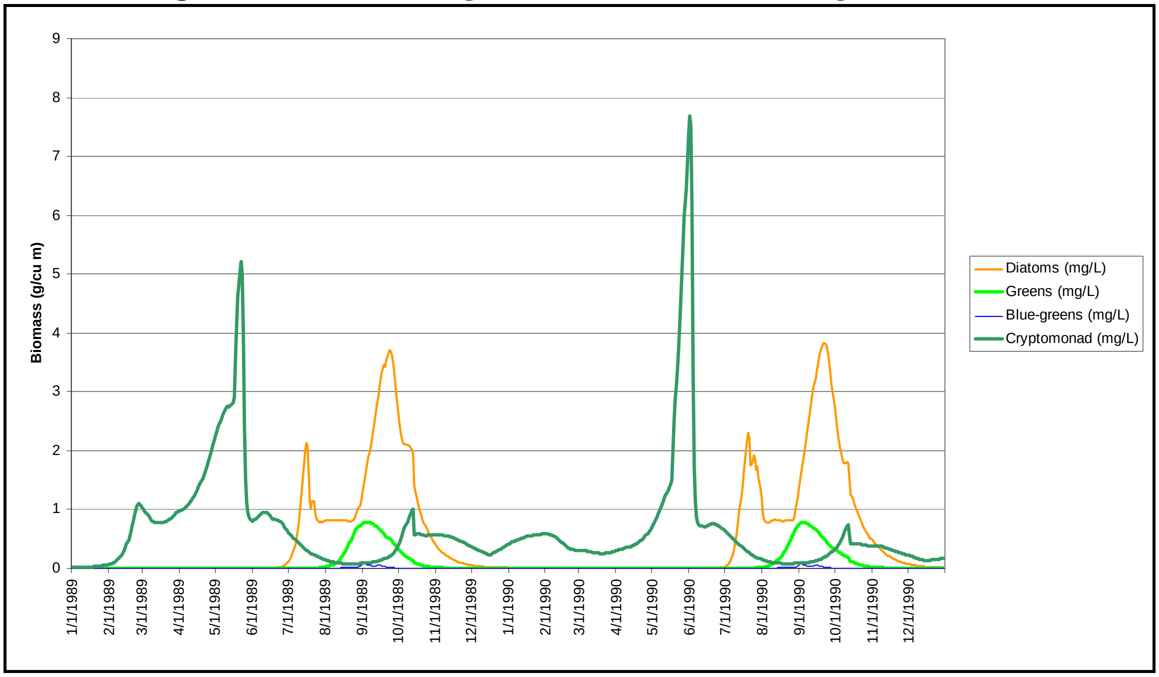
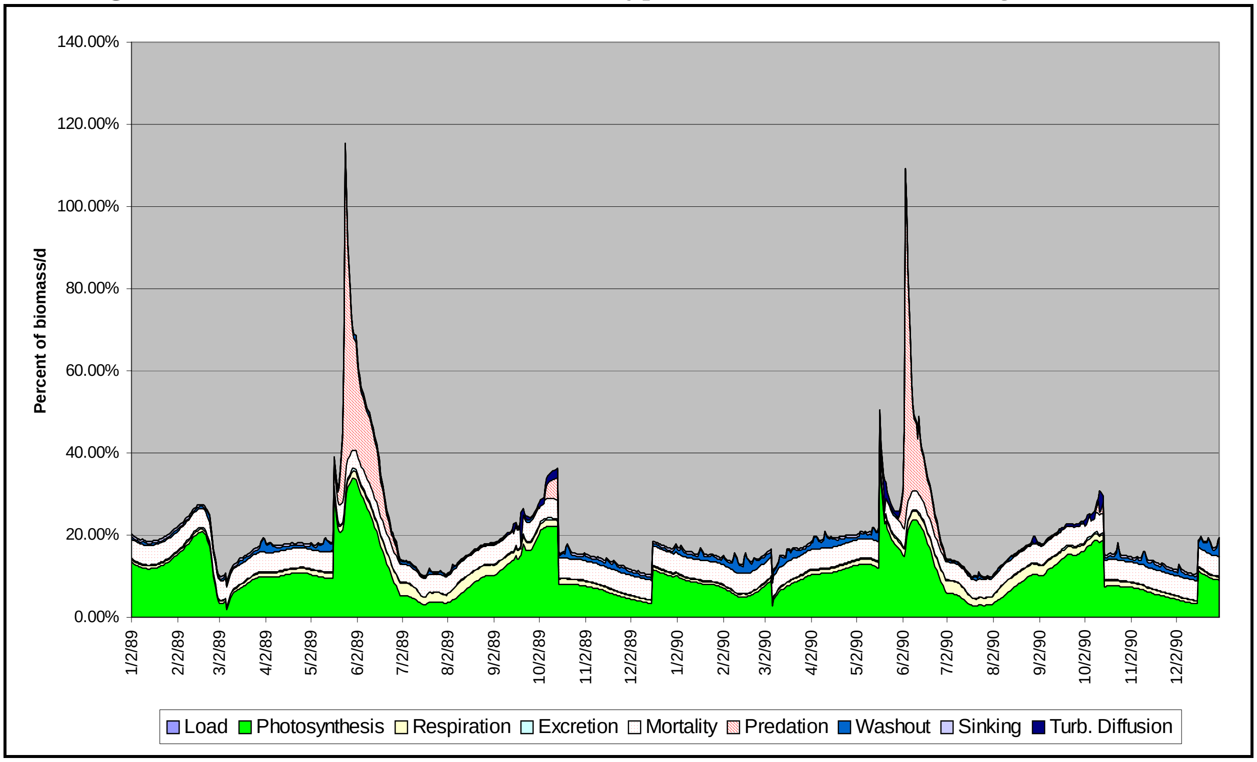


Figure 28. Predicted Process Rates for Cryptomonads in Lake Onondaga, New York



Photosynthesis is modeled as a maximum observed rate multiplied by reduction factors for the effects of toxicants, habitat, and suboptimal light, temperature, current, and nutrients:

$$Photosynthesis = PMax \cdot PProdLimit \cdot Biomass \cdot HabitatLimit \tag{31}$$

The limitation of primary production in phytoplankton is:

$$PProdLimit = LtLimit \cdot NutrLimit \cdot TCorr \cdot FracPhoto \tag{32}$$

Periphyton have an additional limitation based on available substrate, which includes the littoral bottom and the available surfaces of macrophytes. The macrophyte conversion is based on the observation of 24 m^2 periphyton/m^2 bottom (Wetzel, 1996) and assumes that the observation was made with 200 g/m^2 macrophytes.

$$\begin{aligned} PProdLimit = \; & LtLimit \cdot NutrLimit \cdot VLimit \cdot TCorr \cdot FracPhoto \\ & \cdot (FracLittoral + SurfAreaConv \cdot Biomass_{Macro}) \end{aligned} \tag{33}$$

where:

Pmax	=	maximum photosynthetic rate (1/d);
PProdLimit	=	limitation on productivity (unitless);
LtLimit	=	light limitation (unitless), see **(34)**;
NutrLimit	=	nutrient limitation (unitless), see **(47)**;
Vlimit	=	current limitation for periphyton (unitless), see **(48)**;
TCorr	=	limitation due to suboptimal temperature (unitless), see **(51)**;
HabitatLimit	=	in streams, habitat limitation based on plant habitat preferences (unitless), see **(13)**.
FracPhoto	=	reduction factor for effect of toxicant on photosynthesis (unitless), see **(294)**;
FracLittoral	=	fraction of area that is within euphotic zone (unitless) see **(11)**;
SurfAreaConv	=	surface area conversion (0.12 m^2/g);
$Biomass_{Macro}$	=	total biomass of macrophytes in system (g/m^2); and
Biomass	=	biomass of algae (g/m^2).

Under optimal conditions, a reduction factor has a value of 1; otherwise, it has a fractional value. Use of a multiplicative construct implies that the factors are independent. Several authors (for example, Collins, 1980; Straškraba and Gnauck, 1983) have shown that there are interactions among the factors. However, we feel the data are insufficient to generalize to all algae; therefore, the simpler multiplicative construct is used, as in many other models (Chen and Orlob, 1975; Lehman et al., 1975; Jørgensen, 1976; DiToro et al., 1977; Kremer and Nixon, 1978; Park et al., 1985; Ambrose et al., 1991). Default parameter values for the various processes are taken primarily from compilations (for example, Jørgensen, 1979; Collins and Wlosinski, 1983; Bowie et al., 1985); they may be modified as needed.

Light Limitation

Because it is required for photosynthesis, light is a very important limiting variable. It is especially important in controlling competition among plants with differing light requirements. Similar to many other models (for example, Di Toro et al., 1971; Park et al., 1974, 1975, 1979, 1980; Lehman et al., 1975; Canale et al., 1975, 1976; Thomann et al., 1975, 1979; Scavia et al., 1976; Bierman et al., 1980; O'Connor et al., 1981), AQUATOX uses the Steele (1962) formulation for light limitation. Light is specified as average daily radiation. The average radiation is multiplied by the photoperiod, or the fraction of the day with sunlight, based on a simplification of Steele's (1962) equation proposed by Di Toro et al. (1971):

$$LtLimit = 0.85 \cdot \frac{e \cdot Photoperiod \cdot (LtAtDepth - LtAtTop) \cdot PeriphytExt}{Extinct \cdot (Depth_{Bottom} - Depth_{Top})} \qquad \textbf{(34)}$$

where:

LtLimit	=	light limitation (unitless);
e	=	the base of natural logarithms (2.71828, unitless);
Photoperiod	=	fraction of day with daylight (unitless), see **(26)**;
Extinct	=	total light extinction (1/m), see **(35)**;
$Depth_{Bottom}$	=	maximum depth or depth of bottom of layer if stratified (m); if periphyton or macrophyte then limited to euphotic depth;
$Depth_{Top}$	=	depth of top of layer (m);
LtAtDepth	=	intermediate variable for photosynthetic light integral at the bottom of a layer, see **(38)**;
LtAtTop	=	intermediate variable for photosynthetic light integral at the top of a layer, see **(39)**, **(40)**; and
PeriphytExt	=	extinction due to periphyton; only affects periphyton and macrophytes (unitless).

Because the equation overestimates by 15 percent the cumulative effect of light limitation over a 24-hour day, a correction factor of 0.85 is applied (Kremer and Nixon, 1978).

Extinction of light is based on several additive terms: the baseline extinction coefficient for water (which may include suspended sediment if it is not modeled explicitly), the so-called "self-shading" of plants, attenuation due to dissolved organic matter (DOM), and attenuation due to suspended particulate organic matter (POM) and inorganic sediment:

$$\begin{aligned} Extinct = {} & WaterExtinction + PhytoExtinction + ECoeffDOM \cdot DOM \\ & + ECoeffPOM \cdot \Sigma PartDetr + ECoeffSed \cdot InorgSed \end{aligned} \qquad \textbf{(35)}$$

where:

WaterExtinction	=	user-supplied extinction due to water (1/m);

PhytoExtinction	=	user-supplied extinction due to phytoplankton and macrophytes (1/m), see **(35)**, **(36)**;
EcoeffDOM	=	attenuation coefficient for dissolved detritus (0.03/m-g/m^3);
DOM	=	concentration of labile and refractory dissolved organic matter (g/m^3), see **(114)** and **(115)**;
EcoeffPOM	=	attenuation coefficient for particulate detritus (0.12/m-g/m^3);
PartDetr	=	concentration of labile and refractory particulate detritus (g/m^3), see **(112)** and **(113)**;
EcoeffSed	=	attenuation coefficient for suspended inorganic sediment (0.17/m-g/m^3); and
InorgSed	=	concentration of total suspended inorganic sediment (g/m^3), see **(198)**.

For computational reasons, the value of *Extinct* is constrained between 5^{-19} and 25. Light extinction by phytoplankton, periphyton, and macrophytes is a function of the biomass and attenuation coefficient for each group. Not only does this place a constraint in the form of self-shading, but it represents a mechanism for competition and succession among plant taxa. For example, in the model as in nature, an early phytoplankton bloom can restrict growth in macrophytes. Extinction by periphyton is computed differently because it is not depth-dependent but rather pertains to the growing surface:

$$PhytoExtinction = \sum_{plant} (ECoeffPhyto_{plant} \cdot Biomass_{plant}) \tag{36}$$

$$PeriPhytExt = e^{\Sigma_{peri} (- ECoeffPhyto_{peri} \cdot Biomass_{peri})} \tag{37}$$

where:

$ECoeffPhyto_{plant}$	=	attenuation coefficient for given phytoplankton or macrophyte (1/m-g/m^3),
$ECoeffPhyto_{peri}$	=	attenuation coefficient for given periphyton (1/m-g/m^2),
Biomass	=	concentration of given plant (g/m^3 or g/m^2), and

The light effect at depth is computed by:

$$LtAtDepth = e^{-\frac{Light}{LightSat} \cdot e^{-Extinction \cdot DepthBottom}} \tag{38}$$

Light effect at the surface of the water body is computed by:

$$LtAtTop = e^{-\frac{Light}{LightSat}} \tag{39}$$

and light effect at the top of the hypolimnion is computed by:

$$LtAtTop = e^{-\frac{Light}{LightSat} \cdot e^{-Extinction \cdot DepthTop}} \quad \textbf{(40)}$$

where:

Light	=	photosynthetically active radiation (ly/d); and
LightSat	=	light saturation level for photosynthesis (ly/d).

Phytoplankton other than blue-greens are assumed to be mixed throughout the well mixed layer, although subject to sinking. However, healthy blue-green algae tend to float. Therefore, if the nutrient limitation for blue-greens is greater than 0.25 **(47)** and the wind is less than 3 m/s then *DepthBottom* for blue-greens is set to 0.25 m to account for buoyancy due to gas vacuoles. Otherwise it is set to 3 m to represent downward transport by Langmuir circulation. Under the ice, all phytoplankton are represented as occurring in the top 2 m (cf. LeCren and Lowe-McConnell, 1980). As discussed in Section **3.5**, light is decreased to 33% of incident radiation if ice cover is predicted.

Approximately half the incident solar radiation is photosynthetically active (Edmondson, 1956):

$$Light = Solar \cdot 0.5 \quad \textbf{(41)}$$

where:

Solar = average daily light intensity (ly/d), see **(25)**.

The light-limitation function represents both limitation for suboptimal light intensity and photoinhibition at high light intensities (**Figure 29**). However, when the photoperiod for all but the highest latitudes is factored in, photoinhibition disappears (**Figure 30**). When considered over the course of the year, photoinhibition can occur in very clear, shallow systems during summer mid-day hours (**Figure 31**), but it usually is not a factor when considered over 24 hours (**Figure 32**).

The extinction coefficient for pure water varies considerably in the photosynthetically-active 400-700 nm range (Wetzel, 1975, p. 55); a value of 0.016 (1/m) correspond to the extinction of green light. In many models dissolved organic matter and suspended sediment are not considered separately, so a much larger extinction coefficient is used for "water" than in AQUATOX. The attenuation coefficients have units of 1/m-(g/m^3) because they represent the amount of extinction caused by a given concentration (Table 5).

Figure 29
Instantaneous Light Response Function

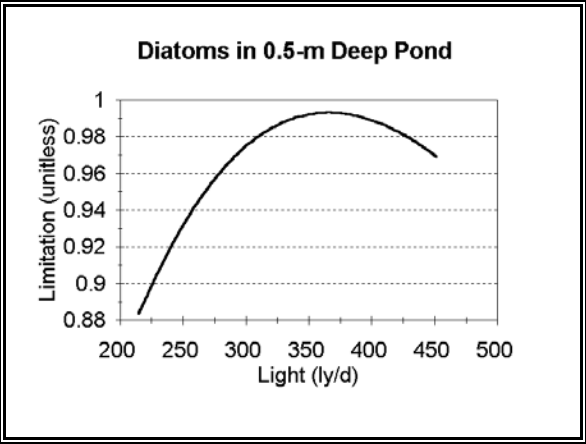


Figure 30
Daily Light Response Function

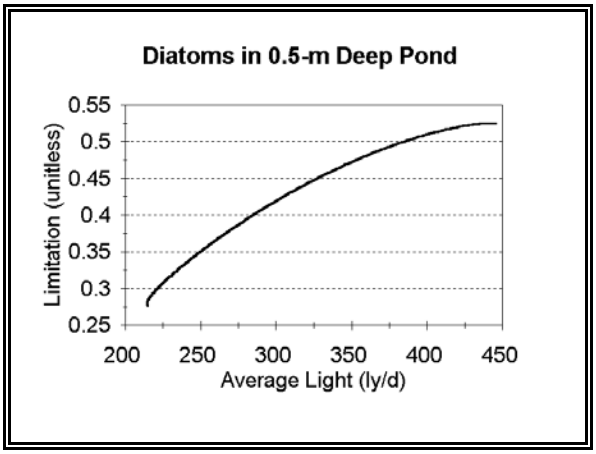


Figure 31
Mid-day Light Limitation

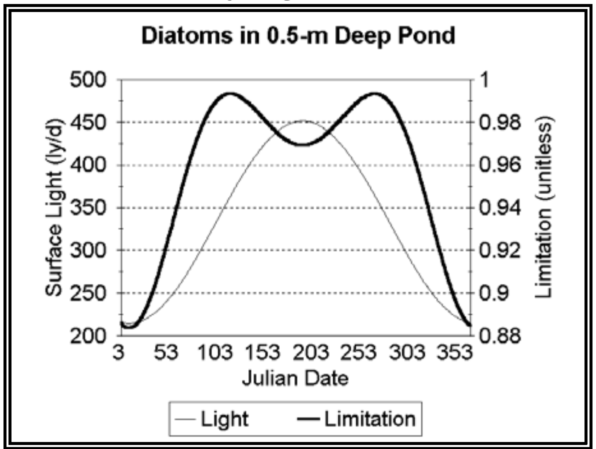


Figure 32
Daily Light Limitation

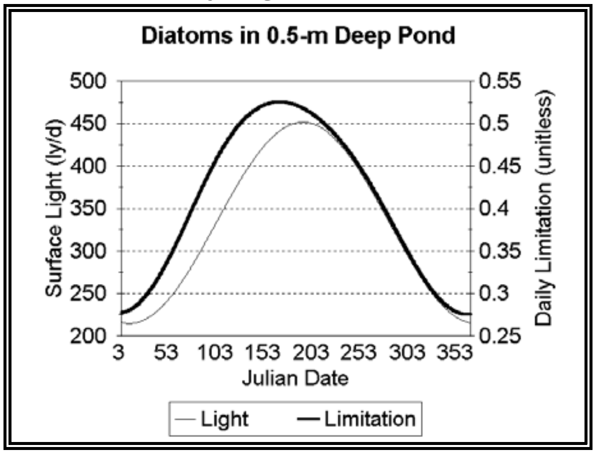


Table 5. Light Extinction and Attenuation Coefficients

WaterExtinction*	0.016 1/m	Wetzel, 1975
ECoeffPhyto$_{diatom}$*	0.014 1/m-(g/m^3)	Collins and Wlosinski, 1980
ECoeffPhyto$_{blue\text{-}green}$ *	0.099 1/m-(g/m^3)	Megard et al., 1979 (calc.)
ECoeffDOM	0.03 1/m-(g/m^3)	Effler et al., 1985 (calc.)
ECoeffPOM	0.12 1/m-(g/m^3)	Verduin, 1982
ECoeffSed	0.03 1/m-(g/m^3)	McIntire and Colby, 1978

* user-supplied

The Secchi depth, the depth at which a Secchi disk disappears from view, is a commonly used indication of turbidity. It is computed as (Straškraba and Gnauck, 1985):

$$Secchi = \frac{1.9}{Extinct} \tag{42}$$

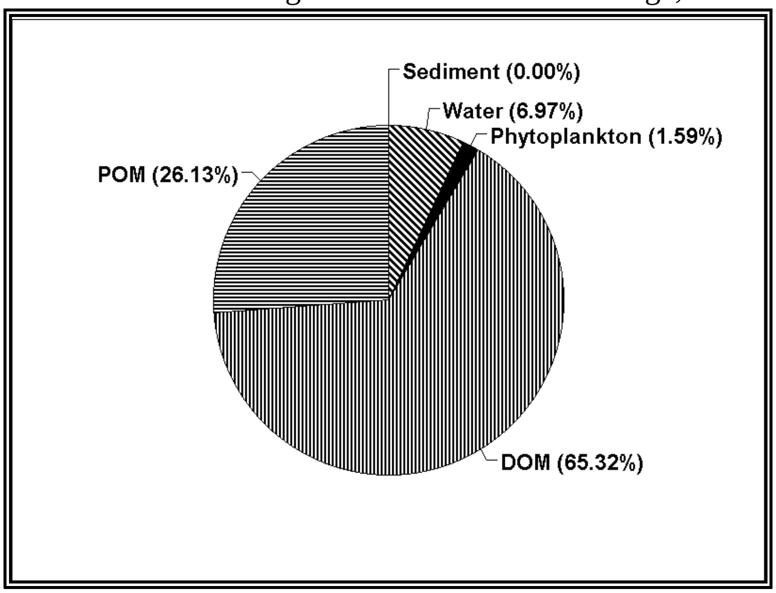
where:

Secchi = Secchi depth (m).

This relationship also could be used to back-calculate an overall Extinction coefficient if only the Secchi depth is known for a site.

As a verification of the extinction computations, the calculated and observed Secchi depths were compared for Lake George, New York. The Secchi depth is estimated to be 8.3 m in Lake George, based on site data for the various components (**Figure 33**). This compares favorably with observed values of 7.5 to 11 (Clifford, 1982).

Figure 33
Contributions to Light Extinction in Lake George, NY



Nutrient Limitation

There are several ways that nutrient limitation has been represented in models. Algae are capable of taking up and storing sufficient nutrients to carry them through several generations, and models have been developed to represent this. However, if the timing of algal blooms is not critical, intracellular storage of nutrients can be ignored, constant stoichiometry can be assumed, and the model is much simpler. Therefore, based on the efficacy of this simplifying assumption, nutrient limitation by external nutrient concentrations is used in AQUATOX, as in many other models (for example, Chen, 1970; Parker, 1972; Lassen and Nielsen, 1972; Larsen et al., 1974; Park et al., 1974; Chen and Orlob, 1975; Patten et al., 1975; Environmental Laboratory, 1982; Ambrose et al., 1991).

For an individual nutrient, saturation kinetics is assumed, using the Michaelis-Menten or Monod equation (**Figure 34**); this approach is founded on numerous studies (cf. Hutchinson, 1967):

$$PLimit = \frac{Phosphorus}{Phosphorus + KP} \tag{43}$$

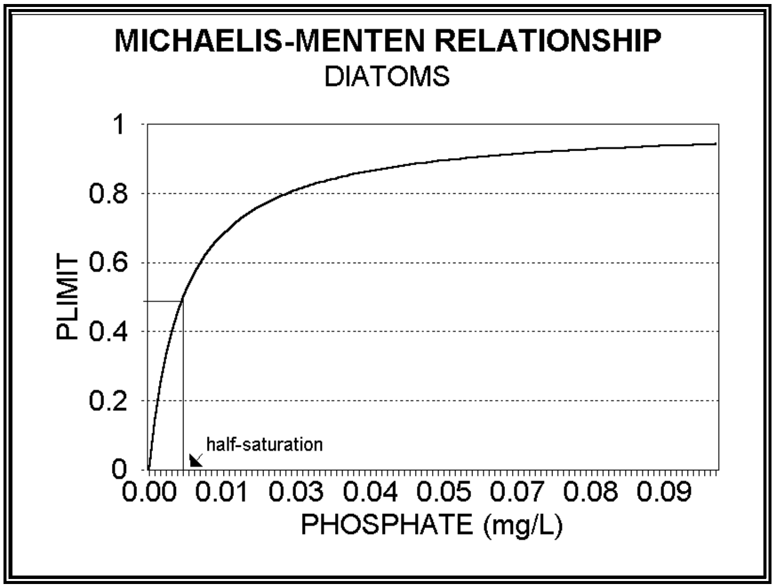
$$NLimit = \frac{Nitrogen}{Nitrogen + KN} \tag{44}$$

$$CLimit = \frac{Carbon}{Carbon + KCO2} \tag{45}$$

where:

PLimit	=	limitation due to phosphorus (unitless);
Phosphorus	=	available soluble phosphorus (gP/m^3);
KP	=	half-saturation constant for phosphorus (gP/m^3);
NLimit	=	limitation due to nitrogen (unitless);
Nitrogen	=	available soluble nitrogen (gN/m^3);
KN	=	half-saturation constant for nitrogen (gN/m^3);
CLimit	=	limitation due to inorganic carbon (unitless);
Carbon	=	available dissolved inorganic carbon (gC/m^3); and
KCO2	=	half-saturation constant for carbon (gC/m^3).

Figure 34
Nutrient Limitation



Nitrogen fixation in blue-green algae is handled by setting *NLimit* to 1.0 if *Nitrogen* is less than half the *KN* value. Otherwise, it is assumed that nitrogen fixation is not operable, and *NLimit* is computed as for the other algae.

Concentrations must be expressed in terms of the chemical element. Because carbon dioxide is computed internally, the concentration of carbon is corrected for the molar weight of the element:

$$Carbon = C2CO2 \cdot CO2 \tag{46}$$

where:

C2CO2	=	ratio of carbon to carbon dioxide (0.27); and
CO2	=	inorganic carbon (g/m^3).

Like many models (for example, Larsen et al., 1973; Baca and Arnett, 1976; Scavia et al., 1976; Smith, 1978; Bierman et al., 1980; Park et al., 1980; Johanson et al., 1980; Grenney and Kraszewski, 1981; Ambrose et al., 1991), AQUATOX uses the minimum limiting nutrient, whereby the Monod equation is evaluated for each nutrient, and the factor for the nutrient that is most limiting at a particular time is used:

$$NutrLimit = \min(PLimit, NLimit, CLimit) \tag{47}$$

where:

NutrLimit = reduction due to limiting nutrient (unitless).

Alternative formulations used in other models include multiplicative and harmonic-mean constructs, but the minimum limiting nutrient construct is well-founded in laboratory studies with individual species.

Current Limitation

Because they are fixed in space, periphyton also are limited by slow currents that do not replenish nutrients and carry away senescent biomass. Based on the work of McIntire (1973) and Colby and McIntire (1978), a factor relating photosynthesis to current velocity is used for periphyton:

$$VLimit = \min(1,\ RedStillWater + \frac{VelCoeff \cdot Velocity}{1 + VelCoeff \cdot Velocity}) \tag{48}$$

where:

VLimit = limitation or enhancement due to current velocity (unitless);
RedStillWater = reduction in photosynthesis in absence of current (unitless);
VelCoeff = empirical proportionality coefficient for velocity (0.057, unitless);

and

Velocity = flow rate (converted to m/s), see **(14)**.

VLimit has a minimum value for photosynthesis in the absence of currents and increases asymptotically to a maximum value for optimal current velocity (?). In high currents scour can limit periphyton; see **(67)**. The value of *RedStillWater* depends on the circumstances under which the maximum photosynthesis rate was measured; if *PMax* was measured in still water then *RedStillWater* = 1, otherwise a value of 0.2 is appropriate (Colby and McIntire, 1978).

Adjustment for Suboptimal Temperature

AQUATOX uses a general but complex formulation to represent the effects of temperature. All organisms exhibit a nonlinear, adaptive response to temperature changes (the so-called Stroganov function). Process rates other than algal respiration increase as the ambient temperature increases until the optimal temperature for the organism is reached; beyond that optimum, process rates decrease until the lethal temperature is reached. This effect is represented by a complex algorithm developed by O'Neill et al. (1972) and modified slightly for application to aquatic systems (Park et al., 1974). An intermediate variable *VT* is computed first; it is the ratio of the difference between the maximum temperature at which a process will occur and the ambient temperature over the difference between the maximum temperature and the optimal temperature for the process:

$$VT = \frac{(TMax + Acclimation) - Temperature}{(TMax + Acclimation) - (TOpt + Acclimation)} \quad \textbf{(49)}$$

where:

Temperature = ambient water temperature (°C);
TMax = maximum temperature at which process will occur (°C);
TOpt = optimal temperature for process to occur (°C); and
Acclimation = temperature acclimation (°C), as described below.

Acclimation to both increasing and decreasing temperature is accounted for with a modification developed by Kitchell et al. (1972):

$$Acclimation = XM \cdot [1 - e^{(-KT \cdot ABS(Temperature - TRef))}] \quad \textbf{(50)}$$

where:

XM = maximum acclimation allowed (°C);
KT = coefficient for decreasing acclimation as temperature approaches T_{ref} (unitless);
ABS = function to obtain absolute value; and
TRef = "adaptation" temperature below which there is no acclimation (°C).

The mathematical sign of the variable *Acclimation* is negative if the ambient temperature is below the temperature at which there is no acclimation; otherwise, it is positive.

If the variable *VT* is less than zero, in other words, if the ambient temperature exceeds (*TMax* + *Acclimation*), then the suboptimal factor for temperature is set equal to zero and the process stops. Otherwise, the suboptimal factor for temperature is calculated as (Park et al., 1974):

$$TCorr = VT^{XT} \cdot e^{(XT \cdot (1 - VT))} \quad \textbf{(51)}$$

where:
TCorr = limitation due to suboptimal temperature (unitless); and

$$XT = \frac{WT^2 \cdot (1 + \sqrt{1 + 40/YT}\ )^2}{400} \quad \textbf{(52)}$$

where:

$$WT = \ln(Q10) \cdot ((TMax + Acclimation) - (TOpt + Acclimation)) \tag{53}$$

and

$$YT = \ln(Q10) \cdot ((TMax + Acclimation) - (TOpt + Acclimation) + 2) \tag{54}$$

where:

Q10 = slope or rate of change per 10°C temperature change (unitless).

This well-founded, robust algorithm for *TCorr* is used in AQUATOX to obtain reduction factors for suboptimal temperatures for all biologic processes in animals and plants, with the exception of algal respiration. By varying the parameters, organisms with both narrow and broad temperature tolerances can be represented (**Figure 35**, **Figure 36**).

Figure 35
Temperature Response of Blue-Greens

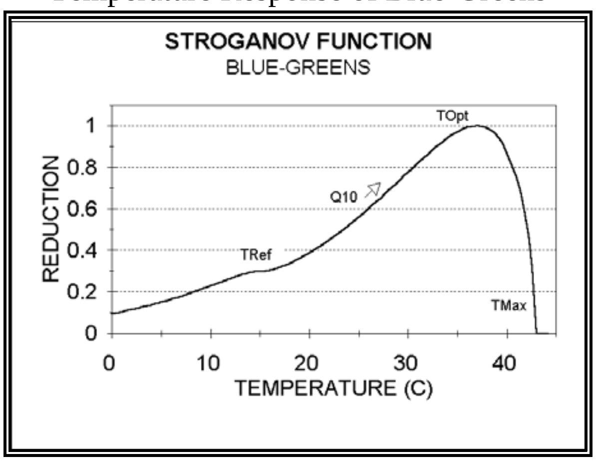
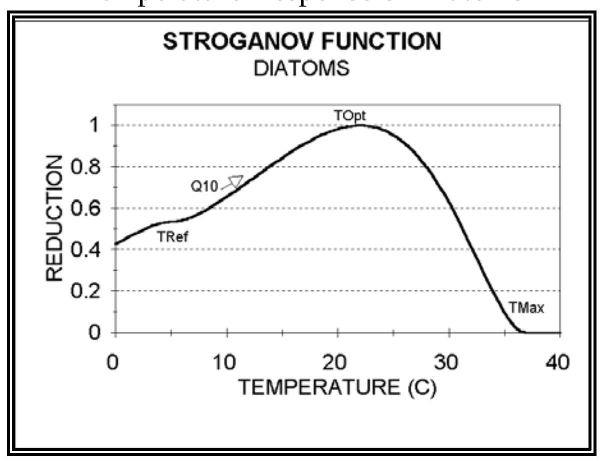


Figure 36
Temperature Response of Diatoms



Algal Respiration

Endogenous or dark respiration is the metabolic process whereby oxygen is taken up by plants for the production of energy for maintenance and carbon dioxide is released (Collins and Wlosinski, 1983). Although it is normally a small loss rate for the organisms, it has been shown to be exponential with temperature (Aruga, 1965). Riley (1963, see also Groden, 1977) derived an equation representing this relationship. Based on data presented by Collins (1980), maximum respiration is constrained to 60% of photosynthesis. Laboratory experiments in support of the CLEANER model confirmed the empirical relationship and provided additional evidence of the correct parameter values (Collins, 1980), as demonstrated by **Figure 37**:

$$Respiration = Resp0 \cdot e^{(TResp \cdot Temperature)} \cdot Biomass \tag{55}$$

where:

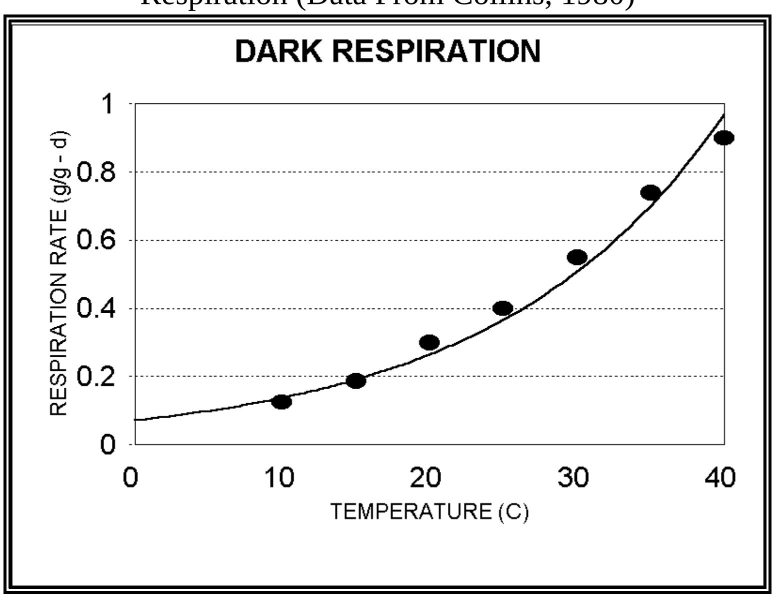
Respiration	=	dark respiration (g/m^{3}"d);
Resp0	=	respiration rate at 0/C (g/g"d);
TResp	=	exponential temperature coefficient (0.065//C);
Temperature	=	ambient water temperature (/C); and
Biomass	=	plant biomass (g/m^3).

This construct also applies to macrophytes. The values for *Resp0* are given in Table 6.

Table 6. Values for respiration rate at 0/C.

Plant group	***Resp0***	**Reference**
Diatoms	0.022	LeCren & Lowe-McConnell, 1980, p. 189
Greens	0.006	LeCren & Lowe-McConnell, 1980, p. 189
Blue-greens	0.072	Collins, 1980
Other algae	0.006	arbitrarily set to the same as greens
Macrophytes	0.015	LeCren & Lowe-McConnell, 1980, p. 195

Figure 37
Respiration (Data From Collins, 1980)



Photorespiration and Excretion

Photorespiration, with the release of carbon dioxide and the concomitant excretion of dissolved organic material, occurs in the presence of light. Environmental conditions that inhibit cell division but still allow photoassimilation result in release of organic compounds. This is especially true for both low and high levels of light (Fogg et al., 1965; Watt, 1966; Nalewajko, 1966; Collins, 1980). AQUATOX uses an equation modified from one by Desormeau (1978) that is the inverse of the light limitation:

$$Excretion = KResp \cdot LightStress \cdot Photosynthesis \qquad \textbf{(56)}$$

where:

Excretion	=	release of photosynthate (g/m^3·d);
KResp	=	coefficient of proportionality between excretion and photosynthesis at optimal light levels (unitless); and
Photosynthesis	=	photosynthesis (g/m^3·d), see **(31)**,

and where:

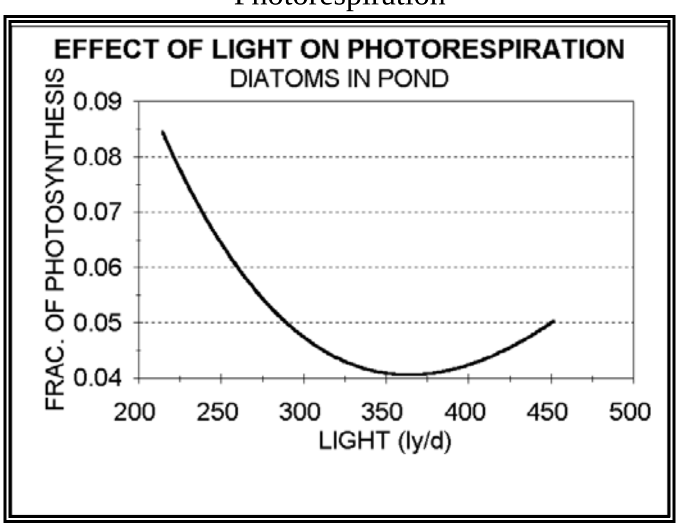
$$LightStress = 1 - LtLimit \qquad \textbf{(57)}$$

where:

LtLimit= light limitation for a given plant (unitless), see **(34)**.

It is a continuous function (**Figure 38**) and has a tendency to overestimate excretion slightly at light levels close to light saturation where experimental evidence suggests a constant relationship (Collins, 1980). The construct for photorespiration also applies to macrophytes.

Figure 38
Photorespiration



Algal Mortality

Nonpredatory algal mortality can occur as a response to toxic chemicals (discussed in **Chapter 8**) and as a response to unfavorable environmental conditions. Phytoplankton under stress may suffer greatly increased mortality due to autolysis and parasitism (Harris, 1986). Therefore, most phytoplankton decay occurs in the water column rather than in the sediments (DePinto, 1979). The rapid remineralization of nutrients in the water column may result in a succession of blooms (Harris, 1986). Sudden changes in the abiotic environment may cause the algal population to crash; stressful changes include nutrient depletion, unfavorable temperature, and damage by light (LeCren and Lowe-McConnell, 1980). These are represented by a mortality term in AQUATOX that includes toxicity, high temperature (Scavia and Park, 1976), and combined nutrient and light limitation (Collins and Park, 1989):

$$Mortality = (KMort + ExcessT + Stress) \cdot Biomass + Poisoned \qquad \textbf{(58)}$$

where:

Mortality	=	nonpredatory mortality (g/m^3"d);
Poisoned	=	mortality rate due to toxicant (g/m^3"d), see ((287));
KMort	=	intrinsic mortality rate (g/g"d); and
Biomass	=	plant biomass (g/m^3),

and where:

$$ExcessT = \frac{e^{(Temperature - TMax)}}{2} \qquad \textbf{(59)}$$

and:

$$Stress = 1 - e^{-EMort \cdot (1 - (NutrLimit \cdot LtLimit))} \qquad \textbf{(60)}$$

where:

ExcessT	=	factor for high temperatures (g/g"d);
TMax	=	maximum temperature tolerated (/ C);
Stress	=	factor for suboptimal light and nutrients (g/g"d),
Emort	=	approximate maximum fraction killed per day with total limitation (g/g"d);
NutrLimit	=	reduction due to limiting nutrient (unitless), see (47)
LtLimit	=	light limitation (unitless), see (34).

Exponential functions are used so that increasing stress leads to rapid increases in mortality, especially with high temperature where mortality is 50% per day at the *TMax* (**Figure 39**), and, to a much lesser degree, with suboptimal nutrients and light (**Figure 40**). This simulated process is responsible in part for maintaining realistically high levels of detritus in the simulated water body. Low temperatures are assumed not to affect algal mortality.

Figure 39
Mortality Due To High Temperatures

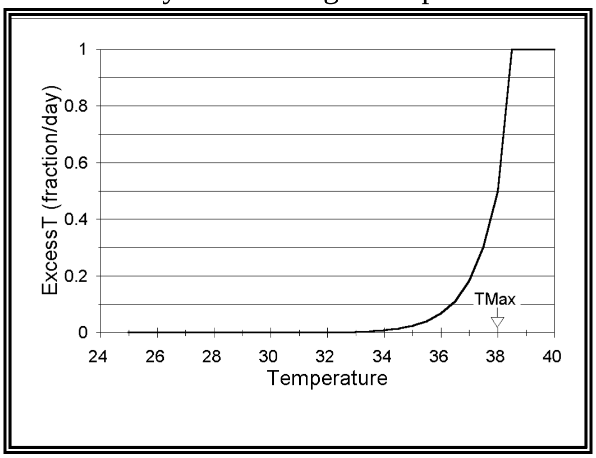
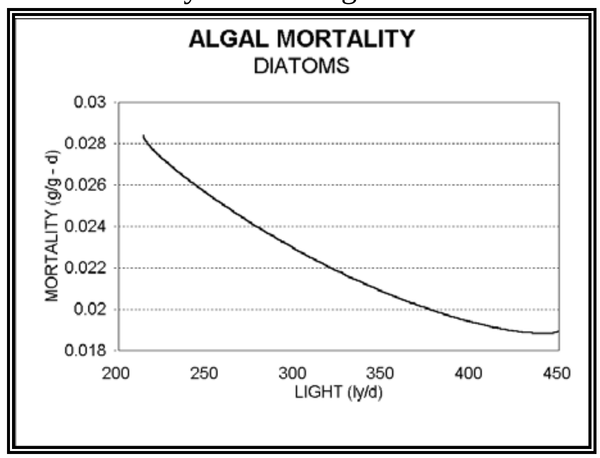


Figure 40
Mortality Due To Light Limitation



Sinking

Sinking of phytoplankton, either between layers or to the bottom sediments, is modeled as a function of physiological state, similar to mortality. Phytoplankton that are not stressed are considered to sink at given rates, which are based on field observations and implicitly account for the effects of averaged water movements (cf. Scavia, 1980). Sinking also is represented as being impeded by turbulence associated with higher discharge (but only when discharge exceeds mean discharge):

$$Sink = \frac{KSed}{Depth} \cdot \frac{MeanDischarge}{Discharge} \cdot SedAccel \cdot Biomass \tag{61}$$

where:

Sink	=	phytoplankton loss due to settling (g/m^{3}"d);
KSed	=	intrinsic settling rate (m/d);
Depth	=	depth of water or, if stratified, thickness of layer (m);
MeanDischarge	=	mean annual discharge (m^3/d);
Discharge	=	daily discharge (m^3/d), see Table 1; and
Biomass	=	phytoplankton biomass (g/m^3).

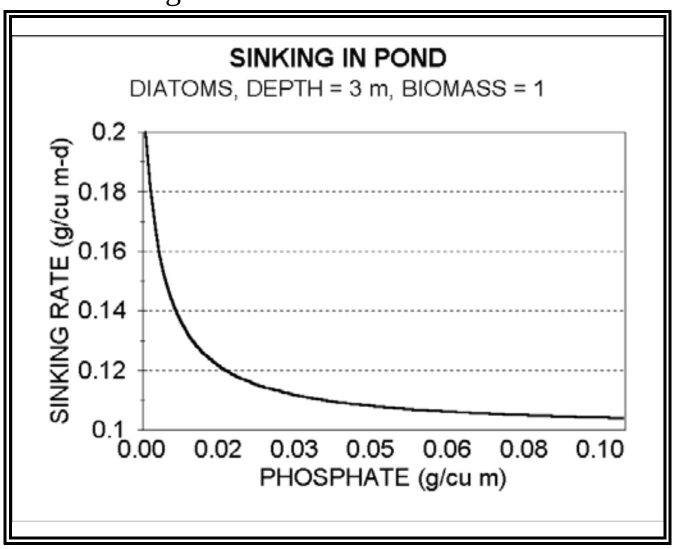
The model is able to mimic high sedimentation loss associated with the crashes of phytoplankton blooms, as discussed by Harris (1986). As the phytoplankton are stressed by toxicants and suboptimal light, nutrients, and temperature, the model computes an exponential increase in sinking (**Figure 41**), as observed by Smayda (1974), and formulated by Collins and Park (1989):

$$SedAccel = e^{ESed \cdot (1 - LtLimit \cdot NutrLimit \cdot TCorr \cdot FracPhoto)} \quad \textbf{(62)}$$

where:

SedAccel	=	increase in sinking due to physiological stress (unitless);
ESed	=	exponential settling coefficient (unitless);
LtLimit	=	light limitation (unitless), see **(33)**;
NutrLimit	=	nutrient limitation (unitless), see **(47)**; and
FracPhoto	=	reduction factor for effect of toxicant on photosynthesis (unitless), see **(294)**;
TCorr	=	temperature limitation (unitless), see **(51)**.

Figure 41
Sinking as a Function of Nutrient Stress



Washout and Sloughing

Phytoplankton are subject to downstream drift. In streams and in lakes and reservoirs with low retention times this may be a significant factor in reducing or even precluding phytoplankton populations (LeCren and Lowe-McConnell, 1980). The process is modeled as a simple function of discharge:

$$Washout_{phytoplankton} = \frac{Discharge}{Volume} \cdot Biomass \quad \textbf{(63)}$$

where:

$Washout_{Phytoplankton}$	=	loss due to downstream drift (g/m^3"d);
$Discharge$	=	daily discharge (m^3/d);
$Volume$	=	volume of site (m^3); and
$Biomass$	=	biomass of phytoplankton (g/m^3).

Periphyton often exhibit a pattern of buildup and then a sharp decline in biomass due to sloughing. Based on extensive experimental data from Walker Branch, Tennessee (Rosemond, 1993), a complex sloughing formulation, extending the approach of Asaeda and Son (2000), was implemented. This function was able to represent a wide range of conditions (**Figure 42** and **Figure 43**):

$$Washout_{Periphyton} = Slough + Dislodge_{Peri,Tox} \qquad \textbf{(64)}$$

where:

$Washout_{Periphyton}$	=	loss due to sloughing (g/m^3"d);
$Slough$	=	loss due to natural causes (g/m^3"d), see **(67)**; and
$Dislodge_{peri,\ Tox}$	=	loss due to toxicant-induced sloughing (g/m^3"d), see **(300)**.

Figure 42. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of both N and P and removal of grazers in Spring, 1989.

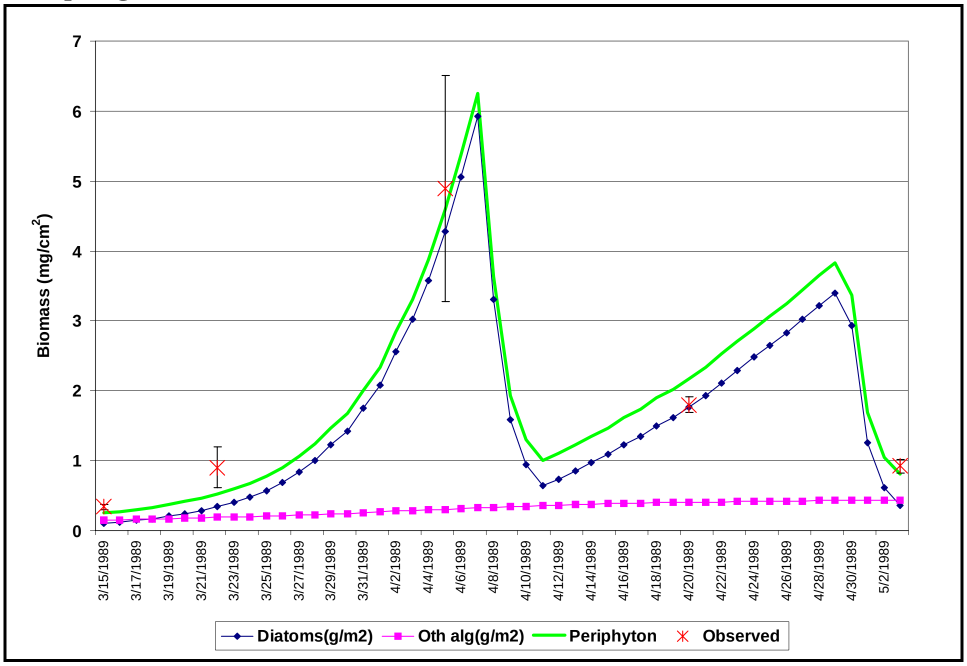
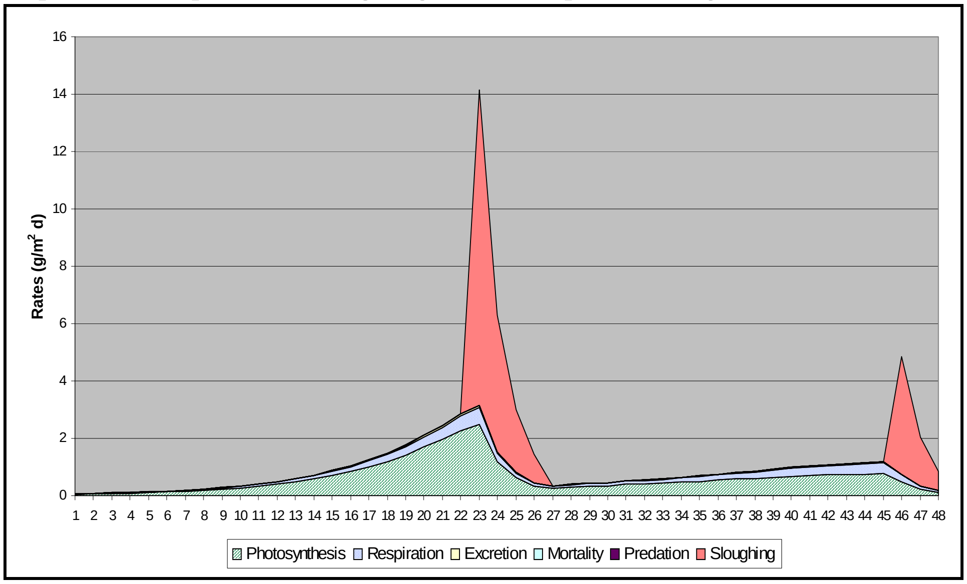


Figure 43. Predicted rates for diatoms in Walker Branch, Tennessee, with addition of both N and P and removal of grazers in Spring, 1989. Note the importance of periodic sloughing. Rates expressed as g/m^2 d.



Natural sloughing is a function of senescence due to suboptimal conditions and the drag force of currents acting on exposed biomass. Drag increases as both biomass and velocity increase:

$$DragForce = Rho \cdot DragCoeff \cdot Vel^2 \cdot (BioVol \cdot UnitArea)^{2/3} \cdot 1E{-}6 \qquad \textbf{(65)}$$

where:

DragForce	=	drag force (kg m/s^2);
Rho	=	density (kg/m^3);
DragCoeff	=	drag coefficient (2.53E-4, unitless);
Vel	=	velocity (converted to m/s) see **(14)**;
BioVol	=	biovolume of algae (mm^3/mm^2);
UnitArea	=	unit area (mm^2);
1E-6	=	conversion factor (m^2/mm^2).

Biovolume is not modeled directly by AQUATOX, so a simplifying assumption is that the empirical relationship between biomass and biovolume is constant for a given growth form, based on observed data from Rosemond (1993):

$$Biovol_{Dia} = \frac{Biomass}{2.08\mathrm{E}{-}9} \qquad \textbf{(66)}$$
$$Biovol_{Fil} = \frac{Biomass}{8.57\mathrm{E}{-}9}$$

where:

$Biovol_{Dia}$	=	biovolume of diatoms (mm^3/mm^2);
$Biovol_{Fil}$	=	biovolume of filamentous algae (mm^3/mm^2);
$Biomass$	=	biomass of given algal group (g/m^2).

Suboptimal light, nutrients, and temperature cause senescence of cells that bind the periphyton and keep them attached to the substrate. This effect is represented by a factor, *Suboptimal*, which is computed in modeling the effects of environmental conditions on photosynthesis. *Suboptimal* decreases the critical force necessary to cause sloughing. If the drag force exceeds the critical force for a given algal group modified by the *Suboptimal* factor and an adaptation factor, then sloughing occurs:

$$\begin{aligned} &\text{If } DragForce > Suboptimal_{Org} \cdot FCrit_{Org} \cdot Adaptation \\ &\quad \text{then } Slough = Biomass \cdot FracSloughed \\ &\quad \text{else } Slough = 0 \end{aligned} \tag{67}$$

where:

$Suboptimal_{Org}$	=	factor for suboptimal nutrient, light, and temperature effect on senescence of given periphyton group (unitless);
$FCrit_{Org}$	=	critical force necessary to dislodge given periphyton group (kg m/s^2);
$Adaptation$	=	factor to adjust for mean discharge of site compared to reference site (unitless);
$Slough$	=	biomass lost by sloughing (g/m^3);
$FracSloughed$	=	fraction of biomass lost at one time (97%, unitless).

$$\begin{aligned} &Suboptimal_{Org} = NutrLimit_{Org} \cdot LtLimit_{Org} \cdot TCorr \\ &\text{If } Suboptimal_{Org} > 1 \text{ then } Suboptimal_{Org} = 1 \end{aligned} \tag{68}$$

where:

$NutrLimit$	=	nutrient limitation for given algal group (unitless) computed by AQUATOX; see **(47)**;
$LtLimit_{Org}$	=	light limitation for given algal group (unitless) computed by AQUATOX; see **(33)**; and
$TCorr$	=	temperature limitation for a given algal group (unitless) computed by AQUATOX; see **(51)**.

The sloughing construct was tested and calibrated (U.S. E.P.A., 2001) with data from experiments with artificial and woodland streams in Tennessee (Rosemond, 1993, **Figure 42**). However, in modeling periphyton at several sites, it was observed that sloughing appears to be triggered at greatly differing mean velocities. The working hypothesis is that periphyton adapt to the ambient conditions of a particular channel. Therefore, a factor is included to adjust for the mean discharge of a given site compared to the reference site in Tennessee. It is still necessary to calibrate

FCrit for each site to account for intangible differences in channel and flow conditions, analogous to the calibration of shear stress by sediment modelers, but the range of calibration needed is reduced by the *Adaptation* factor:

$$Adaptation = \frac{MeanDischarge}{RefDischarge} \qquad \textbf{(69)}$$

where:

MeanDischarge	=	mean discharge for given site, computed over the period of the simulation (m^3/d);
RefDischarge	=	mean discharge for reference experimental stream (3.5 m^3/d).

Detrital Accumulation in Periphyton

In phytoplankton, mortality results in immediate production of detritus, and that transfer is modeled. However, for purposes of modeling, periphyton are defined as including associated detritus. The accumulation of non-living biomass is modeled implicitly by not simulating mortality due to suboptimal conditions. Rather, in the simulation biomass builds up, causing increased self-shading, which in turn makes the periphyton more vulnerable to sudden loss due to sloughing. The fact that part of the biomass is non-living is ignored as a simplification of the model.

Chlorophyll *a*

Chlorophyll *a* is not simulated directly. However, because chlorophyll *a* is commonly measured in aquatic systems and because water quality managers are accustomed to thinking of it as an index of water quality, the model converts phytoplankton biomass estimates into approximate values for chlorophyll *a*. The ratio of carbon to chlorophyll *a* exhibits a wide range of values depending on the nutrient status of the algae (Harris, 1986); blue-green algae often have higher values (cf. Megard et al., 1979). AQUATOX uses a value of 45 μgC/μg chlorophyll *a* for blue-greens and a value of 28 for other phytoplankton as reported in the documentation for WASP (Ambrose et al., 1991). The values are more representative for blooms than for static conditions, but managers are usually most interested in the maxima. The results are presented as total chlorophyll *a* in μg/L; therefore, the computation is:

$$ChlA = \left(\frac{\sum_{Biomass_{BlGr}} \cdot CToOrg}{45} + \frac{\sum_{Biomass_{others}} \cdot CToOrg}{28} \right) \cdot 1000 \qquad \textbf{(70)}$$

where:

ChlA	=	biomass as chlorophyll *a* (μg/L);
$Biomass_{BlGr}$	=	biomass of blue-green algae (mg/L);

$Biomass_{others}$	=	biomass of algae other than blue-greens (mg/L);
$CToOrg$	=	ratio of carbon to biomass (0.526, unitless); and
1000	=	conversion factor for mg to :g (unitless).

Periphytic chlorophyll *a* is computed as a linear conversion from the ash-free dry weight (AFDW) of periphyton; because periphyton can collect inorganic sediments, it is important to measure and model it as AFDW. All biomass computations in AQUATOX are as AFDW. The conversion factor is based on the observed average ratio of chlorophyll a to AFDW for the Cahaba River near Birmingham, Alabama (unpub. data).

$$Perichlor = \Sigma_{Peri} PeriConv \cdot Biomass_{Peri} \qquad \textbf{(71)}$$

where:

$PeriChlor$	=	periphytic chlorophyll *a* (mg/m^2);
$PeriConv$	=	conversion from periphyton AFDW to chlorophyll *a* (6.1 mg/m^2: g/m^2);
$Biomass_{Peri}$	=	biomass of given periphyton (AFDW in g/m^2).

4.2 Macrophytes

Submersed aquatic vegetation or macrophytes can be an important component of shallow aquatic ecosystems. It is not unusual for the majority of the biomass in an ecosystem to be in the form of macrophytes during the growing season. Seasonal macrophyte growth, death, and decomposition can affect nutrient cycling, and detritus and oxygen concentrations. By forming dense cover, they can modify habitat and provide protection from predation for invertebrates and smaller fish (Howick et al., 1993); this function is represented in AQUATOX (see **Figure 49**). Macrophytes also provide direct and indirect food sources for many species of waterfowl, including swans, ducks, and coots (Jupp and Spence, 1977b).

AQUATOX represents macrophytes as occupying the littoral zone, that area of the bottom surface that occurs within the euphotic zone (see **(11)** for computation). Similar to periphyton, the compartment has units of g/m^2. In nature, macrophytes can be greatly reduced if phytoplankton blooms or higher levels of detritus increase the turbidity of the water (cf. Jupp and Spence, 1977a). Because the depth of the euphotic zone is computed as a function of the extinction coefficient **(11)**, the area predicted to be occupied by macrophytes can increase or decrease depending on the clarity of the water.

The macrophyte equations are based on submodels developed for the International Biological Program (Titus et al., 1972; Park et al., 1974) and CLEANER models (Park et al., 1980) and for the Corps of Engineers' CE-QUAL-R1 model (Collins et al., 1985):

$$\frac{dBiomass}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation - Breakage \tag{72}$$

and:

$$Photosynthesis = PMax \cdot LtLimit \cdot TCorr \cdot Biomass \cdot FracLittoral \cdot NutrLimit \cdot FracPhoto \cdot HabitatLimit \tag{73}$$

where:

dBiomass/dt	=	change in biomass with respect to time (g/m^2·d);
Loading	=	loading of macrophyte, usually used as a "seed" in the simulation; may be a moderate value if there is rapid regrowth from rhizomes following breakage or die-back (g/m^2·d);
Photosynthesis	=	rate of photosynthesis (g/m^2·d);
Respiration	=	respiratory loss (g/m^2·d), see **(55)**;
Excretion	=	excretion or photorespiration(g/m^2·d), see **(56)**;
Mortality	=	nonpredatory mortality (g/m^2·d), see **(74)**;
Predation	=	herbivory (g/m^2·d), see **(86)**;
Breakage	=	loss due to breakage (g/m^2·d), see **(75)**;
PMax	=	maximum photosynthetic rate (1/d);
LtLimit	=	light limitation (unitless), see **(34)**;
TCorr	=	correction for suboptimal temperature (unitless), see **(51)**;
HabitatLimit	=	in streams, habitat limitation based on plant habitat preferences (unitless), see **(13)**;
FracLittoral	=	fraction of bottom that is in the euphotic zone (unitless) see **(11)**; and
NutrLimit	=	nutrient limitation for bryophytes only (unitless), see **(47)**;
FracPhoto	=	reduction factor for effect of toxicant on photosynthesis (unitless), see **(294)**.

They share many of the constructs with the algal submodel described above. Temperature limitation is modeled similarly, but with different parameter values. Light limitation also is handled similarly, using the Steele (1962) formulation; the application of this equation has been verified with laboratory data (Collins et al., 1985). Periphyton are epiphytic in the presence of macrophytes; by growing on the leaves they contribute to the light extinction for the macrophytes (Sand-Jensen, 1977). Extinction due to periphyton biomass is computed in AQUATOX, by inclusion in *LtLimit*. Nutrient limitation is not modeled at this time except for bryophytes because most macrophytes can obtain their nutrients from bottom sediments (Bristow and Whitcombe, 1971; Nichols and Keeney, 1976; Barko and Smart, 1980).

Simulation of respiration and excretion utilize the same equations as algae; excretion results in "nutrient pumping" because the nutrients are assumed to come from the sediments but are excreted to the water column. (Because nutrients are not explicitly modeled in bottom sediments, this can result in loss of mass balance, particularly in shallow ponds. This will be addressed in a future version.) Non-predatory mortality is modeled similarly to algae as a function of suboptimal temperature (but not light). However, mortality is a function of low as well as high temperatures, and winter die-back is represented as a result of this control; the response is the inverse of the temperature limitation (**Figure 44**):

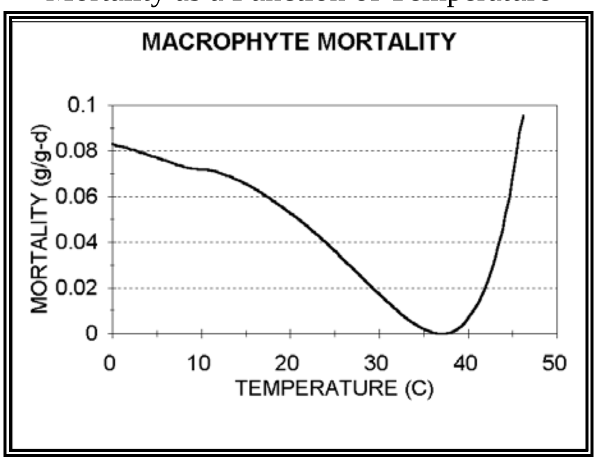
$$Mortality = [KMort + Poisoned + (1 - e^{-EMort \cdot (1 - TCorr)})] \cdot Biomass \qquad \textbf{(74)}$$

where:

KMort	=	intrinsic mortality rate (g/g"d);
Poisoned	=	mortality rate due to toxicant (g/g"d) **(287)**, and
EMort	=	maximum mortality due to suboptimal temperature (g/g"d).

Sloughing of dead leaves can be a significant loss (LeCren and Lowe-McConnell, 1980); it is simulated as an implicit result of mortality (**Figure 44**).

Figure 44
Mortality as a Function of Temperature



Macrophytes are subject to breakage due to higher water velocities; this breakage of live material is different from the sloughing of dead leaves. Although breakage is a function of shoot length and growth form as well as currents (Bartell et al., 2000; Hudon et al., 2000), a simpler construct was developed for AQUATOX (**Figure 45**):

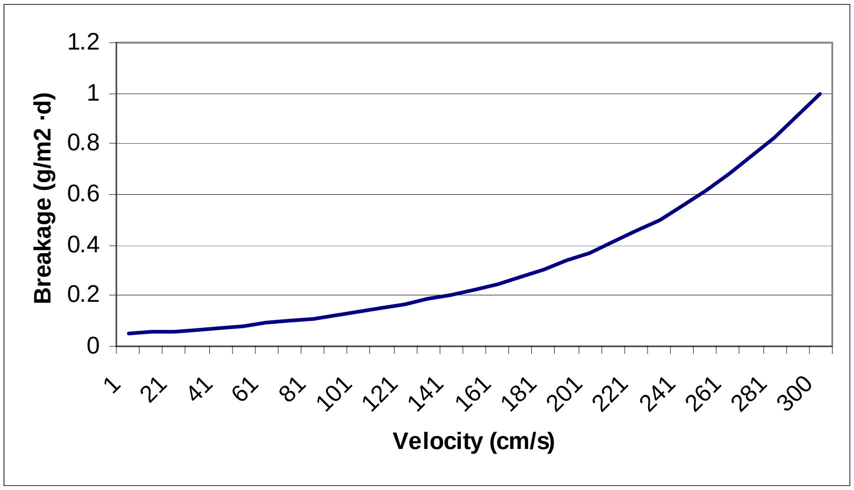
$$Breakage = \frac{Velocity - VelMax}{Gradual \cdot UnitTime} \cdot Biomass \qquad \textbf{(75)}$$

where:

Breakage	=	macrophyte breakage (g/m^2 "d);

Velocity = current velocity (cm/s) see (14);
VelMax = velocity at which total breakage occurs (cm/s);
Gradual = velocity scaling factor (20 cm/s);
UnitTime = unit time for simulation (1 d);
Biomass = macrophyte biomass (g/m^2).

Figure 45. Breakage of macrophytes as a function of current velocity; *VelMax* set to 300 cm/s.



At this time there is no provision for computing velocity due to wave action, so that macrophyte biomass may be overestimated in water bodies where there is significant wave action.

Bryophytes (mosses and liverworts) are a special class of macrophytes that attach to hard substrates, are stimulated by and take up nutrients directly from the water, are resistant to breakage, and decompose very slowly (Stream Bryophyte Group, 1999). Nutrient limitation is enabled when the "Bryophytes" plant type is selected, just as it is for algae. The model assumes that when a bryophyte breaks or dies the result is 75% particulate and 25% dissolved refractory detritus; in contrast, other macrophytes are assumed to yield 38% particulate and 24% dissolved labile detritus and the rest (38%) as refractory detritus. All other differences between bryophytes and other macrophytes in AQUATOX are based on differences in parameter values. These include low saturating light levels, low optimum temperature, very low mortality rates, moderate resistance to breakage, and resistance to herbivory (Arscott et al., 1998; Stream Bryophyte Group, 1999). Because in the field it is difficult to separate bryophyte chlorophyll from that of periphyton, it is computed so that the two can be combined and related to field values:

$$MossChlor = \Sigma(BryoConv \cdot Biomass_{Bryo}) \qquad \textbf{(76)}$$

where:

MossChlor = bryophytic chlorophyll *a* (mg/m^2);

BryoConv	=	conversion from bryophyte AFDW to chlorophyll *a* (8.9 mg/m^2: g/m^2);
$Biomass_{Bryo}$	=	biomass of given bryophyte (AFDW in g/m^2).

Currents and wave agitation can both stimulate and retard macrophyte growth. These effects will be modeled in a future version. Similar to the effect on periphyton, water movement can stimulate photosynthesis in macrophytes (Westlake, 1967); the same function could be used for macrophytes as for periphyton, although with different parameter values. Jupp and Spence (1977b) have shown that wave agitation can severely limit macrophytes; time-varying breakage eventually will be modeled when wave action is simulated.

4.3 Animals

Zooplankton, benthic invertebrates, benthic insects, and fish are modeled, with only slight differences in formulations, with a generalized animal submodel that is parameterized to represent different groups:

$$\begin{aligned}\frac{dBiomass}{dt} = \; & Load + Consumption - Defecation - Respiration \\ & - Excretion - Mortality - Predation - GameteLoss \\ & - Washout \pm Migration - Promotion + Recruit - Entrainment\end{aligned} \qquad \textbf{(77)}$$

where:

dBiomass/dt	=	change in biomass of animal with respect to time (g/m^3"d);
Load	=	biomass loading, usually from upstream (g/m^3"d);
Consumption	=	consumption of food (g/m^3"d), see **(85)**;
Defecation	=	defecation of unassimilated food (g/m^3"d), see **(84)**;
Respiration	=	respiration (g/m^3"d), see **(87)**;
Excretion	=	excretion (g/m^3"d), see **(97)**;
Mortality	=	nonpredatory mortality (g/m^3"d), see **(98)**;
Predation	=	predatory mortality (g/m^3"d), see **(86)**;
GameteLoss	=	loss of gametes during spawning (g/m^3"d), see **(102)**;
Washout	=	loss due to being carried downstream by washout and drift (g/m^3"d), see **(105)** and **(106)**;
Migration	=	loss (or gain) due to vertical migration (g/m^3"d), see **(109)**;
Promotion	=	promotion to next size class or emergence (g/m^3"d), see **(110)**; and
Recruit	=	recruitment from previous size class or through reproduction (g/m^3"d), see **(110)**;
Entrainment	=	entrainment and downstream transport with flood waters (g/m^3"d), see **(108)**.

The change in biomass (**Figure 46**) is a function of a number of processes (**Figure 47**) that are subject to environmental factors, including biotic interactions. Similar to the way algae are treated, parameters for different species of invertebrates and fish are loaded and available for editing by means of the entry screens. Biomass of zoobenthos and fish is expressed as g/m^2 instead of g/m^3.

Figure 46. Predicted Changes in Biomass in a Stream

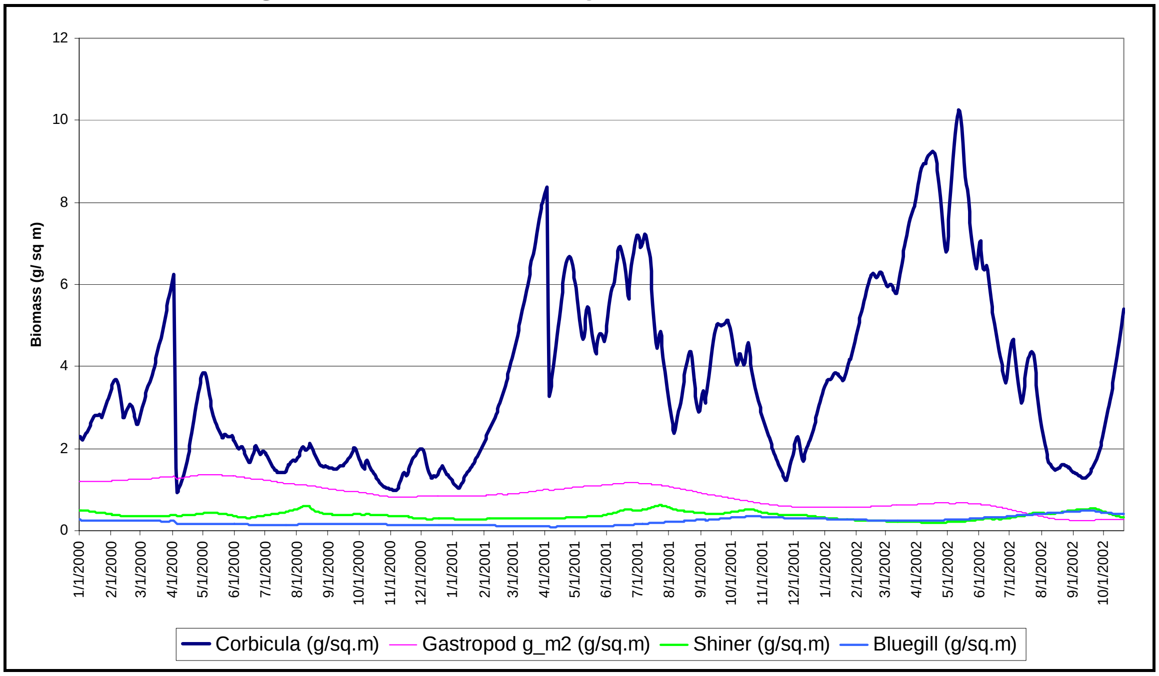
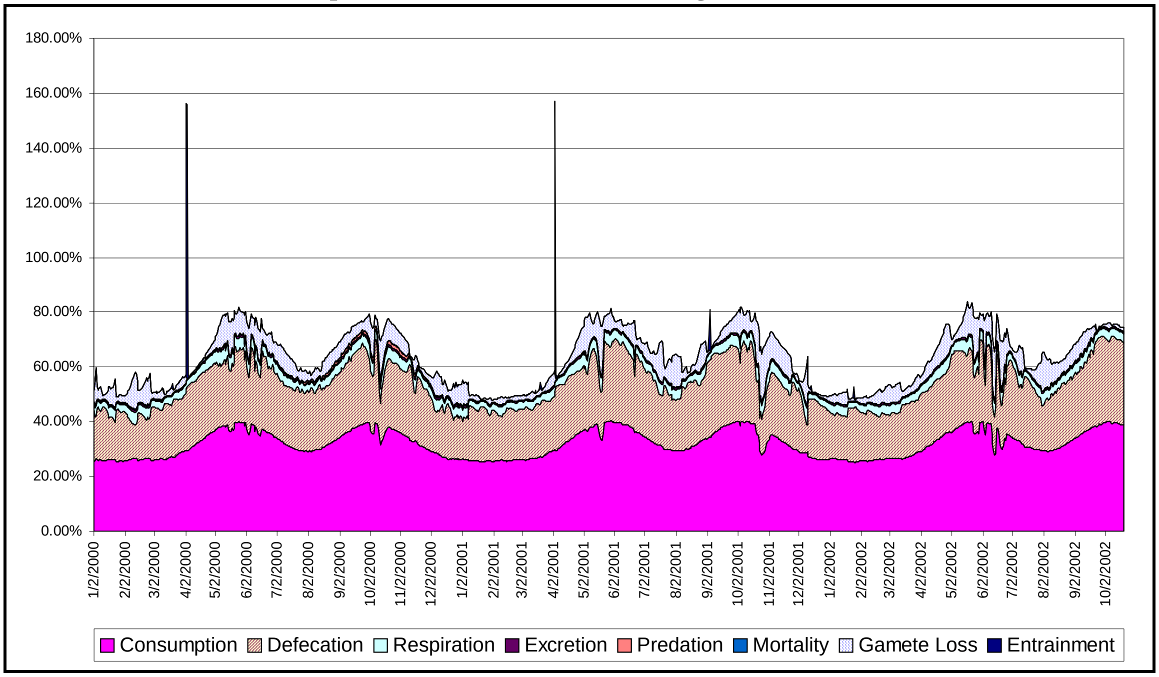


Figure 47. Predicted Process Rates for the Invasive Clam *Corbicula*, Expressed as Percent of Biomass; Spikes are Entrainment During Storm Events



Consumption, Defecation, and Predation

Several formulations have been used in various models to represent consumption of prey, reflecting the fact that there are different modes of feeding and that experimental evidence can be fit by any one of several equations (Mullin et al., 1975; Scavia, 1979; Straškraba and Gnauck, 1985).

Ingestion is represented in AQUATOX by a maximum consumption rate, adjusted for ambient food and temperature conditions, and reduced for sublethal toxicant effects and limitations due to habitat preferences of a given predator or herbivore:

$$Ingestion_{prey,\ pred} = CMax_{pred} \cdot SatFeeding \cdot TCorr_{pred} \cdot HabitatLimit \cdot ToxReduction \cdot Biomass_{pred} \qquad \textbf{(78)}$$

where:

$Ingestion_{prey,\ pred}$ = ingestion of given prey by given predator or herbivore ($g/m^3 \cdot d$);
$Biomass_{pred}$ = concentration of predator or herbivore ($g/m^3 \cdot d$);
$CMax$ = maximum feeding rate for predator or herbivore ($g/g \cdot d$);
$SatFeeding$ = saturation-feeding kinetic factor, see **(80)**;
$TCorr$ = reduction factor for suboptimal temperature (unitless), see **(51)**;
$ToxReduction$ = reduction due to effects of toxicant (see Eq. **(297)**, unitless); and

HabitatLimit = in streams, habitat limitation based on predator habitat preferences (unitless), see (13).

The maximum consumption rate is sensitive to body size, so an alternative to specifying *CMax* for fish is to compute it using an allometric equation and parameters from the Wisconsin Bioenergetics Model (Hewett and Johnson, 1992; Hanson et al., 1997):

$$CMax = CA \cdot MeanWeight^{CB} \tag{79}$$

where:

CA = maximum consumption for a 1-g fish at optimal temperature (g/g"d);
MeanWeight = mean weight for a given fish species (g);
CB = slope of the allometric function for a given fish species.

Many animals adjust their search or filtration in accordance with the concentration of prey; therefore, a saturation-kinetic term is used (Park et al., 1974, 1980; Scavia and Park, 1976):

$$SatFeeding = \frac{Preference_{prey,\,pred} \cdot Food}{\Sigma_{prey}(Preference_{prey,\,pred} \cdot Food) + FHalfSat_{pred}} \tag{80}$$

where:

Preference = preference of predator for prey (unitless);
Food = available biomass of given prey (g/m^3);
FHalfSat = half-saturation constant for feeding by a predator (g/m^3).

The food actually available to a predator may be reduced in two ways:

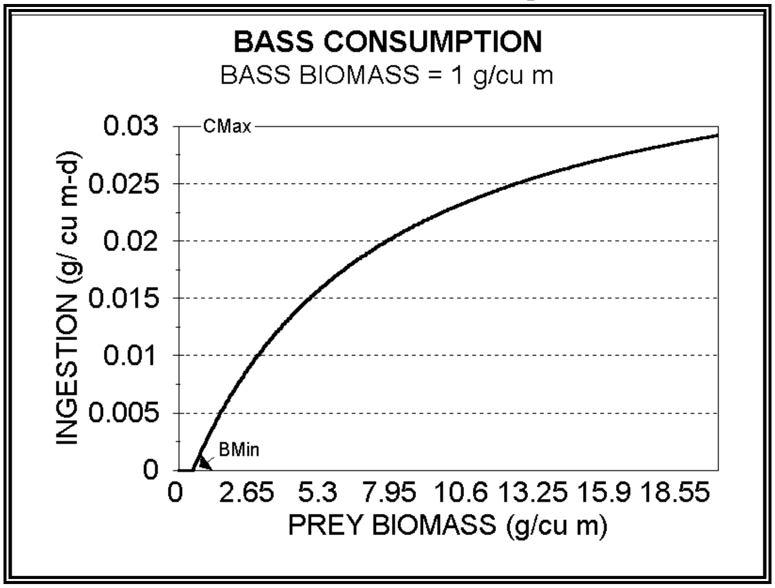
$$Food = (Biomass_{prey} - BMin_{pred}) \cdot Refuge \tag{81}$$

where:

BMin = minimum prey biomass needed to begin feeding (g/m^3); and
Refuge = reduction factor for prey hiding in macrophytes (unitless).

Search or filtration may virtually cease below a minimum prey biomass (*BMin*) to conserve energy (**Figure 48**), so that a minimum food level is incorporated (Parsons et al., 1969; Steele, 1974; Park et al., 1974; Scavia and Park, 1976; Scavia et al., 1976; Steele and Mullin, 1977). However, cladocerans (for example, *Daphnia*) must constantly filter because the filtratory appendages also serve for respiration; therefore, in these animals there is no minimum feeding level and *BMin* is set to 0.

Figure 48
Saturation-kinetic Consumption



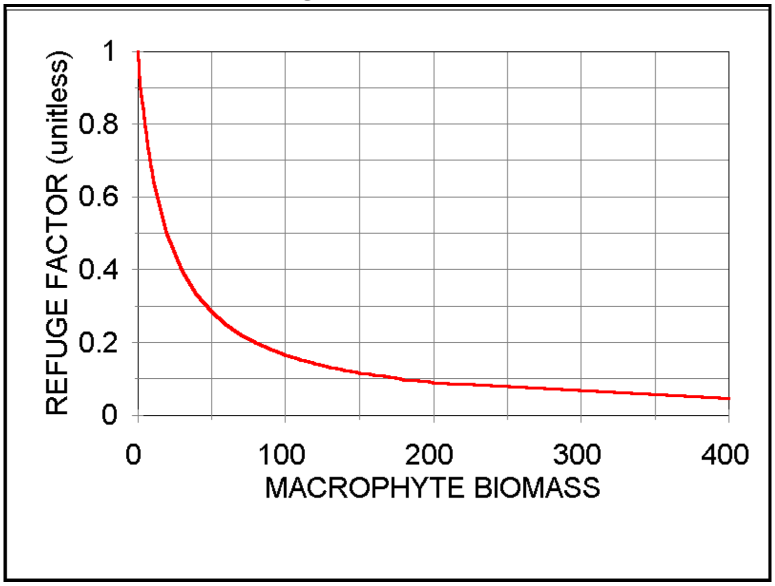
Macrophytes can provide refuge from predation; this is represented by a factor related to the macrophyte biomass that is original with AQUATOX (**Figure 49**):

$$Refuge = 1 - \frac{Biomass_{Macro}}{Biomass_{Macro} + HalfSat} \tag{82}$$

where:

HalfSat	=	half-saturation constant (20, g/m^3), and
$Biomass_{Macro}$	=	biomass of macrophyte (g/m^3).

Figure 49
Refuge From Predation



AQUATOX is a food-web model with multiple potential food sources. Passive size-selective filtering (Mullin, 1963; Lam and Frost, 1976) and active raptorial selection (Burns, 1969; Berman and Richman, 1974; Bogdan and McNaught, 1975; Brandl and Fernando, 1975) occur among aquatic organisms. Relative preferences are represented in AQUATOX by a matrix of preference parameters first proposed by O'Neill (1969) and used in several aquatic models (Bloomfield et al., 1973; Park et al., 1974; Canale et al., 1976; Scavia et al., 1976). Higher values indicate increased preference by a given predator for a particular prey compared to the preferences for all possible prey. In other words, the availability of the prey is weighted by the preference factor.

The preference factors are normalized so that if a potential food source is not modeled or is below the *BMin* value, the other preference factors are modified accordingly, representing adaptive preferences:

$$Preference_{prey,pred} = \frac{Pref_{prey,pred}}{SumPref} \tag{83}$$

where:

$Preference_{prey,pred}$	=	normalized preference of given predator for given prey (unitless);
$Pref_{prey,\ pred}$	=	initial preference value from the animal parameter screen (unitless); and

SumPref	=	sum of preference values for all food sources that are present above the minimum biomass level for feeding during a particular time step (unitless).

Similarly, different prey types have different potentials for assimilation by different predators. The fraction of ingested prey that is egested as feces or discarded (and which is treated as a source of detritus by the model, see **(124)**), is indicated by a matrix of egestion coefficients with the same structure as the preference matrix, so that defecation is computed as (Park et al., 1974):

$$Defecation_{pred} = \Sigma_{prey} (EgestCoeff_{prey,\ pred} + IncrEgest) \cdot Ingestion_{prey,\ pred} \tag{84}$$

where:

$Defecation_{pred}$	=	total defecation for given predator (g/m^{3}"d);
$EgestCoeff_{\mathrm{prey,\ pred}}$	=	fraction of ingested prey that is egested (unitless); and
IncrEgest	=	increased egestion due to toxicant (see Eq. **(298)**, unitless).

Consumption of prey for a predator is also considered predation or grazing for the prey. Therefore, AQUATOX represents consumption as a source term for the predator and as a loss term for the prey:

$$Consumption_{pred} = \Sigma_{prey}(Ingestion_{prey,\ pred}) \tag{85}$$

$$Predation_{prey} = \Sigma_{pred}(Ingestion_{prey,\ pred}) \tag{86}$$

where

$Consumption_{\mathrm{pred}}$	=	total consumption rate by predator (g/m^{3}"d); and
$Predation_{\mathrm{prey}}$	=	total predation or grazing on given prey (g/m^{3}"d).

Respiration

Respiration can be considered as having three components. Standard respiration is a rate at resting in which the organism is expending energy without consumption. Active respiration is modeled only in fish and only when allometric (weight-dependent) equations are used, so standard respiration can be considered as a composite "routine" respiration for invertebrates and in the simpler implementation for fish. The so-called specific dynamic action is the metabolic cost of digesting and assimilating prey. In the model active respiration is combined with standard respiration by means of an activity factor, and specific dynamic action is an additive term (Kitchell et al., 1974):

$$Respiration_{pred} = StdResp_{pred} \cdot Activity_{pred} + SpecDynAction_{pred} \qquad \textbf{(87)}$$

where:

$Respiration_{pred}$	=	respiratory loss of given predator (g/m^3"d);
$StdResp_{pred}$	=	basal respiratory loss modified by temperature (g/m^3"d); see **(88)** and **(89)**;
$Activity_{pred}$	=	a factor for respiratory loss associated with swimming (unitless), see **(92)** and **(94)**; and
$SpecDynAction_{pred}$	=	metabolic cost of processing food (g/m^3"d), see **(96)**.

AQUATOX simulates standard respiration as an optimal observed rate modified by a temperature dependence and, in fish, a density dependence (see Kitchell et al., 1974):

$$StdResp_{pred} = RoutineResp_{pred} \cdot TCorr_{pred} \cdot Biomass_{pred} \cdot DensityDep \qquad \textbf{(88)}$$

where:

$RoutineResp_{pred}$	=	routine respiration rate at optimal temperature for given predator (g/g"d); parameter input by user as “Respiration Rate” or computed as a function of the weight of the animal (see below);
$TCorr_{pred}$	=	Stroganov temperature function (unitless), see **(51)**;
$Biomass_{pred}$	=	concentration of predator (g/m^3); and
$DensityDep$	=	density-dependent respiration factor used in computing standard respiration, applicable only to fish (unitless). See **(95)**

As an alternative formulation, standard respiration in fish can be modeled as a function of the weight of the fish using an allometric equation (Hewett and Johnson, 1992; Hanson et al., 1997):

$$StdResp_{pred} = BasalResp_{pred} \cdot MeanWeight_{pred}^{RB_{pred}} \cdot TFn_{pred} \cdot Biomass_{pred} \cdot DensityDep \qquad \textbf{(89)}$$

where:

$BasalResp_{pred}$	=	basal respiration rate for given predator (g/g"d); computed as a function of the weight of the animal, see **(90)**;
$MeanWeight_{pred}$	=	mean weight for a given fish (g);
RB_{pred}	=	slope of the allometric function for a given fish (1/g);
TFn_{pred}	=	temperature function (unitless), see **(91)**, **(92)**.

The allometric functions are based on the well known Wisconsin Bioenergetics Model and, for convenience, use the published parameter values for that model (Hewett and Johnson, 1992;

Hanson et al., 1997). However, the basal respiration rate in that model is expressed as g of oxygen per g organic matter of fish per day, and this has to be converted to organic matter respired:

$$BasalResp_{pred} = RA_{pred} \cdot 1.5 \tag{90}$$

where:

RA_{pred}	=	basal respiration rate, characterized as the "intercept of the allometric mass function" in the Wisconsin Bioenergetics Model documentation (g O_2/g organic matter "d);
1.5	=	conversion factor (g organic matter/g O_2).

Swimming activity may be large and variable (Hanson et al., 1997) and is subject to calibration for a particular site, considering currents and other factors. Activity can be a complex function of temperature. The Wisconsin Bioenergetics Model (Hewett and Johnson, 1992; Hanson et al., 1997) provides two alternatives. **Equation Set 1** uses an exponential temperature function:

$$TFn = e^{(RQ \cdot Temp)} \tag{91}$$

where:

RQ	=	the Q_{10} or rate of change per 10° C for respiration (1/° C);
$Temp$	=	ambient temperature (° C).

TFn is then factored into the calculation of $StdResp_{pred}$, which is in turn modified by an *Activity* factor as part of the calculation of *Respiration* **(87)**. *Activity* is a complex function for swimming speed as an allometric function of temperature (Hewett and Johnson, 1992; Hanson et al., 1997):

$$\begin{aligned} Activity_{pred} &= e^{(RTO \cdot Vel)} \\ \text{If } Temp > RTL \text{ Then } Vel &= RK1 \cdot MeanWeight^{RK4} \\ \text{Else } Vel &= ACT \cdot MeanWeight^{RK4} \cdot e^{(BACT \cdot Temp)} \end{aligned} \tag{92}$$

where:

RTO	=	coefficient for swimming speed dependence on metabolism (s/cm);
RTL	=	temperature below which swimming activity is an exponential function of temperature (° C);
Vel	=	swimming velocity (cm/s);
$RK1$	=	intercept for swimming speed above the threshold temperature (cm/s);
$RK4$	=	weight-dependent coefficient for swimming speed;
ACT	=	intercept for swimming speed for a 1 g fish at ° C (cm/s); and
$BACT$	=	coefficient for swimming at low temperatures (1/° C),

Equation Set 2 uses the Stroganov function used elsewhere in AQUATOX, see **(51)**:

$$TFn = TCorr \tag{93}$$

and activity is a constant:

$$Activity = ACT \tag{94}$$

where:

ACT = activity factor, which is not the same as ACT in **Equation Set 1** (g/g).

Standard respiration in fish increases with crowding due to competition for spawning sites, interference in feeding, and other factors. This adverse intraspecific interaction helps to constrain the population to the carrying capacity; as the biomass approaches the carrying capacity for a given species the respiration is increased proportionately (Kitchell et al., 1974):

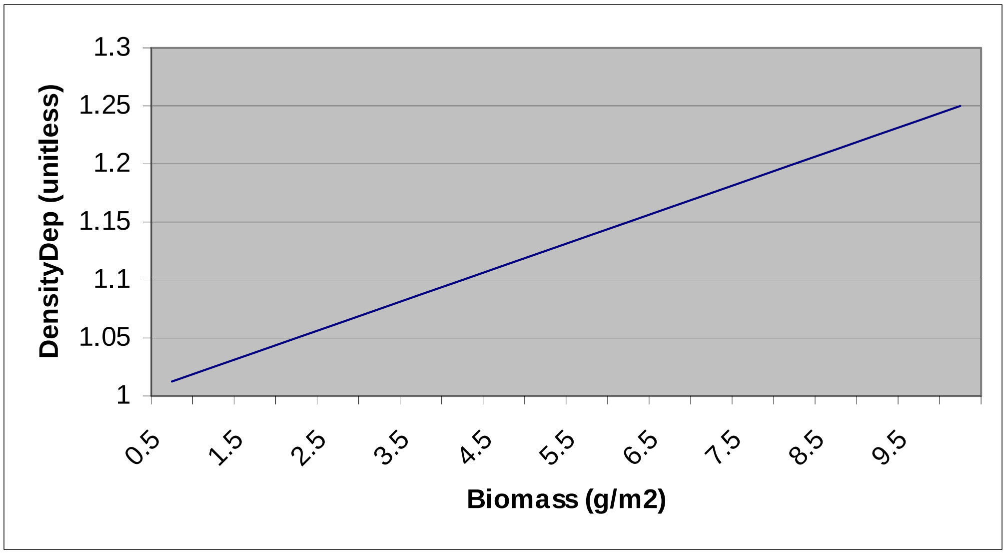
$$DensityDep = 1 + \frac{IncrResp \cdot Biomass}{KCap} \tag{95}$$

where:

$IncrResp$ = increase in respiration at carrying capacity (0.25);
$KCap$ = carrying capacity (g/m^3).

With the $IncrResp$ value of 0.25, which is a conservative estimate, respiration is increased by 25% at carrying capacity (Kitchell et al., 1974), as shown in **Figure 50**. This density-dependence is used only for fish, and not for invertebrates.

Figure 50. Density-dependent factor for increase in respiration as fish biomass approaches the carrying capacity (10.0 in this example).



As a simplification, specific dynamic action is represented as proportional to food assimilated (Hewett and Johnson, 1992; see also Kitchell et al., 1974; Park et al., 1974):

$$SpecDynAction_{pred} = KResp_{pred} \cdot (Consumption_{pred} - Defecation_{pred}) \tag{96}$$

where:

$KResp_{pred}$ = proportion of assimilated energy lost to specific dynamic action (unitless); parameter input by user as “Specific Dynamic Action;”

$Consumption_{\mathrm{pred}}$ = ingestion ($g/m^3 \cdot d$); and

$Defecation_{\mathrm{pred}}$ = egestion of unassimilated food ($g/m^3 \cdot d$).

Excretion

As respiration occurs, biomass is lost and nitrogen and phosphorus are excreted directly to the water (Horne and Goldman 1994); see **(139)** and **(147)**. Ganf and Blažka (1974) have reported that this process is important to the dynamics of the Lake George, Uganda, ecosystem. Their data were converted by Scavia and Park (1976) to obtain a proportionality constant relating excretion to respiration:

$$Excretion_{pred} = KExcr_{pred} \cdot Respiration_{pred} \tag{97}$$

where:

$Excretion_{pred}$ = excretion rate ($g/m^3 \cdot d$);

$KExcr_{pred}$ = proportionality constant for excretion:respiration (unitless); and

$Respiration_{pred}$ = respiration rate ($g/m^3 \cdot d$).

Excretion is approximately 17 percent of respiration, which is not an important biomass loss term for animals, but it is important in nutrient recycling.

Nonpredatory Mortality

Nonpredatory mortality is a result of both environmental conditions and the toxicity of pollutants:

$$Mortality_{pred} = D_{pred} \cdot Biomass_{pred} + Poisoned_{pred} \tag{98}$$

where:

$Mortality_{pred}$ = nonpredatory mortality ($g/m^3 \cdot d$);

D_{pred}	=	environmental mortality rate; the maximum value of three computations, (99), (100), and (101), is used (1/d);
$Biomass_{pred}$	=	biomass of given animal (g/m^3); and
$Poisoned$	=	mortality due to toxic effects (g/m^3"d), see (287).

Under normal conditions a baseline mortality rate is used:

$$D_{pred} = KMort_{pred} \tag{99}$$

where:

$KMort_{pred}$	=	normal nonpredatory mortality rate (1/d).

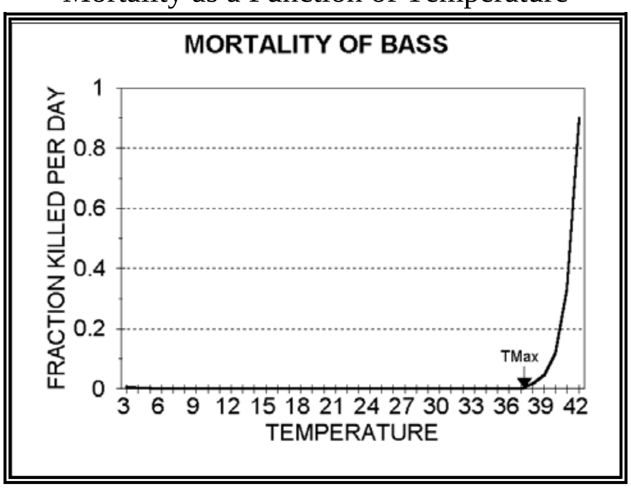
An exponential function is used for temperatures above the maximum (**Figure 51**):

$$D_{pred} = KMort_{pred} + \frac{e^{Temperature - TMax_{pred}}}{2} \tag{100}$$

where:

$Temperature$	=	ambient water temperature (/C); and
$TMax_{pred}$	=	maximum temperature tolerated (/C).

Figure 51
Mortality as a Function of Temperature



The lower lethal temperature is often 0/C (Leidy and Jenkins, 1976), so it is ignored at this time. Total mortality is assumed when dissolved oxygen drops below 0.25 g/m^3, recognizing that the predicted level is an average for the entire water column or epilimnetic or hypolimnetic segment:

$$Dead = 1.0 \text{ if } Oxygen < 0.25 \tag{101}$$

Gamete Loss and Recruitment

Eggs and sperm can be a significant fraction of adult biomass; in bluegills these can be 13 percent and 5 percent, respectively (Toetz, 1967), giving an average of 9 percent if the proportion of sexes is equal. Because only a small fraction of these gametes results in viable young when shed at the time of spawning, the remaining fraction is lost to detritus in the model.

There are two options for determining the date or dates on which spawning will take place. A user can specify up to three dates on which spawning will take place. Alternatively, one may use a construct that was modified from a formulation by Kitchell et al. (1974). As a simplification, rather than requiring species-specific spawning temperatures, it assumes that spawning occurs when the temperature first enters the range from six tenths of the optimum temperature to 1/ less than the optimal temperature. This is based on a comparison of the optimal temperatures with the species-specific spawning temperatures reported by Kitchell et al. (1974). Depending on the range of temperatures, this simplifying assumption usually will result in one or two spawnings per year in a temperate ecosystem when a simple sinusoidal temperature function is used. However, the user also can specify a maximum number of spawnings.

$$\text{If } (0.6 \cdot TOpt) < Temperature < (TOpt - 1.0) \text{ then}$$

$$GameteLoss = (GMort + IncrMort) \cdot FracAdults \cdot PctGamete \cdot Biomass \tag{102}$$

$$\text{else } GameteLoss = 0$$

where:

Temperature	=	ambient water temperature (/C);
TOpt	=	optimum temperature (/C);
GameteLoss	=	loss rate for gametes (g/m^{3}"d);
GMort	=	gamete mortality (1/d);
IncrMort	=	increased gamete and embryo mortality due to toxicant (1/d); see **(299)**;
Biomass	=	biomass of predator (g/m^{3});
PctGamete	=	fraction of adult predator biomass that is in gametes (unitless); and
FracAdults	=	fraction of biomass that is adult (unitless).

As the biomass of a population reaches its carrying capacity, reproduction is usually reduced due to stress; this results in a population that is primarily adults. Therefore, the proportion of adults and the fraction of biomass in gametes are assumed to be at a maximum when the biomass is at the carrying capacity (**Figure 52**):

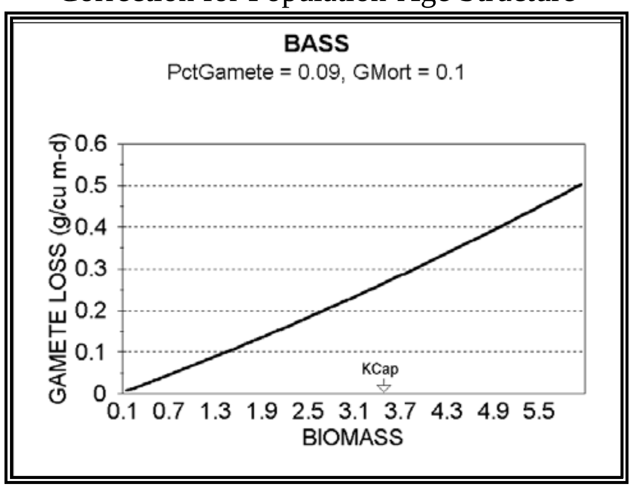
$$FracAdults = 1.0 - \left(\frac{Capacity}{KCap} \right) \tag{103}$$

$$\text{if } Biomass > KCap \text{ then } Capacity = 0 \textit{ else } Capacity = KCap - Biomass$$

where:

KCap	=	carrying capacity (g/m^3).

Figure 52
Correction for Population-Age Structure



Spawning in large fish results in an increase in the biomass of small fish if both small and large size classes are of the same species. Gametes are lost from the large fish, and the small fish gain the viable biomass through recruitment:

$$Recruit = (1 - (GMort + IncrMort)) \cdot FracAdults \cdot PctGamete \cdot Biomass \tag{104}$$

where:

Recruit	=	biomass gained from successful spawning ($g/m^{3} \cdot d$).

Washout, Drift, and Entrainment

Downstream transport is an important loss term for invertebrates. Zooplankton are subject to transport downstream similar to phytoplankton:

$$Washout = \frac{Discharge}{Volume} \cdot Biomass \qquad \textbf{(105)}$$

where:

Washout	=	loss of zooplankton due to downstream transport (g/m^3"d);
Discharge	=	discharge (m^3/d), see **Table 1**;
Volume	=	volume of site (m^3), see **(2)**; and
Biomass	=	biomass of invertebrate (g/m^3).

Likewise, zoobenthos exhibit drift, which is detachment followed by washout, and it is represented by a construct that is original with AQUATOX:

$$Drift = (Dislodge + Dislodge_{Tox}) \cdot Biomass \qquad \textbf{(106)}$$

where:

Drift	=	loss of zoobenthos due to downstream drift (g/m^3"d);
Dislodge	=	fraction of biomass subject to drift per day (fraction/d), see **(107)**; and
$Dislodge_{Tox}$	=	fraction of biomass subject to drift per day because of toxicant stress (fraction/d), see **(301)**.

Nocturnal drift is a natural phenomenon:

$$Dislodge = AveDrift \qquad \textbf{(107)}$$

where:

AveDrift	=	fraction of biomass subject to normal drift per day (fraction/d).

Animals also are subject to entrainment and downstream transport in flood waters. In fact, annual variations in fish populations in streams are due largely to variations in flow, with almost 100% loss during large floods in Shenandoah National Park (NPS, 1997). A simple exponential loss function was developed for AQUATOX:

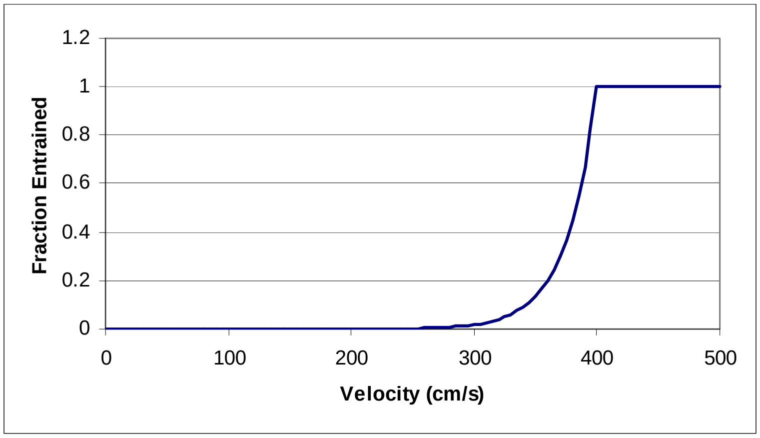
$$Entrainment = Biomass \cdot MaxRate \cdot e^{\frac{Vel - VelMax}{Gradual}} \qquad \textbf{(108)}$$

where:

Entrainment	=	entrainment and downstream transport (g/m^3"d);
Biomass	=	biomass of given animal (g/m^3);
MaxRate	=	maximum loss per day (1/d);
Vel	=	velocity of water (cm/s), **(14)**;
VelMax	=	velocity at which there is total loss of biomass (cm/s); and

Gradual = slope of exponential, set to 25 (cm/s).

Figure 53
Entrainment of animals as a function of stream velocity with *VelMax* of 400 cm/s



Vertical Migration

When presented with unfavorable conditions, most animals will attempt to migrate to an adjacent area with more favorable conditions. The current version of AQUATOX, following the example of CLEANER (Park et al., 1980), assumes that zooplankton and fish will exhibit avoidance behavior by migrating vertically from an anoxic hypolimnion to the epilimnion. Anoxic conditions are taken to occur when dissolved oxygen levels are less than 0.25 mg/L. The assumption is that anoxic conditions will persist until overturn. The construct calculates the absolute mass of the given group of organisms in the hypolimnion, then divides by the volume of the epilimnion to obtain the biomass being added to the epilimnion:

$$\text{If } VSeg = Hypo \text{ and } Anoxic$$

$$Migration = \frac{HypVolume \cdot Biomass_{pred,\ hypo}}{EpiVolume} \tag{109}$$

where:

VSeg = vertical segment;
Hypo = hypolimnion;
Anoxic = boolean variable for anoxic conditions when $O_2 < 0.25$ mg/L;
Migration = rate of migration ($g/m^3 \cdot d$);
HypVolume = volume of hypolimnion (m^3), see **Figure 19**;

EpiVolume	=	volume of epilimnion (m^3), see **Figure 19**; and
$Biomass_{pred,hypo}$	=	biomass of given predator in hypolimnion (g/m^3).

This does not include horizontal migration or avoidance of toxicants and stressful temperatures.

Promotion

Although AQUATOX is an ecosystem model, promotion to the next size class is important in representing the emergence of aquatic insects, and therefore loss of biomass from the system, and in predicting bioaccumulation of hydrophobic organic compounds in larger fish. The model assumes that promotion is determined by the rate of growth. Growth is considered to be the sum of consumption and the loss terms other than mortality and migration; a fraction of the growth goes into promotion to the next size class (cf. Park et al., 1980):

$$Promotion = KPro_{pred} \cdot (Consumption - Defecation - Respiration - Excretion - GameteLoss) \quad \textbf{(110)}$$

where:

Promotion	=	rate of promotion ($g/m^3 \cdot d$);
KPro	=	fraction of growth that goes to promotion or emergence (0.5, unitless);
Consumption	=	rate of consumption ($g/m^3 \cdot d$), see **(85)**;
Defecation	=	rate of defecation ($g/m^3 \cdot d$), see **(84)**;
Respiration	=	rate of respiration ($g/m^3 \cdot d$), see **(87)**;
Excretion	=	rate of excretion ($g/m^3 \cdot d$), see **(97)**; and
GameteLoss	=	loss rate for gametes ($g/m^3 \cdot d$), see **(102)**.

This is a simplification of a complex response that depends on the mean weight of the individuals. However, simulation of mean weight would require modeling both biomass and numbers of individuals (Park et al., 1979, 1980), and that is beyond the scope of this model at present.

Promotion of multi-age fish is straightforward; each age class is promoted to the next age class on the first spawning date each year. The oldest age class merely increments biomass from the previous age class to any remaining biomass in the class. Of course, any associated toxicant is transferred to the next class as well. Recruitment to the youngest age class is the fraction of gametes that are not subject to mortality at spawning. Note that the user specifies the age at which spawning begins on the multi-age fish screen.

Insect emergence can be an important factor in the dynamics of an aquatic ecosystem. Often there is synchrony in the emergence; in AQUATOX this is assumed to be cued to temperature with additional forcing as twice the promotion that would ordinarily be computed, and is represented by:

$$\text{If } Temperature > (0.8 \cdot TOpt) \textit{ and } Temperature < (TOpt - 1.0) \textit{ then}$$
$$EmergeInsect = 2 \cdot Promotion \qquad \textbf{(111)}$$

where:

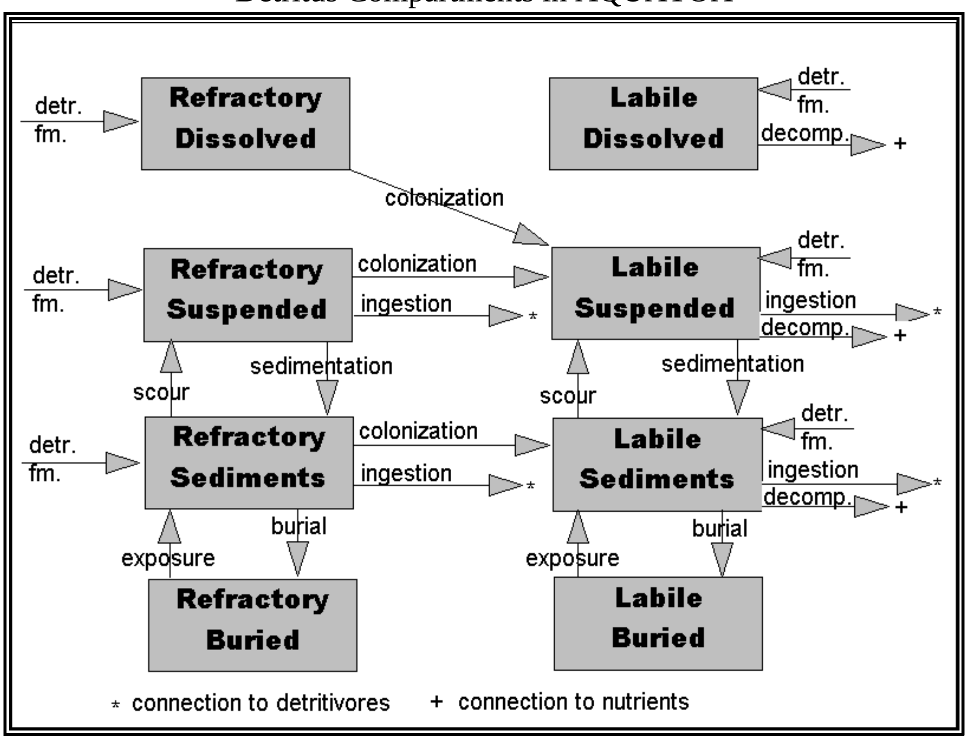
EmergeInsect	=	insect emergence (mg/L·d);
Temperature	=	ambient water temperature (°C); and
TOpt	=	optimum temperature (°C);

5 REMINERALIZATION

5.1 Detritus

For the purposes of AQUATOX, the term "detritus" is used to include all non-living organic material and associated decomposers (bacteria and fungi). As such, it includes both particulate and dissolved material in the sense of Wetzel (1975), but it also includes the microflora and is analogous to “biodetritus” of Odum and de la Cruz (1963) . Detritus is modeled as eight compartments: refractory (resistant) dissolved, suspended, sedimented, and buried detritus; and labile (readily decomposed) dissolved, suspended, sedimented, and buried detritus (**Figure 54**). This degree of disaggregation is considered necessary to provide more realistic simulations of the detrital food web; the bioavailability of toxicants, with orders-of-magnitude differences in partitioning; and biological oxygen demand, which depends largely on the decomposition rates. Buried detritus is considered to be taken out of active participation in the functioning of the ecosystem. In general, dissolved organic material is about ten times that of suspended particulate matter in lakes and streams (Saunders, 1980), and refractory compounds usually predominate; however, the proportions are modeled dynamically.

Figure 54
Detritus Compartments in AQUATOX



The concentrations of detritus in these eight compartments are the result of several competing processes:

$$\frac{dSuspRefrDetr}{dt} = Loading + DetrFm - Colonization - Washout - Sedimentation - Ingestion + Scour \pm Sinking \pm TurbDiff \tag{112}$$

$$\frac{dSuspLabDetr}{dt} = Loading + DetrFm + Colonization - Decomposition - Washout - Sedimentation - Ingestion + Scour \pm Sinking \pm TurbDiff \tag{113}$$

$$\frac{dDissRefrDetr}{dt} = Loading + DetrFm - Colonization - Washout \pm TurbDiff \tag{114}$$

$$\frac{dDissLabDetr}{dt} = Loading + DetrFm - Decomposition - Washout \pm TurbDiff \tag{115}$$

$$\frac{dSedRefrDetr}{dt} = Loading + DetrFm + Sedimentation + Exposure - Colonization - Ingestion - Scour - Burial \tag{116}$$

$$\frac{dSedLabileDetr}{dt} = Loading + DetrFm + Sedimentation + Colonization - Ingestion - Decomposition - Scour + Exposure - Burial \tag{117}$$

$$\frac{dBuriedRefrDetr}{dt} = Sedimentation + Burial - Scour - Exposure \tag{118}$$

$$\frac{d BuriedLabileDetr}{dt} = Sedimentation + Burial - Scour - Exposure \qquad \textbf{(119)}$$

where:

d*SuspRefrDetr*/dt	=	change in concentration of suspended refractory detritus with respect to time (g/m^3·d);
d*SuspLabileDetr*/dt	=	change in concentration of suspended labile detritus with respect to time (g/m^3·d);
d*DissRefrDetr*/dt	=	change in concentration of dissolved refractory detritus with respect to time (g/m^3·d);
d*DissLabDetr*/dt	=	change in concentration of dissolved labile detritus with respect to time (g/m^3·d);
d*SedRefrDetr*/dt	=	change in concentration of sedimented refractory detritus with respect to time (g/m^3·d);
d*SedLabileDetr*/dt	=	change in concentration of sedimented labile detritus with respect to time (g/m^3·d);
d*BuriedRefrDetr*/dt	=	change in concentration of buried refractory detritus with respect to time (g/m^3·d);
d*BuriedLabileDetr*/dt	=	change in concentration of buried labile detritus with respect to time (g/m^3·d);
Loading	=	loading of given detritus from nonpoint and point sources, or from upstream (g/m^3·d);
DetrFm	=	detrital formation (g/m^3·d);
Colonization	=	colonization of refractory detritus by decomposers (g/m^3·d), see **(126)**;
Decomposition	=	loss due to microbial decomposition (g/m^3·d), see **(130)**;
Sedimentation	=	transfer from suspended detritus to sedimented detritus by sinking (g/m^3·d); in streams with the inorganic sediment model attached see **(189)**, for all other systems see **(135)**;
Scour	=	resuspension from sedimented detritus (g/m^3·d); in streams with the inorganic sediment model attached see **(187)**, for all other systems see **(135)** (resuspension);
Exposure	=	transfer from buried to sedimented by scour of overlying sediments (g/m^3·d);
Burial	=	transfer from sedimented to buried due to deposition of sediments (g/m^3·d), see **(184)**;
Washout	=	loss due to being carried downstream (g/m^3·d), see **(16)**;
Ingestion	=	loss due to ingestion by detritivores and filter feeders (g/m^3·d), see **(78)**;

Sinking	=	detrital sinking from epilimnion and to hypolimnion under stratified conditions, see **(135)**; and
TurbDiff	=	transfer between epilimnion and hypolimnion due to turbulent diffusion (g/m^3·d), see **(22)** and **(23)**.

As a simplification, refractory detritus is considered not to decompose directly, but rather to be converted to labile detritus through microbial colonization, especially through ingestion then egestion by detritivores (organisms that feed on detritus). Labile detritus is then available for both decomposition and assimilation by detritivores. Because detritivores digest microbes and defecate the remaining organic material, detritus has to be conditioned through microbial colonization before it is suitable food. Therefore, the assimilation efficiency of detritivores for refractory material is usually set to 0.0, and the assimilation efficiency for labile material is increased accordingly. Sedimentation and scour, or resuspension, are opposite processes. In shallow systems there may be no long-term sedimentation (Wetzel et al., 1972), while in deep systems there may be little resuspension. In this version sedimentation is a function of flow, ice cover and, in very shallow water, wind based on simplifying assumptions. Burial, scour and exposure are applicable only in streams where they are keyed to the behavior of clay and silt. Scour as an explicit function of wave and current action is not implemented.

Detrital Formation

Detritus is formed in several ways: through mortality, gamete loss, sinking of phytoplankton, excretion and defecation:

$$DetrFm_{SuspRefrDetr} = \Sigma_{biota}(Mort2_{detr,\ biota} \cdot Mortality_{biota}) \tag{120}$$

$$DetrFm_{DissRefrDetr} = \Sigma_{biota}(Mort2_{detr,biota} \cdot Mortality_{biota}) + \Sigma_{biota}(Excr2_{detr,biota} \cdot Excretion) \tag{121}$$

$$DetrFm_{DissLabileDetr} = \Sigma_{biota}(Mort2_{detr,biota} \cdot Mortality_{biota}) + \Sigma_{biota}(Excr2_{detr,biota} \cdot Excretion) \tag{122}$$

$$DetrFm_{SuspLabileDetr} = \Sigma_{biota}(Mort2_{detr,biota} \cdot Mortality_{biota}) + \Sigma_{animals}\ GameteLoss \tag{123}$$

$$DetrFm_{SedLabileDetr} = \Sigma_{pred}(Def2_{detr,pred} \cdot Defecation_{pred}) + \Sigma_{compartment}(Sink_{compartment}) \tag{124}$$

$$DetrFm_{SedRefrDetr} = \Sigma_{pred}(Def2_{detr,pred} \cdot Defecation_{pred}) + \Sigma_{compartment}(Sedimentation_{compartment} \cdot PlantSinkToDetr) \quad \mathbf{(125)}$$

where:

$DetrFm$	=	formation of detritus (g/m³·d);
$Mort2_{\mathrm{detr,\,biota}}$	=	fraction of given dead organism that goes to given detritus (unitless);
$Excr2_{detr,\,biota}$	=	fraction of excretion that goes to given detritus (unitless);
$Mortality_{biota}$	=	death rate for organism (g/m³·d), see **(58)**, **(74)** and **(98)**;
$Excretion$	=	excretion rate for organism (g/m³·d), see **(56)** and **(97)** for plants and animals, respectively;
$GameteLoss$	=	loss rate for gametes (g/m³·d), see **(102)**;
$Def2_{detr,\,biota}$	=	fraction of defecation that goes to given detritus (unitless);
$Defecation_{\mathrm{pred}}$	=	defecation rate for organism (g/m³·d), see **(84)**;
$Sedimentation$	=	loss of phytoplankton to bottom sediments (g/m³·d), see **(61)**; and
$PlantSinkToDetr$	=	labile and refractory portions of phytoplankton (unitless, 0.92 and 0.08 respectively).

A fraction of mortality, including sloughing of leaves from macrophytes, is assumed to go to refractory detritus; a much larger fraction goes to labile detritus. Excreted material goes to both refractory and labile detritus, while gametes are considered to be labile. Half the defecated material is assumed to be labile because of the conditioning due to ingestion and subsequent inoculation with bacteria in the gut (LeCren and Lowe-McConnell, 1980); fecal pellets sink rapidly (Smayda, 1971), so defecation is treated as if it were directly to sediments. Phytoplankton that sink to the bottom are considered to become detritus; most are consumed quickly by zoobenthos (LeCren and Lowe-McConnell, 1980) and are not available to be resuspended.

Colonization

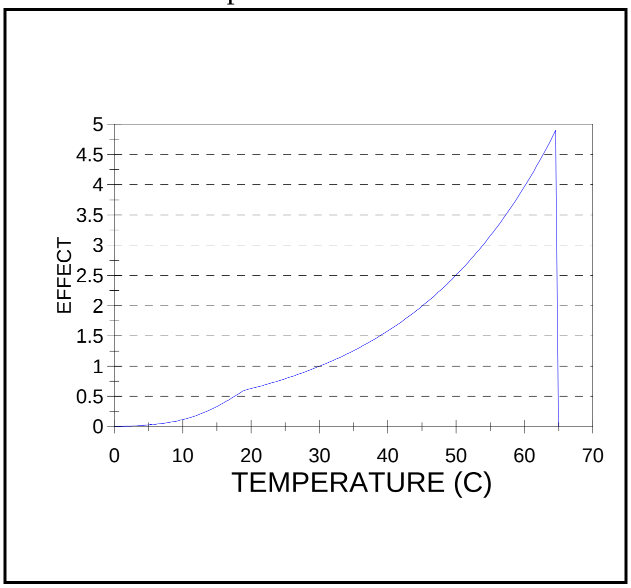
Refractory detritus is converted to labile detritus through microbial colonization. When bacteria and fungi colonize dissolved refractory organic matter, they are in effect turning it into particulate matter. Detritus is often refractory because it has a deficiency of nitrogen compared to microbial biomass. In order for microbes to colonize refractory detritus, they have to take up additional nitrogen from the water (Saunders et al., 1980). Thus, colonization is nitrogen-limited, as well as being limited by suboptimal temperature, pH, and dissolved oxygen:

$$Colonization = ColonizeMax \cdot DecTCorr \cdot NLimit \cdot pHCorr \cdot DOCorrection \cdot RefrDetr \quad \mathbf{(126)}$$

where:

Colonization = rate of conversion of refractory to labile detritus ($g/m^3 \cdot d$);

Figure 55. Colonization and Decomposition as an Effect of Temperature



ColonizeMax	=	maximum colonization rate under ideal conditions ($g/g \cdot d$);
Nlimit	=	limitation due to suboptimal nitrogen levels (unitless), see **(128)**;
DecTCorr	=	the effect of temperature (unitless), see **(127)**;
pHCorr	=	limitation due to suboptimal pH level (unitless), see **(133)**;
DOCorrection	=	limitation due to suboptimal oxygen level (unitless), see **(131)**; and
RefrDetr	=	concentration of refractory detritus in suspension, sedimented, or dissolved (g/m^3).

Because microbial colonization and decomposition involves microflora with a wide range of temperature tolerances, the effect of temperature is modeled in the traditional way (Thomann and Mueller, 1987), taking the rate at an observed temperature and correcting it for the ambient temperature up to a user-defined, high maximum temperature, at which point it drops to 0:

$$
\begin{aligned}
DecTCorr &= Theta^{Temp - TObs} \text{ where} \\
Theta &= 1.047 \text{ if } Temp \geq 19° \text{ else} \\
Theta &= 1.185 - 0.00729 \cdot Temp
\end{aligned}
\qquad \textbf{(127)}
$$

$$\text{If } Temp > TMax \quad \text{Then } DecTCorr = 0$$

The resulting curve has a shoulder similar to the Stroganov curve, but the effect increases up to the maximum rate (**Figure 55**).

The nitrogen limitation construct, which is original with AQUATOX, is parameterized using an analysis of data presented by Egglishaw (1972) for Scottish streams. It is computed by:

$$NLimit = \frac{N - MinN}{N - MinN + HalfSatN} \tag{128}$$

$$N = Ammonia + Nitrate \tag{129}$$

where:

N	=	total available nitrogen (g/m^3);
MinN	=	minimum level of nitrogen for colonization (= 0.1 g/m^3);
HalfSatN	=	half-saturation constant for nitrogen stimulation (= 0.15 g/m^3);
Ammonia	=	concentration of ammonia (g/m^3); and
Nitrate	=	concentration of nitrite and nitrate (g/m^3).

Although it can be changed by the user, a default maximum colonization rate of 0.007 (g/g"d) per day is provided, based on McIntire and Colby (1978, after Sedell et al., 1975). The rates of decomposition (or colonization) of refractory dissolved organic matter are comparable to those for particulate matter. Saunders (1980) reported values of 0.007 (g/g"d) for a eutrophic lake and 0.008 (g/g"d) for a tundra pond. Anaerobic rates were reported by Gunnison et al. (1985).

Decomposition

Decomposition is the process by which detritus is broken down by bacteria and fungi, yielding constituent nutrients, including nitrogen, phosphorus, and inorganic carbon. Therefore, it is a critical process in modeling nutrient recycling. In AQUATOX, following a concept first advanced by Park et al. (1974), the process is modeled as a first-order equation with multiplicative limitations for suboptimal environmental conditions (see **section 4.1** for a discussion of similar construct for photosynthesis):

$$Decomposition = DecayMax \cdot DOCorrection \cdot DecTCorr \cdot pHCorr \cdot Detritus \tag{130}$$

where:

Decomposition	=	loss due to microbial decomposition (g/m^3"d);
DecayMax	=	maximum decomposition rate under aerobic conditions (g/g"d);
DOCorrection	=	correction for anaerobic conditions (unitless), see **(131)**;
DecTCorr	=	the effect of temperature (unitless), see **(127)**;
pHCorr	=	correction for suboptimal pH (unitless), see **(133)**, **(134)**; and
Detritus	=	concentration of detritus, including dissolved but not buried (g/m^3).

Note that biomass of bacteria is not explicitly modeled in AQUATOX, rather it is considered part of the detritus. In some models (for example, EXAMS, Burns et al., 1982) decomposition is represented by a second-order equation using an empirical estimate of bacteria biomass. However, using bacterial biomass as a site constant constrains the model, potentially forcing the rate. Decomposers were modeled explicitly as a part of the CLEAN model (Clesceri et al., 1977). However, if conditions are favorable, decomposers can double in 20 minutes; this can result in stiff equations, adding significantly to the computational time. Ordinarily, decomposers will grow rapidly as long as conditions are favorable. The only time the biomass of decomposers might need to be considered explicitly is when a new organic chemical is introduced and the microbial assemblage requires time to become adapted to using it as a substrate.

The effect of temperature on biodegradation is represented by Equation **(127)**, which also is used for colonization. The function for dissolved oxygen, formulated for AQUATOX, is:

$$DOCorrection = Factor + (1 - Factor) \cdot \frac{KAnaerobic}{DecayMax} \tag{131}$$

where the predicted DO concentrations are entered into a Michaelis-Menten formulation to determine the extent to which degradation rates are affected by ambient DO concentrations (Clesceri, 1980; Park et al., 1982):

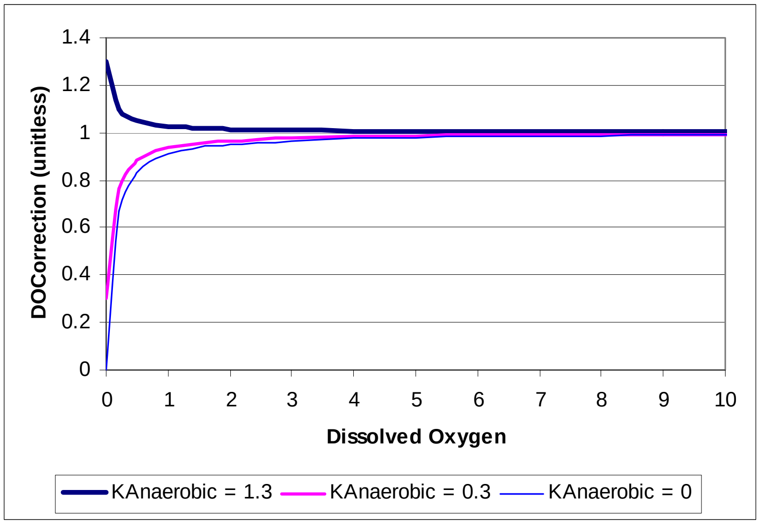
$$Factor = \frac{Oxygen}{HalfSatO + Oxygen} \tag{132}$$

and:

Factor	=	Michaelis-Menten factor (unitless);
KAnaerobic	=	decomposition rate at 0 g/m^3 oxygen (g/g"d);
Oxygen	=	dissolved oxygen concentration (g/m^3); and
HalfSatO	=	half-saturation constant for oxygen (g/m^3).

DOCorrection accounts for both decreased and increased (**Figure 56**) degradation rates under anaerobic conditions, with *KAnaerobic/DecayMax* having values less than one and greater than one, respectively. Detritus will always decompose more slowly under anaerobic conditions; but some organic chemicals, such as some halogenated compounds (Hill and McCarty, 1967), will degrade more rapidly. Half-saturation constants of 0.1 to 1.4 g/m^3 have been reported (Bowie et al., 1985); a value of 0.1 g/m^3 is used.

Figure 56. Correction for Dissolved Oxygen



Another important environmental control on the rate of microbial degradation is pH. Most fungi grow optimally between pH 5 and 6 (Lyman et al., 1990), and most bacteria grow between pH 6 to about 9 (Alexander, 1977). Microbial oxidation is most rapid between pH 6 and 8 (Lyman et al., 1990). Within the pH range of 5 and 8.5, therefore, pH is assumed to not affect the rate of microbial degradation, and the suboptimal factor for pH is set to 1.0. In the absence of good data on the rates of biodegradation under extreme pH conditions, biodegradation is represented as decreasing exponentially beyond the optimal range (Park et al., 1980a; Park et al., 1982). If the pH is below the lower end of the optimal range, the following equation is used:

$$pHCorr = e^{(pH - pHMin)} \qquad \textbf{(133)}$$

where:

pH	=	ambient pH, and
pHMin	=	minimum pH below which limitation on biodegradation rate occurs.

If the pH is above the upper end of the optimal range for microbial degradation, the following equation is used:

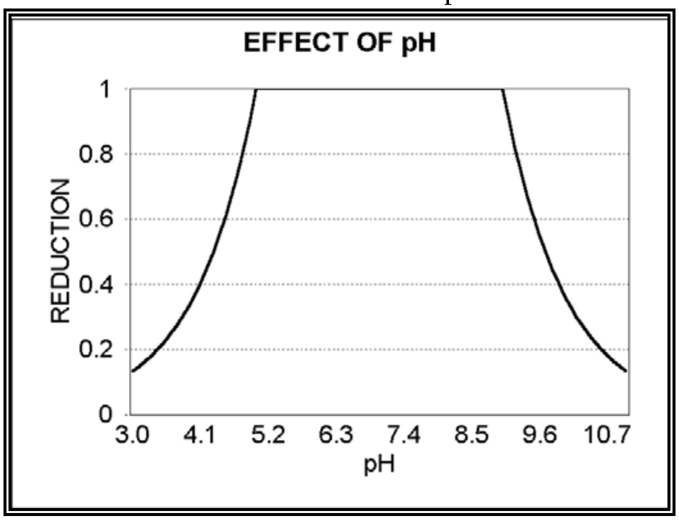
$$pHCorr = e^{(pHMmax - pH)} \qquad \textbf{(134)}$$

where:

pHMax	=	maximum pH above which limitation on biodegradation rate occurs.

These responses are shown in **Figure 57**.

Figure 57
Limitation Due To pH



Sedimentation and Resuspension

When the inorganic sediment model is not included in a simulation, the sedimentation of suspended particulate detritus to bottom sediments and the resuspension of bottom sediments to suspended detritus are modeled using simplifying assumptions. The constructs are intended to provide general responses to environmental factors, but they should not be considered as anything more than place holders for more realistic hydrodynamic functions to be incorporated in later versions. When the inorganic sediment model is included, the sedimentation and deposition of detritus is assumed to mimic the sedimentation and resuspension of silt (see **(187)** and **(189)**). Otherwise:

$$Sedimentation = \frac{KSed}{Thick} \cdot Decel \cdot State \qquad \textbf{(135)}$$

where:

Sedimentation	=	transfer from suspended to sedimented by sinking ($g/m^3 \cdot d$), see **(135)**;
KSed	=	sedimentation rate (m/d);
Thick	=	depth of water or thickness of layer if stratified (m);
Decel	=	deceleration factor (unitless), see **(136)**; and
State	=	concentration of particulate detrital compartment (g/m^3).

If the discharge exceeds the mean discharge then sedimentation is slowed proportionately (**Figure 58**):

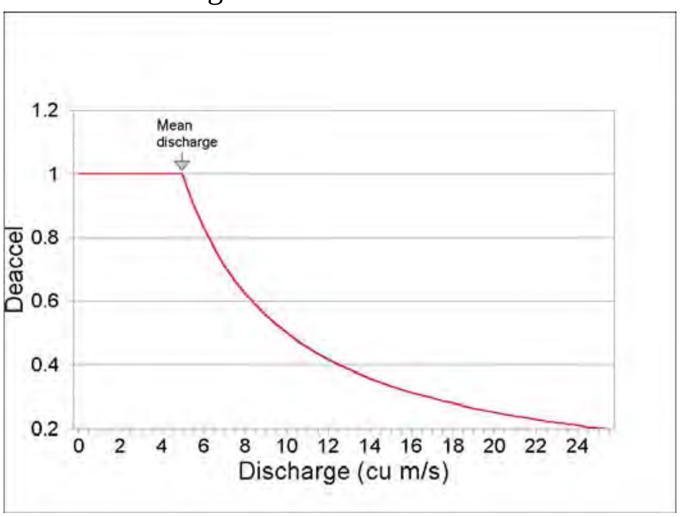
$$\text{If } TotDischarge > MeanDischarge \text{ then} \quad Decel = \frac{MeanDischarge}{TotDischarge} \quad \text{else } Decel = 1.0 \qquad \textbf{(136)}$$

where:

TotDischarge = total epilimnetic and hypolimnetic discharge (m^3/d); and
MeanDischarge = mean discharge over the course of the simulation (m^3/d).

If the depth of water is less than or equal to 1.0 m and wind speed is greater than or equal to 5.5 m/s then the sedimentation rate is negative, effectively becoming the rate of resuspension. If there is ice cover, then the sedimentation rate is doubled to represent the lack of turbulence.

Figure 58. Relationship of *Decel* to Discharge with a Mean Discharge of 5 m^3/s.



5.2 Nitrogen

Two nitrogen compartments, ammonia and nitrate, are modeled (**Figure 59**). Nitrite occurs in very low concentrations and is rapidly transformed through nitrification and denitrification (Wetzel, 1975); therefore, it is modeled with nitrate. Likewise, un-ionized ammonia (NH_3) is not modeled as a separate state variable. Ammonia is assimilated by algae and macrophytes and is converted to nitrate as a result of nitrification:

$$\frac{\mathrm{d}Ammonia}{\mathrm{d}t} = Loading + Excrete + Decompose - Nitrify - Assimilation_{Ammonia} - Washout \pm TurbDiff \quad \textbf{(137)}$$

where:

d*Ammonia*/d*t*	=	change in concentration of ammonia with time ($g/m^3 \cdot d$);
Loading	=	loading of nutrient from inflow ($g/m^3 \cdot d$);
Excrete	=	ammonia derived from excretion by animals ($g/m^3 \cdot d$), see **(139)**;
Decompose	=	ammonia derived from decomposition of detritus ($g/m^3 \cdot d$), see **(138)**;
Nitrify	=	nitrification ($g/m^3 \cdot d$), see **(144)**;
Assimilation	=	assimilation of nutrient by plants ($g/m^3 \cdot d$), see **(141)** and **(142)**;
Washout	=	loss of nutrient due to being carried downstream ($g/m^3 \cdot d$), see **(16)**

and;

TurbDiff	=	depth-averaged turbulent diffusion between epilimnion and hypolimnion if stratified ($g/m^3 \cdot d$), see **(22)** and **(23)**.

Ammonia is a product of decomposition:

$$Decompose = \Sigma_{Detritus}(Org2Ammonia \cdot Decomposition_{Detritus}) \quad \textbf{(138)}$$

It also is excreted directly by animals:

$$Excrete = \Sigma_{Biota}(Org2Ammonia \cdot Excretion_{Organism}) \quad \textbf{(139)}$$

where:

Org2Ammonia	=	ratio of ammonia to organic matter (unitless);
Decomposition	=	decomposition rate of given type of detritus, ($g/m^3 \cdot d$), see **(130)**; and
Excretion	=	excretion rate of given animal ($g/m^3 \cdot d$), see **(97)**.

Nitrate is assimilated by plants and is converted to free nitrogen (and lost) through denitrification:

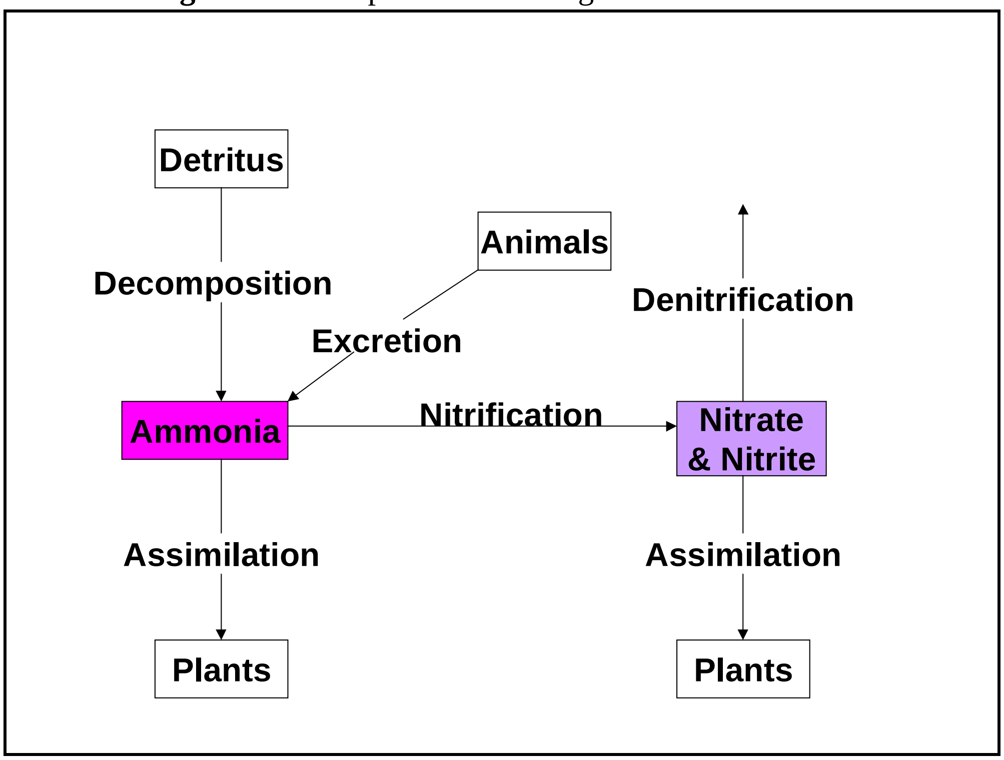
$$\frac{\mathrm{d}Nitrate}{\mathrm{d}t} = Loading + Nitrify - Denitrify - Assimilation_{Nitrate} - Washout \pm TurbDiff \quad \textbf{(140)}$$

where:

d*Nitrate*/dt	=	change in concentration of nitrate with time ($g/m^3 \cdot d$);
Loading	=	user entered loading of nitrate, including atmospheric deposition; and
Denitrify	=	denitrification ($g/m^3 \cdot d$); see **(145)**.

Free nitrogen can be fixed by blue-green algae. Both nitrogen fixation and denitrification are subject to environmental controls and are difficult to model with any accuracy; therefore, the nitrogen cycle is represented with considerable uncertainty.

Figure 59. Components of Nitrogen Remineralization



Assimilation

Nitrogen compounds are assimilated by plants as a function of photosynthesis in the respective groups (Ambrose et al., 1991):

$$Assimilation_{Ammonia} = \Sigma_{Plant}(Photosynthesis_{Plant} \cdot Uptake_{Nitrogen} \cdot NH4Pref) \quad \textbf{(141)}$$

$$Assimilation_{Nitrate} = \Sigma_{Plant}(Photosynthesis_{Plant} \cdot Uptake_{Nitrogen} \cdot (1 - NH4Pref)) \quad \textbf{(142)}$$

where:

Assimilation	=	assimilation rate for given nutrient (g/m^{3}"d);
Photosynthesis	=	rate of photosynthesis (g/m^{3}"d), see **(31)**;
$Uptake_{Nitrogen}$	=	fraction of photosynthate that is nitrogen (unitless, 0.01975 if nitrogen-fixing, otherwise 0.079);
NH4Pref	=	ammonia preference factor (unitless).

Only 23 percent of nitrate is nitrogen, but 78 percent of ammonia is nitrogen. This results in an apparent preference for ammonia. The preference factor is calculated with an equation developed by Thomann and Fitzpatrick (1982) and cited and used in WASP (Ambrose et al., 1991):

$$NH4Pref = \frac{N2NH4 \cdot Ammonia \cdot N2NO3 \cdot Nitrate}{(KN + N2NH4 \cdot Ammonia) \cdot (KN + N2NO3 \cdot Nitrate)} + \frac{N2NH4 \cdot Ammonia \cdot KN}{(N2NH4 \cdot Ammonia + N2NO3 \cdot Nitrate) \cdot (KN + N2NO3 \cdot Nitrate)} \quad \textbf{(143)}$$

where:

N2NH4	=	ratio of nitrogen to ammonia (0.78);
N2NO3	=	ratio of nitrogen to nitrate (0.23);
KN	=	half-saturation constant for nitrogen uptake (g N/m^{3});
Ammonia	=	concentration of ammonia (g/m^{3}); and
Nitrate	=	concentration of nitrate (g/m^{3}).

For algae other than blue-greens, *Uptake* is the Redfield (1958) ratio; although other ratios (cf. Harris, 1986) may be used by editing the parameter screen. At this time nitrogen fixation by blue-greens is represented by using a smaller uptake ratio, thus "creating" nitrogen.

Nitrification and Denitrification

Nitrification is the conversion of ammonia to nitrite and then to nitrate by nitrifying bacteria; it occurs primarily at the sediment-water interface (Effler et al., 1996). The maximum rate of nitrification, corrected for the area to volume ratio, is reduced by limitation factors for suboptimal dissolved oxygen and pH, similar to the way that decomposition is modeled, but using the more restrictive correction for suboptimal temperature used for plants and animals:

$$Nitrify = KNitri \cdot \frac{Area}{Volume} \cdot DOCorrection \cdot TCorr \cdot pHCorr \cdot Ammonia \qquad \textbf{(144)}$$

where:

Nitrify	=	nitrification rate ($g/m^3 \cdot d$);
KNitri	=	maximum rate of nitrification (0.135 m/d, according to Effler et al., 1996);
Area	=	area of site or segment (m^2);
Volume	=	volume of site or segment (m^3); see **(2)**;
DOCorrection	=	correction for anaerobic conditions (unitless) see **(131)**;
TCorr	=	correction for suboptimal temperature (unitless); see **(51)**;
pHCorr	=	correction for suboptimal pH (unitless), see **(133)**; and
Ammonia	=	concentration of ammonia (g/m^3).

The nitrifying bacteria have narrow environmental optima; according to Bowie et al. (1985) they require aerobic conditions with a pH between 7 and 9.8, an optimal temperature of 30°, and minimum and maximum temperatures of 10° and 60° respectively (**Figure 60**, **Figure 61**).

Figure 60
Response to pH, Nitrification

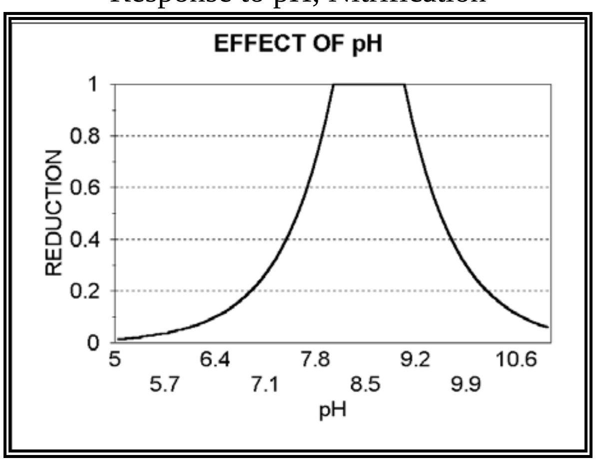
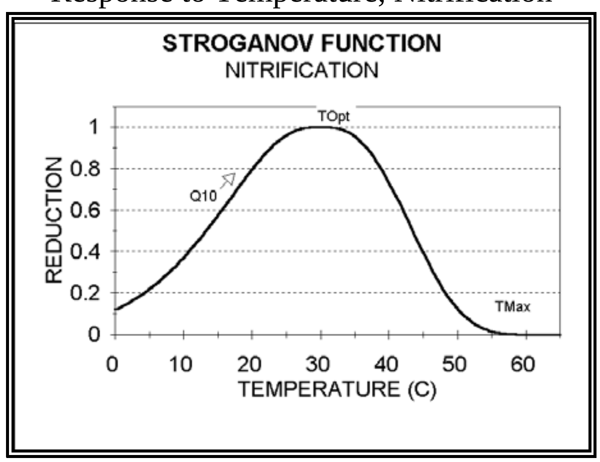


Figure 61
Response to Temperature, Nitrification



In contrast, denitrification (the conversion of nitrate and nitrite to free nitrogen) is an anaerobic process, so that *DOCorrection* enhances the process (Ambrose et al., 1991):

$$Denitrify = KDenitri \cdot (1 - DOCorrection) \cdot TCorr \cdot pHCorr \cdot Nitrate \qquad \textbf{(145)}$$

where:

Denitrify	=	denitrification rate (g/m^{3}"d);
KDenitri	=	maximum rate of denitrification (0.1 m/d, according to Di Toro, 2001); and
Nitrate	=	concentration of nitrate (g/m^{3}).

Furthermore, it is accomplished by a large number of reducing bacteria under anaerobic conditions and with broad environmental tolerances (Bowie et al., 1985; **Figure 62**,**Figure 63**).

Figure 62
Response to pH, Denitrification

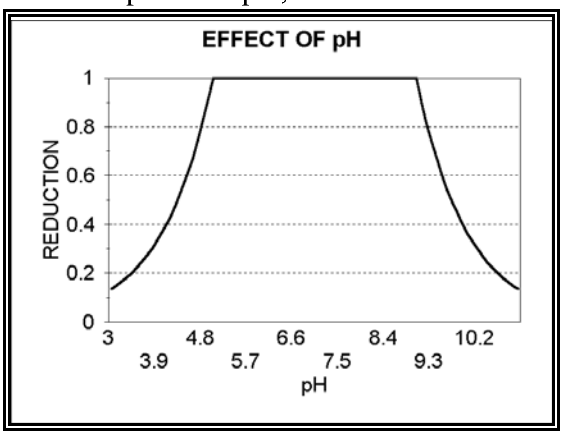
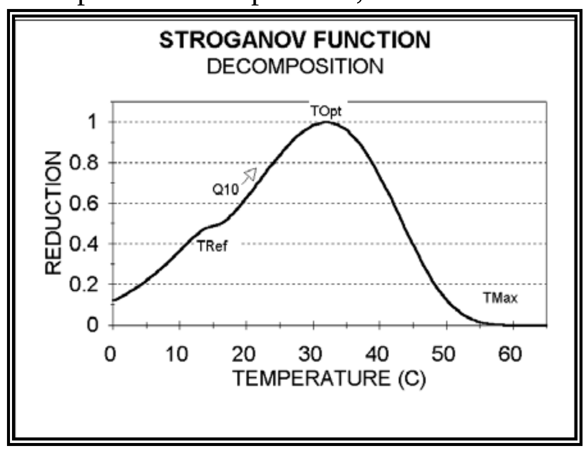


Figure 63
Response to Temperature, Denitrification



5.3 Phosphorus

The phosphorus cycle is much simpler than the nitrogen cycle. Decomposition, excretion, and assimilation are important processes that are similar to those described above:

$$\frac{dPhosphate}{dt} = Loading \cdot FracAvail + Excrete + Decompose - Assimilation_{Phosphate} - Washout \pm TurbDiff \quad \textbf{(146)}$$

$$Excrete = \Sigma_{Biota}(Org2Phosphate \cdot Excretion_{Biota}) \quad \textbf{(147)}$$

$$Decompose = \Sigma_{Detritus}(Org2Phosphate \cdot Decomposition_{Detritus}) \quad \textbf{(148)}$$

$$Assimilation = \Sigma_{Plant}(Photosynthesis_{Plant} \cdot Uptake_{Phosphorus}) \quad \textbf{(149)}$$

where:

d*Phosphate*/dt = change in concentration of phosphate with time ($g/m^3 \cdot d$);
Loading = loading of nutrient from inflow and atmospheric deposition ($g/m^3 \cdot d$);
FracAvail = fraction of phosphate loading that is available (unitless);
Excrete = phosphate derived from excretion by biota ($g/m^3 \cdot d$); see **(56)** and **(97)** for plants and animals, respectively;
Decompose = phosphate derived from decomposition of detritus ($g/m^3 \cdot d$);
Assimilation = assimilation by plants ($g/m^3 \cdot d$);
Washout = loss due to being carried downstream ($g/m^3 \cdot d$), see **(16)**;
Area = area of site (m^2);
Volume = volume of water at site (m^3); see **(2)**;
Org2Phosphate = ratio of phosphate to organic matter (unitless);
Excretion = excretion rate for given organism ($g/m^3 \cdot d$), see **(56)** and **(97)** for plants and animals, respectively;
Decomposition = decomposition rate for given detrital compartment ($g/m^3 \cdot d$), see **(130)**;
Photosynthesis = rate of photosynthesis ($g/m^3 \cdot d$), see **(31)**, and
Uptake = fraction of photosynthate that is phosphate (unitless, 0.018).

At this time AQUATOX models only phosphate available for plants; a correction factor in the loading screen allows the user to scale total phosphate loadings to available phosphate. A future enhancement could be to consider phosphate precipitated with calcium carbonate, which would better represent the dynamics of marl lakes; however, that process is ignored in the current version. A default value is provided for average atmospheric deposition, but this should be adjusted for site conditions. In particular, entrainment of dust from tilled fields and new highway construction can cause significant increases in phosphate loadings. As with nitrogen, the uptake parameter is the Redfield (1958) ratio; it may be edited if a different ratio is desired (cf. Harris, 1986).

$$\frac{dOxygen}{dt} = Loading + Reaeration + Photosynthesized - BOD - NitroDemand - Washout \pm TurbDiff \quad \textbf{(150)}$$

5.4 Dissolved Oxygen

Oxygen is an important regulatory endpoint; very low levels can result in mass mortality for fish and other organisms, mobilization of nutrients and metals, and decreased degradation of toxic organic materials. Dissolved oxygen is simulated as a daily average and does not account for diurnal fluctuations. It is a function of reaeration, photosynthesis, respiration, decomposition, and nitrification:

$$Photosynthesized = O2Photo \cdot \Sigma_{Plant}(Photosynthesis_{Plant}) \quad \textbf{(151)}$$

$$BOD = O2Biomass \cdot (\Sigma_{Detritus}(Decomposition_{Detritus}) + \Sigma_{Organisms}(Respiration_{Organisms})) \quad \textbf{(152)}$$

$$NitroDemand = O2N \cdot Nitrify \quad \textbf{(153)}$$

where:

d*Oxygen*/dt	=	change in concentration of dissolved oxygen ($g/m^3 \cdot d$);
Loading	=	loading from inflow ($g/m^3 \cdot d$);
Reaeration	=	atmospheric exchange of oxygen ($g/m^3 \cdot d$);
Photosynthesized	=	oxygen produced by photosynthesis ($g/m^3 \cdot d$);
O2Photo	=	ratio of oxygen to photosynthesis (1.6, unitless);
BOD	=	instantaneous biological oxygen demand ($g/m^3 \cdot d$);
NitroDemand	=	oxygen taken up by nitrification ($g/m^3 \cdot d$);
Washout	=	loss due to being carried downstream ($g/m^3 \cdot d$), see **(16)**;
O2Biomass	=	ratio of oxygen to organic matter (mg oxygen/mg biomass; 0.575, but user can change in remineralization screen);
Photosynthesis	=	rate of photosynthesis ($g/m^3 \cdot d$), see **(31)**, **(73)**;
Decomposition	=	rate of decomposition ($g/m^3 \cdot d$), see **(130)**;
Respiration	=	rate of respiration ($g/m^3 \cdot d$), see **(55)** and **(87)**;
O2N	=	ratio of oxygen to nitrogen (unitless; 4.57, but user can change in remineralization screen); and
Nitrify	=	rate of nitrification ($g\ N/m^3 \cdot d$).

Reaeration is a function of the depth-averaged mass transfer coefficient *KReaer*, corrected for ambient temperature, multiplied by the difference between the dissolved oxygen level and the saturation level (cf. Bowie et al., 1985):

$$Reaeration = KReaer \cdot (O2Sat - Oxygen) \quad \textbf{(154)}$$

where:

Reaeration	=	mass transfer of oxygen ($g/m^3 \cdot d$);
KReaer	=	depth-averaged reaeration coefficient (1/d);
O2Sat	=	saturation concentration of oxygen (g/m^3), see **(163)**; and
Oxygen	=	concentration of oxygen (g/m^3).

In standing water *KReaer* is computed as a minimum transfer velocity plus the effect of wind on the transfer velocity (Schwarzenbach et al., 1993) divided by the thickness of the mixed layer to obtain a depth-averaged coefficient (**Figure 64**):

$$KReaer = \frac{(4E-4 + 4E-5 \cdot Wind^2) \cdot 864}{Thick} \tag{155}$$

where:

Wind	=	wind velocity 10 m above the water (m/sec);
864	=	conversion factor (cm/sec to m/d); and
Thick	=	thickness of mixed layer (m).

Algal blooms can generate dissolved oxygen levels that are as much as 400% of saturation (Wetzel, 2001). However, near-surface blue-green algal blooms, which are modeled as being in the top 0.33 m, produce high levels of oxygen that do not extend significantly into deeper water. An adjustment is made in the code so that if the blue-green algal biomass exceeds 1 mg/L and is greater than other phytoplankton biomass, the thickness subject to oxygen reaeration is set to 0.33 m. This does not affect the *KReaer* that is used in computing volatilization.

In streams, reaeration is a function of current velocity and water depth (**Figure 65**) following the approach of Covar (1978, see Bowie et al., 1985) and used in WASP (Ambrose et al., 1991). The decision rules for which equation to use are taken from the WASP5 code (Ambrose et al., 1991).

If *Vel* < 0.518 m/sec:

$$TransitionDepth = 0 \tag{156}$$

else:

$$TransitionDepth = 4.411 \cdot Vel^{2.9135} \tag{157}$$

where:

Vel	=	velocity of stream (converted to m/sec) see **(14)**; and
TransitionDepth	=	intermediate variable (m).

If *Depth* < 0.61 m, the equation of Owens et al. (1964, cited in Ambrose et al., 1991) is used:

$$KReaer = 5.349 \cdot Vel^{0.67} \cdot Depth^{-1.85} \tag{158}$$

where:

Depth = mean depth of stream (m).

Otherwise, if *Depth* is > *TransitionDepth*, the equation of O'Connor and Dobbins (1958, cited in Ambrose et al., 1991) is used:

$$KReaer = 3.93 \cdot Vel^{0.50} \cdot Depth^{-1.50} \tag{159}$$

Else, if *Depth* # *TransitionDepth*, the equation of Churchill et al. (1962, cited in Ambrose et al., 1991) is used:

$$KReaer = 5.049 \cdot Vel^{0.97} \cdot Depth^{-1.67} \tag{160}$$

In extremely shallow streams, especially experimental streams where depth is < 0.06 m, an equation developed by Krenkel and Orlob (1962, cited in Bowie et al. 1985) from flume data is used:

$$KReaer = \frac{234 \cdot (U \cdot Slope)^{0.408}}{H^{0.66}}$$

where:

U = velocity (converted to fps);
Slope = longitudinal channel slope (m/m); and
H = water depth (converted to ft).

If reaeration due to wind exceeds that due to current velocity, the equation for standing water is used. Reaeration is set to 0 if ice cover is expected (i.e., when the depth-averaged temperature < 3°C).

Figure 64
Reaeration as a Function of Wind

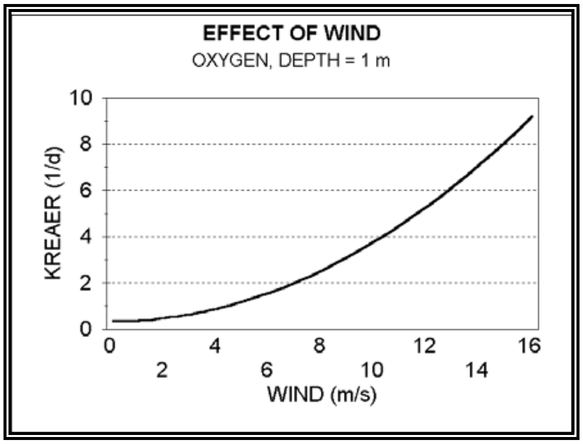
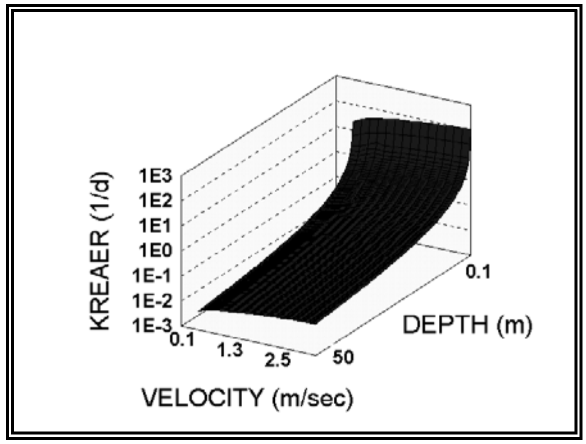


Figure 65
Reaeration in Streams



Reaeration is assumed to be representative of 20°C, so it is adjusted for ambient water temperature using (Thomann and Mueller 1987):

$$KReaer_T = KReaer_{20} \cdot Theta^{(Temperature - 20)} \tag{162}$$

where:

$KReaer_T$	=	Reaeration coefficient at ambient temperature (1/d);
$Kreaer_{20}$	=	Reaeration coefficient for 20°C (1/d);
Theta	=	temperature coefficient (1.024); and
Temperature	=	ambient water temperature (°C).

Oxygen saturation, as a function of both temperature (**Figure 66**) and salinity (**Figure 67**), is based on Weiss (1970, cited in Bowie et al., 1985):

$$O2Sat = 1.4277 \cdot \exp[-173.4927 + \frac{24963.39}{TKelvin} + 143.3483 \ln\left(\frac{TKelvin}{100}\right) - 0.21849 \cdot TKelvin + S \cdot (-0.033096 + 0.00014259 \cdot TKelvin - 1.7\ 10^{-7} \cdot \sqrt{TKelvin})] \tag{163}$$

where:

TKelvin	=	Kelvin temperature, and
S	=	salinity (ppt).

According to Bowie et al. (1985), it gives results that are not significantly different from those computed by the more complex APHA (1985) equations that are used in WASP (Ambrose et al., 1993). At the present time salinity is set to 0; although, it has little effect on reaeration.

Figure 66
Saturation as a Function of Temperature

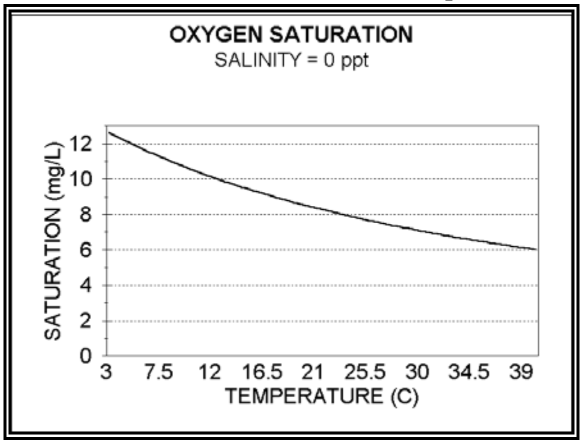
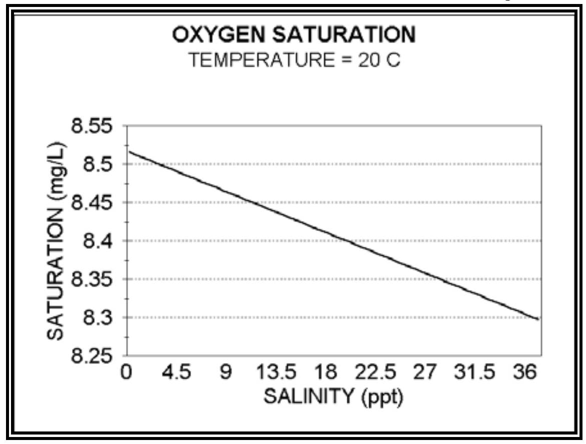


Figure 67
Saturation as a Function of Salinity



5.5 Inorganic Carbon

Many models ignore carbon dioxide as an ecosystem component (Bowie et al., 1985). However, it can be an important limiting nutrient. Similar to other nutrients, it is produced by decomposition and is assimilated by plants; it also is respired by organisms:

$$\frac{dCO2}{dt} = Loading + Respired + Decompose - Assimilation - Washout \pm CO2AtmosExch \pm TurbDiff \quad \textbf{(164)}$$

where:

$$Respired = CO2Biomass \cdot \Sigma_{Organism}(Respiration_{Organism}) \quad \textbf{(165)}$$

$$Assimilation = \Sigma_{Plant}(Photosynthesis_{Plant} \cdot UptakeCO2) \quad \textbf{(166)}$$

$$Decompose = CO2Biomass \cdot \Sigma_{Detritus}(Decomp_{Detritus}) \quad \textbf{(167)}$$

and where:

d*CO2*/dt	=	change in concentration of carbon dioxide (g/m$^3\cdot$d);
Loading	=	loading of carbon dioxide from inflow (g/m$^3\cdot$d);
Respired	=	carbon dioxide produced by respiration (g/m$^3\cdot$d);
Decompose	=	carbon dioxide derived from decomposition (g/m$^3\cdot$d);
Assimilation	=	assimilation of carbon dioxide by plants (g/m$^3\cdot$d);
Washout	=	loss due to being carried downstream (g/m$^3\cdot$d), see **(16)**;
CO2AtmosExch	=	interchange of carbon dioxide with atmosphere (g/m$^3\cdot$d);
TurbDiff	=	depth-averaged turbulent diffusion between epilimnion and hypolimnion if stratified (g/m$^3\cdot$d), see **(22)** and **(23)**;
CO2Biomass	=	ratio of carbon dioxide to organic matter (unitless; 0.526, according to Winberg, 1971);
Respiration	=	rate of respiration (g/m$^3\cdot$d), see **(55)** and **(87)**;
Decomposition	=	rate of decomposition (g/m$^3\cdot$d), see **(130)**;
Photosynthesis	=	rate of photosynthesis (g/m$^3\cdot$d), see **(31)**; and
UptakeCO2	=	ratio of carbon dioxide to photosynthate (= 0.53).

Carbon dioxide also is exchanged with the atmosphere; this process is important, but is not instantaneous: significant undersaturation and oversaturation are possible (Stumm and Morgan, 1996). The treatment of atmospheric exchange is similar to that for oxygen:

$$CO2AtmosExch = KLiqCO2 \cdot (CO2Sat - CO2) \qquad \textbf{(168)}$$

In fact, the mass transfer coefficient is based on the well-established reaeration coefficient for oxygen, corrected for the difference in diffusivity of carbon dioxide as recommended by Schwarzenbach et al. (1993):

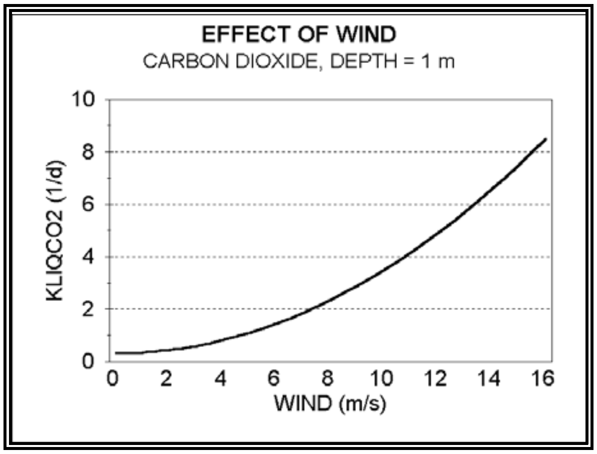
$$KLiqCO2 = KReaer \cdot \left(\frac{MolWtO2}{MolWtCO2} \right)^{0.25} \qquad \textbf{(169)}$$

where:

CO2AtmosExch	=	interchange of carbon dioxide with atmosphere (g/m$^3\cdot$d);
KLiqCO2	=	depth-averaged liquid-phase mass transfer coefficient (1/d);
CO2	=	concentration of carbon dioxide (g/m^3);
CO2Sat	=	saturation concentration of carbon dioxide (g/m^3), see **(170)**;
KReaer	=	depth-averaged reaeration coefficient for oxygen (1/d), see **(155)**-**(162)**;
MolWtO2	=	molecular weight of oxygen (=32); and
MolWtCO2	=	molecular weight of carbon dioxide (= 44).

Keying the mass-transfer coefficient for carbon dioxide to the reaeration coefficient for oxygen is very powerful in that the effects of wind (**Figure 68**) and the velocity and depth of streams can be represented, using the oxygen equations (Equations **(155)**- **(160)**).

Figure 68
Carbon Dioxide Mass Transfer



Based on this approach, the predicted mass transfer under still conditions is 0.92, compared to the observed value of 0.89 ± 0.03 (Lyman et al., 1982). This same approach is used, with minor modifications, to predict the volatilization of other chemicals (see Section **7.5**). Computation of saturation of carbon dioxide is based on the method in Bowie et al. (1985; see also Chapra and Reckhow, 1983) using Henry's law constant, with its temperature dependency (**Figure 69**), and the partial pressure of carbon dioxide:

$$CO2Sat = CO2Henry \cdot pCO2 \tag{170}$$

where:

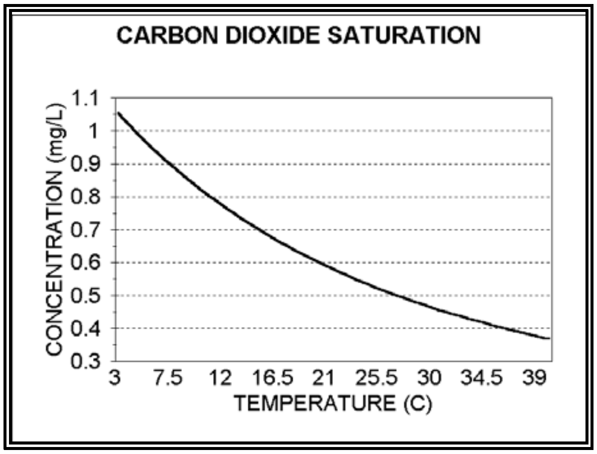
$$CO2Henry = MCO2 \cdot 10^{\frac{2385.73}{TKelvin} - 14.0184 + 0.0152642 \cdot TKelvin} \tag{171}$$

$$TKelvin = 273.15 + Temperature \tag{172}$$

and where:

CO2Sat	=	saturation concentration of carbon dioxide (g/m^3);
CO2Henry	=	Henry's law constant for carbon dioxide (g/m^3-atm)
pCO2	=	atmospheric partial pressure of carbon dioxide (= 0.00035);
MCO2	=	mg carbon dioxide per mole (= 44000);
TKelvin	=	temperature in °K, and
Temperature	=	ambient water temperature (°C).

Figure 69
Saturation of Carbon Dioxide



6 INORGANIC SEDIMENTS[1]

The sediment transport component of AQUATOX simulates scour, deposition and transport of sediments and calculates the concentration of sediments in the water column and sediment bed within a river reach. For running waters, the sediment is divided into three categories according to the particle size: 1) sand, with particle sizes between 0.062 to 2.0 millimeters (mm), 2) silt (0.004 to 0.062 mm), and 3) clay (0.00024 to 0.004 mm). Wash load (primarily clay and silt) is deposited or eroded within the channel reach depending on the daily flow regime. Sand transport is also computed within the channel reach. At present, inorganic sediments in standing water are computed based on total suspended solids loadings, described in section 6.3.

The river reach is assumed to be short and well mixed so that concentration does not vary longitudinally. Flow routing is not performed within the river reach. The daily average flow regime determines the amount of scour, deposition and transport of sediment. Scour, deposition and transport quantities are also limited by the amount of solids available in the bed sediments and the water column.

Inorganic sediments are important to the functioning of natural and perturbed ecosystems for several reasons. When suspended, they increase light extinction and decrease photosynthesis. When sedimented, they can temporarily or permanently remove toxicants from the active ecosystem through deep burial. Scour can adversely affect periphyton and zoobenthos. All these processes are represented to a certain degree in AQUATOX. In addition, rapid sedimentation also can adversely affect periphyton and some zoobenthos; and the ratio of inorganic to organic sediments can be used as an indicator of aerobic or anaerobic conditions in the bottom sediments. These are not simulated in the model at this time.

The mass of sediment in each of the three sediment size classes is a function of the previous mass, and the mass of sediment in the overlying water column lost through deposition, and gained through scour:

$$MassBed_{Sed} = MassBed_{Sed,\ t=-1} + (Deposit_{Sed} - Scour_{Sed}) \cdot Volume_{Water} \tag{173}$$

where:

$MassBed_{Sed}$	=	mass of sediment in channel bed (kg);
$MassBed_{Sed,\ t=-1}$	=	mass of sediment in channel bed on previous day (kg);
$Deposit_{Sed}$	=	amount of suspended sediment deposited (kg/m^3); see **(184)**;
$Scour_{Sed}$	=	amount of silt or clay resuspended (kg/m^3); see **(181)**; and
$Volume_{Water}$	=	volume of stream reach (m^3); see page 3-1.

[1] Original version contributed by Rodolfo Camacho of Abt Associates Inc.

The volumes of the respective sediment size classes are calculated as:

$$Volume_{Sed} = \frac{MassBed_{Sed}}{Rho_{Sed}} \tag{174}$$

where:

$Volume_{Sed}$	=	volume of given sediment size class (m^3);
$MassBed_{Sed}$	=	mass of the given sediment size class (kg); see **(173)**;
Rho_{Sed}	=	density of given sediment size class (kg/m^3);
Rho_{Sand}	=	2600 (kg/m^3); and
$Rho_{Silt, Clay}$	=	2400 (kg/m^3).

The porosity of the bed is calculated as the volume weighted average of the porosity of its components:

$$BedPorosity = \sum Frac_{Sed} \cdot Porosity_{Sed} \tag{175}$$

where:

$BedPorosity$	=	porosity of the bed (fraction);
$Frac_{Sed}$	=	fraction of the bed that is composed of given sediment class; and
$Porosity_{Sed}$	=	porosity of given sediment class.

The total volume of the bed is calculated as:

$$BedVolume = \frac{Volume_{Sand} + Volume_{Silt} + Volume_{Clay}}{1 - BedPorosity} \tag{176}$$

where:

$BedVolume$	=	volume of the bed (m^3).

The depth of the bed is calculated as

$$BedDepth = \frac{BedVolume}{ChannelLength \cdot ChannelWidth} \tag{177}$$

where:

$BedDepth$	=	depth of the sediment bed (m);
$ChannelLength$	=	length of the channel (m); and
$ChannelWidth$	=	width of the channel (m).

The concentrations of silt and clay in the water column are computed similarly to the mass of those sediments in the bed, with the addition of loadings from upstream and losses downstream:

$$\frac{dConc_{Sed}}{dt} = Load_{Sed} + Scour_{Sed} - Deposit_{Sed} - Wash_{Sed} \tag{178}$$

where:

$Conc_{Sed}$	=	concentration of silt or clay in water column (kg/m^3);
$Load_{Sed}$	=	loading of clay or silt (kg/m^3 d);
$Scour_{Sed}$	=	amount of silt or clay resuspended (kg/m^3 d); see **(181)**;
$Deposit_{Sed}$	=	amount of suspended sediment deposited (kg/m^3 d); see **(184)**; and
$Wash_{Sed}$	=	amount of sediment lost through downstream transport (kg/m^3 d); see **(185)**.

The concentration of sand is computed using a totally different approach, which is described in Section **6.2**.

6.1 Deposition and Scour of Silt and Clay

Relationships for scour and deposition of cohesive sediments (silts and clays) used in AQUATOX are the same as the ones used by the Hydrologic Simulation Program in Fortran (HSPF, US EPA 1991). Deposition and scour of silts and clay are modeled using the relationships for deposition (Krone, 1962) and scour (Partheniades, 1965) as summarized by Partheniades (1971).

Shear stress is computed as (Bicknell et al., 1992):

$$Tau = H2ODensity \cdot Slope \cdot HRadius \tag{179}$$

where:

Tau	=	shear stress (kg/m^2);
$H2ODensity$	=	density of water (1000 kg/m^3);
$Slope$	=	slope of channel (m/m);

and hydraulic radius (*HRadius*) is (Colby and McIntire, 1978):

$$HRadius = \frac{Y \cdot Width}{2 \cdot Y + Width} \tag{180}$$

where:

$HRadius$	=	hydraulic radius (m);
Y	=	average depth over reach (m); and
$Width$	=	channel width (m).

Resuspension or scour of bed sediments is predicted to occur when the computed shear stress is greater than the critical shear stress for scour:

$$\text{if } Tau > TauScour_{Sed} \text{ then}$$
$$Scour_{Sed} = \frac{Erodibility_{Sed}}{Y} \cdot \left(\frac{Tau}{TauScour_{Sed}} - 1 \right) \tag{181}$$

where:

$Scour_{Sed}$ = resuspension of silt or clay (kg/m^3); see also **(183)**;
$Erodibility_{Sed}$ = erodibility coefficient, (0.244 kg/m^2); and
$TauScour_{Sed}$ = critical shear stress for scour of silt or clay (kg/m^2); default values are given in stream data screen, but may be changed by the user.

The amount of sediment that is resuspended is constrained by the mass of sediments stored in the bed. An intermediate variable representing the maximum potential mass that can be scoured is calculated; if the mass available is less than the potential, then scour is set to the lower amount:

$$Check_{Sed} = Scour_{Sed} \cdot Volume_{Water} \tag{182}$$

$$\text{if } Mass_{Sed} \leq Check_{Sed} \text{ then}$$
$$Scour_{Sed} = \frac{Mass_{Sed}}{Volume_{Water}} \tag{183}$$

where:

$Check_{Sed}$ = maximum potential mass (kg); and
$Mass_{Sed}$ = mass of silt or clay in bed (kg); see **(173)**.

Deposition occurs when the computed shear stress is less than the critical depositional shear stress:

$$\text{if } Tau < TauDep_{Sed} \text{ then}$$
$$Deposit_{Sed} = Conc_{Sed} \cdot \left(1 - e^{\frac{-VT_{Sed} \cdot SecPerDay}{Y} \cdot (1 - \frac{Tau}{TauDep_{Sed}})} \right) \tag{184}$$

where:

$Deposit_{Sed}$ = amount of sediment deposited (kg/m^3 day);
$TauDep_{Sed}$ = critical depositional shear stress (kg/m^2); default values are given in stream data screen, but may be changed by the user;

$Conc_{Sed}$	=	concentration of suspended silt or clay (kg/m^3); see **(178)**;
VT_{Sed}	=	terminal fall velocity of given sediment type (m/s); default values are given in stream data screen, but may be changed by the user; and
$SecPerDay$	=	86400 (seconds / day).

Downstream transport is an important mechanism for loss of suspended sediment from a given stream reach:

$$Wash_{Sed} = \frac{Disch \cdot Conc_{Sed}}{SegVolume} \tag{185}$$

where:

$Wash_{Sed}$	=	amount of given sediment lost to downstream transport (kg/m^3 day);
$Disch$	=	discharge of water from the segment (m^3/day);
$Conc_{Sed}$	=	concentration of suspended sediment (kg/m^3);
$SegVolume$	=	volume of segment (m^3); see page 3-1.

When the inorganic sediment model is included in an AQUATOX stream simulation, the deposition and erosion of detritus mimics the deposition and erosion of silt. The fraction of detritus that is being scoured or deposited is assumed to equal the fraction of silt that is being scoured or deposited. The following equations are used to calculate the scour and deposition of detritus:

$$FracScour_{Detritus} = FracScour_{Silt} = Scour_{Silt} \cdot \frac{Volume_{Silt}}{Mass_{Silt}} \tag{186}$$

$$Scour_{Detritus} = FracScour_{Detritus} \cdot Conc_{AllSedDetritus} \cdot 1000 \tag{187}$$

where:

$FracScour$	=	fraction of scour per day (fraction/day);
$Scour_{Silt}$	=	amount of silt scoured (kg/m^3 day) see **(181)**;
$Volume_{Silt}$	=	volume of silt in the bed (m^3); see **(174)**;
$Mass_{Silt}$	=	mass of silt in the bed (kg); see **(173)**;
$Conc_{AllSedDetritus}$	=	all sedimented detritus (labile and refractory) in the stream bed (kg/m^3);
$Scour_{Detritus}$	=	amount of detritus scoured (g/m^3 day); and
1000	=	conversion of kg to g.

The equations for deposition of detritus are similar:

$$FracDeposition_{Detritus} = FracDeposition_{Silt} = \frac{Deposition_{Silt} \cdot 1000}{Conc_{Silt}} \quad (188)$$

$$Deposition_{Detritus} = FracDeposition_{Detritus} \cdot Conc_{SuspDetritus} \quad (189)$$

where:

$Deposition_{Silt}$	=	amount of silt deposited (kg/m^3 day) see **(184)**;
$Conc_{Silt}$	=	amount of silt initially in the water (g/m^3);
$FracDeposition$	=	fraction of deposition per day (frac / day); and
$Conc_{SuspDetritus}$	=	amount of suspended detritus initially in the water (g/m^3); and
$Deposition_{Detritus}$	=	amount of detritus deposited (g/m^3 day).

6.2 Scour, Deposition and Transport of Sand

Scour, deposition and transport of sand are simulated using the Engelund and Hansen (1967) sediment transport relationships as presented by Brownlie (1981). This relationship was selected because of its simplicity and accuracy. Brownlie (1981) shows that this relationship gives good results when compared to 13 others using a field and laboratory data set of about 7,000 records.

$$PotConc_{Sand} = 0.05 \cdot \frac{Rho}{Rho_{Sand} - Rho} \cdot \frac{Velocity \cdot Slope}{\sqrt{\frac{Rho_{Sand} - Rho}{Rho} \cdot g \cdot D_{Sand}/1000}} \cdot \sqrt{TauStar} \quad (190)$$

where:

$PotConc_{Sand}$	=	potential concentration of suspended sand (kg/m^3);
Rho	=	density of water (1000 kg/m3)
Rho_{Sand}	=	density of sand (2650 kg/m^3);
$Velocity$	=	flow velocity (converted to m/s);
$Slope$	=	slope of stream (m/m);
D_{Sand}	=	mean diameter of sand particle (0.30 mm converted to m); and
$TauStar$	=	dimensionless shear stress.

The dimensionless shear stress is calculated by:

$$TauStar = \frac{Rho}{Rho_{Sand} - Rho} \cdot HRadius \cdot \frac{Slope}{D_{Sand}/1000} \quad (191)$$

where:

HRadius = hydraulic radius (m).

Once the potential concentration has been determined for the given flow rate and channel characteristics, it is compared with the present concentration. If the potential concentration is greater, the difference is considered to be made available through scour, up to the limit of the bed. If the potential concentration is less than what is in suspension, the difference is considered to be deposited:

$$Check_{Sand} = PotConc_{Sand} \cdot Volume_{Water} \tag{192}$$

$$MassSusp_{Sand} = Conc_{Sand} \cdot Volume_{Water} \tag{193}$$

$$TotalMass_{Sand} = MassSusp_{Sand} + MassBed_{Sand} \tag{194}$$

$$\begin{gathered} \text{if } Check_{Sand} \le MassSusp_{Sand} \text{ then} \\ Deposit_{Sand} = MassSusp_{Sand} - Check_{Sand} \\ Conc_{Sand} = PotConc_{Sand} \end{gathered} \tag{195}$$

$$\begin{gathered} \text{if } Check_{Sand} \ge TotalMass_{Sand} \ \textit{then} \\ MassBed_{Sand} = 0 \\ Conc_{Sand} = \frac{TotalMass_{Sand}}{Volume_{Water}} \end{gathered} \tag{196}$$

$$\text{if } Check_{Sand} > MassSusp_{Sand} \text{ and } < TotalMass_{Sand} \text{ then}$$

$$Scour_{Sand} = Check_{Sand} - MassSusp_{Sand}$$
$$Conc_{Sand} = \frac{MassSusp_{Sand} + Scour_{Sand}}{Volume_{Water}} \tag{197}$$

where:

$Check_{Sand}$	=	maximum potential mass (kg);
$MassBed_{Sand}$	=	mass of sand in bed (kg);
$MassSusp_{Sand}$	=	mass of sand in water column (kg);
$Conc_{Sand}$	=	concentration of sand in water column (kg/m^3);
$Scour_{Sand}$	=	amount of sand resuspended (kg/m^3 d);
$Deposit_{Sand}$	=	amount of suspended sand deposited (kg/m^3 d);
$PotConc_{Sand}$	=	potential concentration of suspended sand (kg/m^3); see **(190)**;
Volume	=	volume of reach (m^3); see page 3-1.

6.3 Suspended Inorganic Sediments in Standing Water

At present, AQUATOX does not compute settling of inorganic sediments in standing water or scour as a function of wave action. However, suspended sediments are important in creating turbidity and limiting light, especially in reservoirs and shallow lakes. Therefore, the user can provide loadings of total suspended solids (TSS), and the model will back-calculate suspended inorganic sediment concentrations by subtracting the simulated phytoplankton and suspended detritus concentrations:

$$InorgSed = TSS - \sum Phyto - \sum PartDetr \tag{198}$$

where:

InorgSed	=	concentration of suspended inorganic sediments (g/m^3);
TSS	=	observed concentration of total suspended solids (g/m^3);
Phyto	=	predicted phytoplankton concentrations (g/m^3), see **(29)**, **(30)**; and
PartDetr	=	predicted suspended detritus concentrations (g/m^3), see **(112)**, **(113)**.

The concentration of suspended inorganic sediments is used solely to calculate their contribution to the extinction coefficient, which affects the depth of the euphotic zone and the Secchi depth (see **(35)**, **(36)**).

7 TOXIC ORGANIC CHEMICALS

The chemical fate module of AQUATOX predicts the partitioning of a compound between water, sediment, and biota (**Figure 70**), and estimates the rate of degradation of the compound (**Figure 71**). Microbial degradation, biotransformation, photolysis, hydrolysis, and volatilization are modeled in AQUATOX. Each of these processes is described generally, and again in more detail below.

Nonequilibrium concentrations, as represented by kinetic equations, depend on sorption, desorption, and elimination as functions of the chemical and exposure through water and food as a function of bioenergetics of the organism. Equilibrium partitioning is computed as a constraint on sorption and for purposes of computing critical body residues for ecotoxicity, but it is no longer an output from AQUATOX. Partitioning to inorganic sediments is not modeled at this time.

Microbial degradation is modeled by entering a maximum biodegradation rate for a particular organic toxicant, which is subsequently reduced to account for suboptimal temperature, pH, and dissolved oxygen. Biotransformation is represented by user-supplied first-order rate constants with the option of also modeling multiple daughter products. Photolysis is modeled by using a light screening factor (Schwarzenbach et al., 1993) and the near-surface, direct photolysis first-order rate constant for each pollutant. The light screening factor is a function of both the diffuse attenuation coefficient near the surface and the average diffuse attenuation coefficient for the whole water column. For those organic chemicals that undergo hydrolysis, neutral, acid-, and base-catalyzed reaction rates are entered into AQUATOX as applicable. Volatilization is modeled using a stagnant two-film model, with the air and water transfer velocities approximated by empirical equations based on reaeration of oxygen (Schwarzenbach et al., 1993).

Figure 70. In-situ Uptake and Release of Chlorpyrifos in a Pond

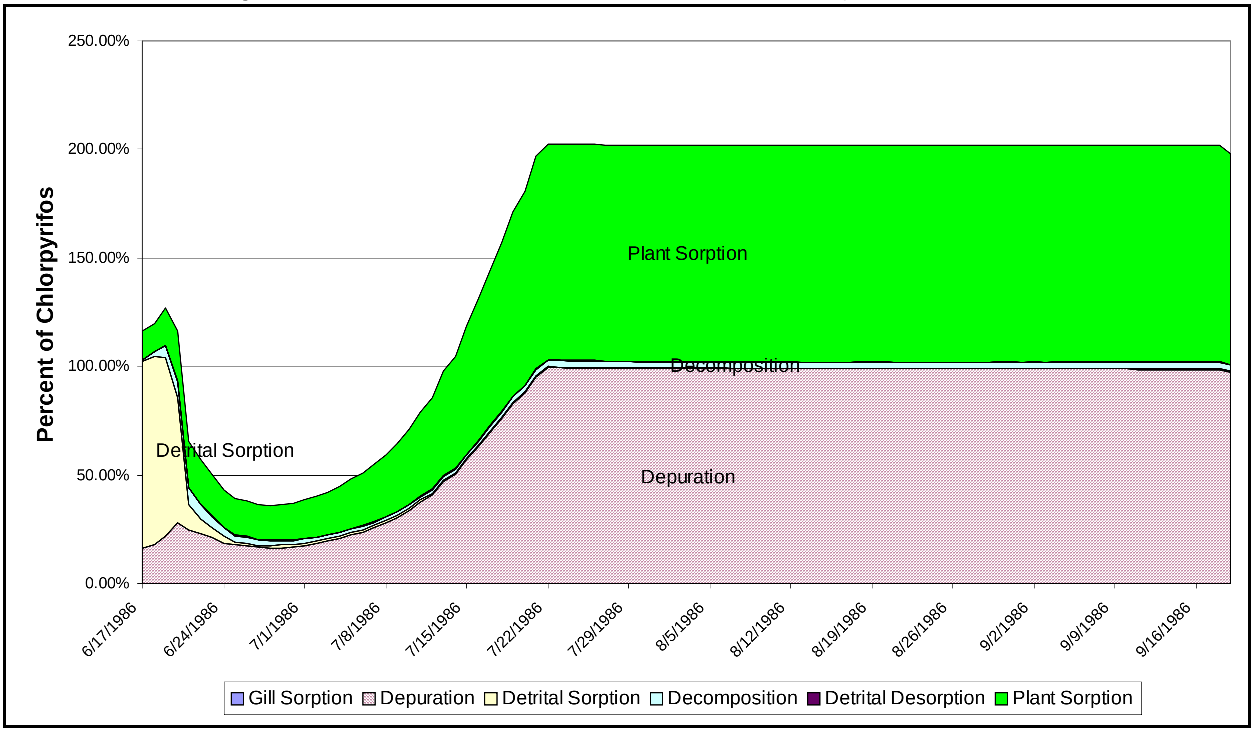
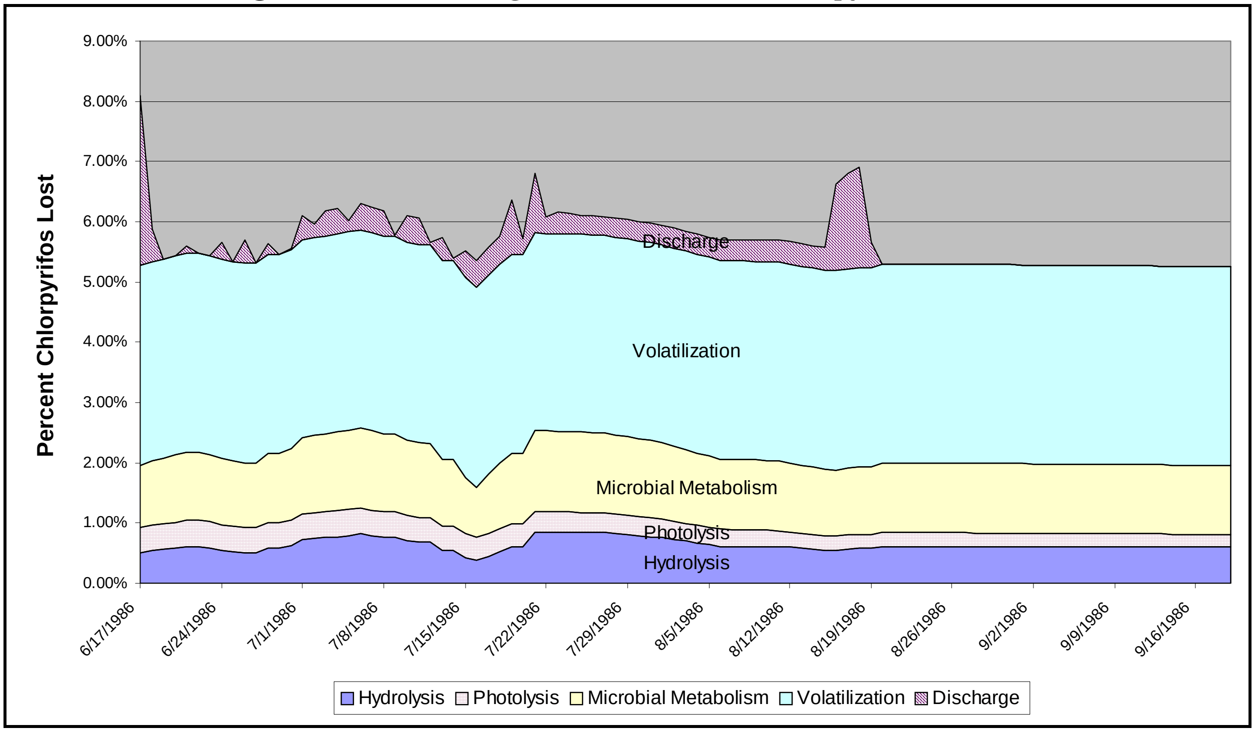


Figure 71. In-situ Degradation Rates for Chlorpyrifos in Pond



The mass balance equations follow. For computational ease, the concentrations of all toxicants are converted to μg/L of water (they also are computed as ppb in each carrier). The change in mass of toxicant in the water includes explicit representations of mobilization of the toxicant from sediment to water as a result of decomposition of the labile sediment detritus compartment, sorption to and desorption from the detrital sediment compartments, uptake by algae and macrophytes, uptake across the gills of animals, depuration by organisms, and turbulent diffusion between epilimnion and hypolimnion:

$$\begin{aligned}\frac{dToxicant_{Water}}{dt} = {} & Loading + \sum_{LabileDetr} (Decomposition_{LabileDetr} \cdot PPB_{LabileDetr} \cdot 1e-6) \\ & + \sum Desorption_{DetrTox} + \sum Depuration_{Org} - \sum Sorption_{DetrTox} \\ & - \sum GillUptake - MacroUptake - \sum AlgalUptake_{Alga} \\ & - Hydrolysis - Photolysis - MicrobialDegrdn + Volatilization \\ & - Discharge + Biotransform_{Microb\ In} \pm TurbDiff\end{aligned} \qquad (199)$$

The equations for the toxicant associated with the two sediment detritus compartments are rather involved, involving direct processes such as sorption and indirect conversions such as defecation. However, photolysis is not included based on the assumption that it is not a significant process for detrital sediments. Either scour or resuspension is simulated, depending on whether or not inorganic sediments are modeled (scour of detritus is linked to scour of silt).

$$\frac{dToxicant_{SedLabileDetr}}{dt} = Sorption - Desorption + (Colonization \cdot PPB_{SedRefrDetr} \cdot 1e-6) + \sum_{Pred}\sum_{Prey} Def2SedLabile \cdot DefecationTox_{Pred,\,Prey} - (Resuspension + Scour + Decomposition) \cdot PPB_{SedLabileDetr} \cdot 1e-6 - \sum_{Pred} Ingestion_{Pred,\,SedLabileDetr} \cdot PPB_{SedLabileDetr} \cdot 1e-6 + (Sedimentation + Deposition) \cdot PPB_{SuspLabileDetr} \cdot 1e-6 + \sum (Sed2Detr \cdot Sink_{Phyto} \cdot PPB_{Phyto} \cdot 1e-6) - Hydrolysis - MicrobialDegrdn - Burial + Expose \pm Biotransform_{Microbial} \quad \textbf{(200)}$$

$$\frac{dToxicant_{SedRefrDetr}}{dt} = Sorption - Desorption + \sum_{Pred}\sum_{Prey} (1 - Def2SedLabile) \cdot DefecationTox_{Pred,\,Prey} - (Resuspension + Scour + Colonization) \cdot PPB_{SedRefrDetr} \cdot 1e-6 - \sum_{Pred} Ingestion_{Pred,\,SedRefrDetr} \cdot PPB_{SedRefrDetr} \cdot 1e-6 + (Sedimentation + Deposition) \cdot PPB_{SuspRefrDetr} \cdot 1e-6 + \sum (Sed2Detr \cdot Sink_{Phyto} \cdot PPB_{Phyto} \cdot 1e-6) - Hydrolysis - MicrobialDegrdn - Burial + Expose \pm Biotransform_{Microbial} \quad \textbf{(201)}$$

The equations are similar for the toxicant associated with suspended and dissolved detritus, with deposition or sedimentation, depending on whether or not inorganic sediments are modeled:

$$\frac{dToxicant_{SuspLabileDetr}}{dt} = Loading + Sorption - Desorption + \sum_{Org} ((Mort2Detr \cdot Mortality_{Org} + GameteLoss_{Org}) \cdot PPB_{Org} \cdot 1e-6) - (Sedimentation + Deposition + Washout + Decomposition + \sum_{Pred} Ingestion_{Pred,\,SuspLabileDetr}) \cdot PPB_{SuspLabileDetr} \cdot 1e-6 + Colonization \cdot PPB_{SuspRefrDetr} \cdot 1e-6 \pm Biotransform_{Microbial} + (Resuspension + Scour) \cdot PPB_{SedLabileDetr} \cdot 1e-6 \pm SedToHyp - Hydrolysis - Photolysis - MicrobialDegrdn \pm TurbDiff \quad \textbf{(202)}$$

$$\frac{dToxicant_{SuspRefrDetr}}{dt} = Loading + Sorption - Desorption + \sum_{Org} (Mort2Ref \cdot Mortality_{Org} \cdot PPB_{Org} \cdot 1e-6) - (Sedimentation + Deposition + Washout + Colonization \pm Biotransform_{Microbial} + \sum_{Pred} Ingestion_{SuspRefrDetr}) \cdot PPB_{SuspRefrDetr} \cdot 1e-6 + (Resuspension + Scour) \cdot PPB_{SedRefrDetr} \cdot 1e-6 \pm SedToHyp - Hydrolysis - Photolysis - MicrobialDegrdn \pm TurbDiff \tag{203}$$

$$\frac{dToxicant_{DissLabileDetr}}{dt} = Loading + Sorption - Desorption + \sum ExcrToxToDiss_{Org} + \sum_{Org} (Mort2Detr \cdot Mortality_{Org} \cdot PPB_{Org} \cdot 1e-6) - (Washout + Decomposition) \cdot PPB_{DissLabileDetr} \cdot 1e-6 \pm Biotransform_{Microbial} - Hydrolysis - Photolysis - MicrobialDegrdn \pm TurbDiff \tag{204}$$

$$\frac{dToxicant_{DissRefrDetr}}{dt} = Loading + Sorption - Desorption + \sum ExcToxToDiss_{Org} + \sum_{Org} (Mort2Ref \cdot Mortality_{Org} \cdot PPB_{Org} \cdot 1e-6) - (Washout + Colonization) \cdot PPB_{DissRefrDetr} \cdot 1e-6 \pm Biotransform_{Microbial} - Hydrolysis - Photolysis - MicrobialDegrdn \pm TurbDiff \tag{205}$$

Note that there are no equations for buried detritus, as they are considered to be sequestered and outside of the influence of any processes which would change the concentrations of their associated toxicants.

Algae are represented as:

$$\frac{dToxicant_{Alga}}{dt} = Loading + AlgalUptake - Depuration \pm TurbDiff - (Excretion + Washout + \sum_{Pred} Predation_{Pred,\, Alga} + Mortality + Sink \pm SinkToHypo) \cdot PPB_{Alga} \cdot 1e-6 \pm Biotransform_{Alga} \tag{206}$$

Macrophytes are represented similarly, but reflecting the fact that they are stationary:

$$\frac{dToxicant_{Macrophyte}}{dt} = Loading + MacroUptake - Depuration - (Excretion + \sum_{Pred} Predation_{Pred,\ Macro} + Mortality + Breakage) \cdot PPB_{Macro} \cdot 1e-6 \pm Biotransform_{Macrophyte} \quad \textbf{(208)}$$

$$\frac{dToxicant_{Animal}}{dt} = Loading + GillUptake + \sum_{Prey} DietUptake \pm TurbDiff - (Depuration + \sum_{Pred} Predation_{Pred,\ Animal} + Mortality + Recruit \pm Promotion + GameteLoss + Drift + Migration + EmergeInsect) \cdot PPB_{Animal} \cdot 1e-6 \pm Biotransform_{Animal} \quad \textbf{(207)}$$

The toxicant associated with animals is represented by an involved kinetic equation because of the various routes of exposure and transfer:
where:

$Toxicant_{Water}$	=	toxicant in dissolved phase in unit volume of water (:g/L);
$Toxicant_{SedDetr}$	=	mass of toxicant associated with each of the two sediment detritus compartments in unit volume of water (:g/L);
$Toxicant_{SuspDetr}$	=	mass of toxicant associated with each of the two suspended detritus compartments in unit volume of water (:g/L);
$Toxicant_{DissDetr}$	=	mass of toxicant associated with each of the two dissolved organic compartments in unit volume of water (:g/L);
$Toxicant_{Alga}$	=	mass of toxicant associated with given alga in unit volume of water (:g/L);
$Toxicant_{Macrophyte}$	=	mass of toxicant associated with macrophyte in unit volume of water (:g/L);
$Toxicant_{Animal}$	=	mass of toxicant associated with given animal in unit volume of water (:g/L);
$PPB_{SedDetr}$	=	concentration of toxicant in sediment detritus (:g/kg), see **(209)**;
$PPB_{SuspDetr}$	=	concentration of toxicant in suspended detritus (:g/kg);
$PPB_{DissDetr}$	=	concentration of toxicant in dissolved organics (:g/kg);
PPB_{Alga}	=	concentration of toxicant in given alga (:g/kg);
$PPB_{Macrophyte}$	=	concentration of toxicant in macrophyte (:g/kg);
PPB_{Animal}	=	concentration of toxicant in given animal (:g/kg);
1 e -6	=	units conversion (kg/mg);
Loading	=	loading of toxicant from external sources (:g/L"d);
TurbDiff	=	depth-averaged turbulent diffusion between epilimnion and hypolimnion (:g/L"d), see **(22)** and **(23)**.
Hydrolysis	=	rate of loss due to hydrolysis (:g/L"d), see **(212)**;
$Biotransform_{Microbial}$	=	biotransformation to or from given organic chemical in given detrital compartment due to microbial decomposition (:g/L"d), see **(273)**;

$Biotransform_{Org}$	=	biotransformation to or from given organic chemical within the given organism (:g/L"d);
Photolysis	=	rate of loss due to direct photolysis (:g/L"d), see **(219)**; assumed not to be significant for bottom sediments;
MicrobialDegrdn	=	rate of loss due to microbial degradation (:g/L"d), see **(225)**;
Volatilization	=	rate of loss due to volatilization (:g/L"d), see **(230)**;
Discharge	=	rate of loss of toxicant due to discharge downstream (:g/L"d), see **Table 1**;
Burial	=	rate of loss due to deep burial (:g/L"d) see **(184)**;
Expose	=	rate of exposure due to resuspension of overlying sediments (:g/L"d), see **(181)**;
Decomposition	=	rate of decomposition of given detritus (mg/L"d), see **(130)**;
Depuration	=	elimination rate for toxicant due to clearance (:g/L"d), see **(262)** and **(269)**;
Sorption	=	rate of sorption to given compartment (:g/L"d), see **(249)**;
Desorption	=	rate of desorption from given compartment (:g/L"d), see **(250)**;
Colonization	=	rate of conversion of refractory to labile detritus (g/m3"d), see **(126)**;
$DefecationTox_{Pred, Prey}$	=	rate of transfer of toxicant due to defecation of given prey by given predator (:g/L"d), see **(276)**;
Def2SedLabile	=	fraction of defecation that goes to sediment labile detritus;
Resuspension	=	rate of resuspension of given sediment detritus (mg/L"d) without the inorganic sediment model attached, see **(135)**;
Scour	=	rate of resuspension of given sediment detritus (mg/L"d) in streams with the inorganic sediment model attached, see **(187)**;
Sedimentation	=	rate of sedimentation of given suspended detritus (mg/L"d), without the inorganic sediment model attached, see **(135)**;
Deposition	=	rate of sedimentation of given suspended detritus (mg/L"d) in streams with the inorganic sediment model attached, see **(189)**;
Sed2Detr	=	fraction of sinking phytoplankton that goes to given detrital compartment;
Sink	=	loss rate of phytoplankton to bottom sediments (mg/L"d), see **(61)**;
$Mortality_{Org}$	=	nonpredatory mortality of given organism (mg/L"d), see **(98)**;
Mort2Detr	=	fraction of dead organism that is labile (unitless);
GameteLoss	=	loss rate for gametes (g/m3"d), see **(102)**;
Mort2Ref	=	fraction of dead organism that is refractory (unitless);
Washout or *Drift*	=	rate of loss of given suspended detritus or organism due to being carried downstream (mg/L"d), see **(16)**, **(63)**, **(67)**, **(105)**, and **(106)**;
SedToHyp	=	rate of settling loss to hypolimnion from epilimnion (mg/L"d). May be positive or negative depending on segment being simulated;

$Ingestion_{Pred, Prey}$	=	rate of ingestion of given food or prey by given predator (mg/L·d), see **(78)**;
$Predation_{Pred, Prey}$	=	predatory mortality by given predator on given prey (mg/L·d), see **(86)**;
$ExcToxToDiss_{Org}$	=	toxicant excretion from plants to dissolved organics (mg/L·d);
Excretion	=	excretion rate for given plant (g/m^3·d), see **(97)**;
SinkToHypo	=	rate of transfer of phytoplankton to hypolimnion (mg/L·d). May be positive or negative depending on segment being modeled;
AlgalUptake	=	rate of sorption by algae (μg/L - d), see **(260)**;
MacroUptake	=	rate of sorption by macrophytes (μg/L - d), see **(256)**;
GillUptake	=	rate of absorption of toxicant by the gills (μg/L - d), see **(265)**;
$DietUptake_{Prey}$	=	rate of dietary absorption of toxicant associated with given prey (μg/L·d), see **(268)**;
Recruit	=	biomass gained from successful spawning (g/m^3·d), see **(104)**;
Promotion	=	promotion from one age class to the next (mg/L·d), see **(110)**;
Migration	=	rate of migration (g/m^3·d), see **(109)**; and
EmergeInsect	=	insect emergence (mg/L·d), see **(111)**.

The concentration in each carrier is given by:

$$PPB_i = \frac{ToxState_i}{CarrierState_i} \cdot 1e6 \qquad \textbf{(209)}$$

where:

PPB_i	=	concentration of chemical in carrier *i* (μg/kg);
$ToxState_i$	=	mass of chemical in carrier *i* (ug/L);
CarrierState	=	biomass of carrier (mg/L); and
1e6	=	conversion factor (mg/kg).

7.1 Ionization

Dissociation of an organic acid or base in water can have a significant effect on its environmental properties. In particular, solubility, volatilization, photolysis, sorption, and bioconcentration of an ionized compound can be affected. Rather than modeling ionization products, the approach taken in AQUATOX is to represent the modifications to the fate and transport of the neutral species, based on the fraction that is not dissociated. The acid dissociation constant is expressed as the negative log, *pKa*, and the fraction that is not ionized is:

$$Nondissoc = \frac{1}{1 + 10^{(pH - pKa)}} \qquad \textbf{(210)}$$

where:

Nondissoc = nondissociated fraction (unitless).

If the compound is a base then the fraction not ionized is:

$$Nondissoc = \frac{1}{1 + 10^{(pKa - pH)}} \tag{211}$$

When $pKa = pH$ half the compound is ionized and half is not (**Figure 72**). At ambient environmental pH values, compounds with a pKa in the range of 4 to 9 will exhibit significant dissociation (**Figure 73**).

Figure 72
Dissociation of Pentachlorophenol (pKa = 4.75) at Higher pH Values

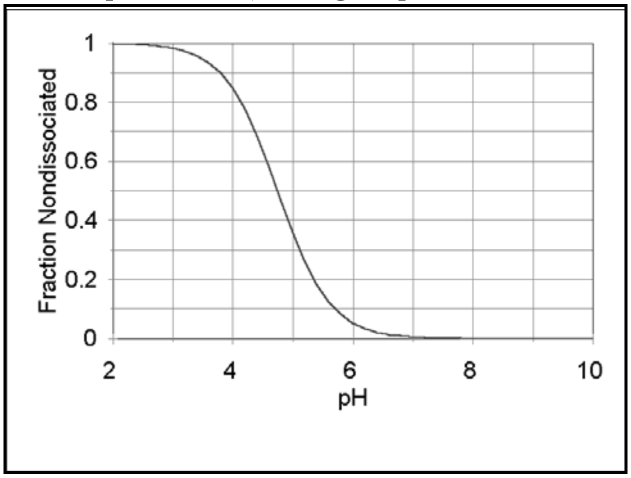
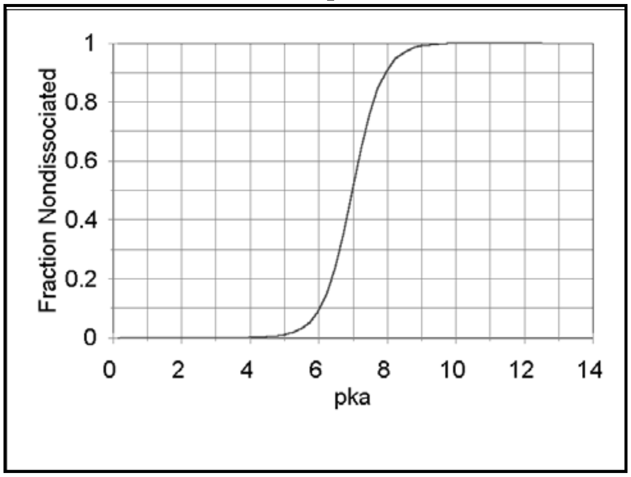


Figure 73
Dissociation as a Function of pKa at an Ambient pH of 7



7.2 Hydrolysis

Hydrolysis is the degradation of a compound through reaction with water. During hydrolysis, both a pollutant molecule and a water molecule are split, and the two water molecule fragments (H^+ and OH^-) join to the two pollutant fragments to form new chemicals. Neutral and acid- and base-catalyzed hydrolysis are modeled using the approach of Mabey and Mill (1978) in which an overall pseudo-first-order rate constant is computed for a given pH, adjusted for the ambient temperature of the water:

$$Hydrolysis = KHyd \cdot Toxicant_{Phase} \tag{212}$$

where:

$$KHyd = (KAcidExp + KBaseExp + KUncat) \cdot Arrhen \qquad \textbf{(213)}$$

and where:

KHyd = overall pseudo-first-order rate constant for a given pH and temperature (1/d);
KAcidExp = pseudo-first-order acid-catalyzed rate constant for a given pH (1/d);
KBaseExp = pseudo-first-order base-catalyzed rate constant for a given pH (1/d);
KUncat = the measured first-order reaction rate at pH 7 (1/d); and
Arrhen = temperature adjustment (unitless), see **(218)**.

There are three types of hydrolysis: acid-catalyzed, base-catalyzed, and neutral. In neutral hydrolysis reactions, the pollutant reacts with a water molecule (H_2O) and the concentration of water is usually included in *KUncat*. In acid-catalyzed hydrolysis, the hydrogen ion reacts with the pollutant, and a first-order decay rate for a given pH can be estimated as follows:

$$KAcidExp = KAcid \cdot HIon \qquad \textbf{(214)}$$

where:

$$HIon = 10^{-pH} \qquad \textbf{(215)}$$

and where:

KAcid = acid-catalyzed rate constant (L/mol · d);
HIon = concentration of hydrogen ions (mol/L); and
pH = pH of water column.

Likewise for base-catalyzed hydrolysis, the first-order rate constant for a reaction between the hydroxide ion and the pollutant at a given pH (**Figure 74**) can be described as:

$$KBaseExp = KBase \cdot OHIon \qquad \textbf{(216)}$$

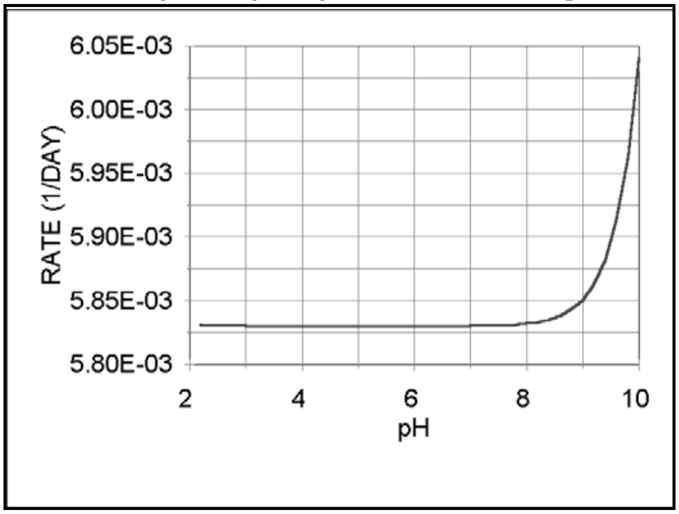
where:

$$OHIon = 10^{pH - 14} \qquad \textbf{(217)}$$

and where:

KBase = base-catalyzed rate constant (L/mol · d); and
OHIon = concentration of hydroxide ions (mol/L).

Figure 74
Base-catalyzed Hydrolysis of Pentachlorophenol



Hydrolysis reaction rates were adjusted for the temperature of the waterbody being modeled by using the Arrhenius rate law (Hemond and Fechner 1994). An activation energy value of 18,000 cal/mol (a mid-range value for organic chemicals) was used as a default:

$$Arrhen = e^{-(\frac{En}{R \cdot KelvinT} - \frac{En}{R \cdot TObs})} \quad \textbf{(218)}$$

where:

En	=	Arrhenius activation energy (cal/mol);
R	=	universal gas constant (cal/mol @ Kelvin);
KelvinT	=	temperature for which rate constant is to be predicted (Kelvin); and
TObs	=	temperature at which known rate constant was measured (Kelvin).

7.3 Photolysis

Direct photolysis is the process by which a compound absorbs light and undergoes transformation:

$$Photolysis = KPhot \cdot Toxicant_{Phase} \quad \textbf{(219)}$$

where:

Photolysis	=	rate of loss due to photodegradation (: g/L"d); and
KPhot	=	direct photolysis first-order rate constant (1/day).

For consistency, photolysis is computed for both the epilimnion and hypolimnion in stratified systems. However, it is not a significant factor at hypolimnetic depths.

Ionization may result in a significant shift in the absorption of light (Lyman et al., 1982; Schwarzenbach et al., 1993). However, there is a general absence of information on the effects of light on ionized species. The user provides an observed rate constant for photolysis (*PhotRate*), and this is usually determined either with distilled water or with water from a representative site, so that ionization may be included in the calculated lumped parameter *KPhot*.

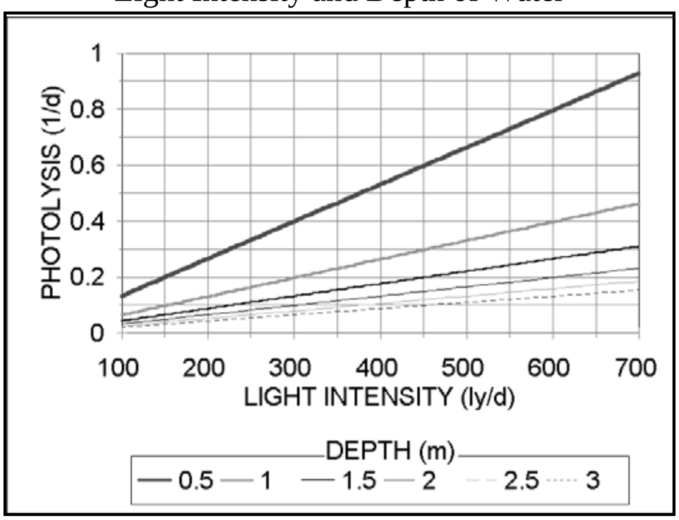
Based on the approach of Thomann and Mueller (1987; see also Schwarzenbach et al. 1993), the observed first-order rate constant for the compound is modified by a light attenuation factor for ultraviolet light so that the process as represented is depth-sensitive (**Figure 75**); it also is adjusted by a factor for time-varying light:

$$KPhot = PhotRate \cdot ScreeningFactor \cdot LightFactor \tag{220}$$

where:

PhotRate	=	direct, observed photolysis first-order rate constant (1/day);
ScreeningFactor	=	a light screening factor (unitless), see **(221)**; and
LightFactor	=	a time-varying light factor (unitless), see **(222)**.

Figure 75
Photolysis of Pentachlorophenol as a Function of
Light Intensity and Depth of Water



A light screening factor adjusts the observed laboratory photolytic transformation rate of a given pollutant for field conditions with variable light attenuation and depth (Thomann and Mueller, 1987):

$$ScreeningFactor = \frac{RadDistr}{RadDistr0} \cdot \frac{1 - \exp^{(-Extinct \cdot Thick)}}{Extinct \cdot Thick} \tag{221}$$

where:

RadDistr	=	radiance distribution function, which is the ratio of the average pathlength to the depth (see Schwarzenbach et al., 1993) (taken to be 1.6, unitless);
RadDistr0	=	radiance distribution function for the top of the segment (taken to be 1.2 for the top of the epilimnion and 1.6 for the top of the hypolimnion, unitless);
Extinct	=	light extinction coefficient (1/m) not including periphyton, see **(30)**; and
Thick	=	thickness of the water body segment if stratified or maximum depth if unstratified (m).

The equation presented above implicitly makes the following assumptions:

- quantum yield is independent of wavelength; and,
- the value used for *PhotRate* is a representative near-surface, first-order rate constant for direct photolysis.

The rate is modified further to represent seasonally varying light conditions and the effect of ice cover:

$$LightFactor = \frac{Solar0}{AveSolar} \tag{222}$$

where:

Solar0	=	time-varying average light intensity at the top of the segment (ly/day); and
AveSolar	=	average light intensity for late spring or early summer, corresponding to time when photolytic half-life is often measured (500 Ly/day).

If the system is unstratified or if the epilimnion is being modeled, the light intensity is the light loading:

$$Solar0 = Solar \tag{223}$$

otherwise we are interested in the intensity at the top of the hypolimnion and the attenuation of light is given as a logarithmic decrease over the thickness of the epilimnion:

$$Solar0 = Solar \cdot \exp^{(-Alpha \cdot MaxZMix)} \tag{224}$$

where:

Solar	=	incident solar radiation loading (ly/d), see **(25)**; and
MaxZMix	=	depth of the mixing zone (m), see **(17)**.

Because the ultraviolet light intensity exhibits greater seasonal variation than the visible spectrum (Lyman et al., 1982), decreasing markedly when the angle of the sun is low, this construct could predict higher rates of photolysis in the winter than might actually occur. However, the model also accounts for significant attenuation of light due to ice cover so that photolysis, as modeled, is not an important process in northern waters in the winter.

7.4 Microbial Degradation

Not only can microorganisms decompose the detrital organic material in ecosystems, they also can degrade xenobiotic organic compounds such as fuels, solvents, and pesticides to obtain energy. In AQUATOX this process of biodegradation of pollutants, whether they are dissolved in the water column or adsorbed to organic detritus in the water column or sediments, is modeled using the same equations as for decomposition of detritus, substituting the pollutant and its degradation parameters for detritus in Equation **(130)** and supporting equations:

$$\begin{aligned} MicrobialDegrdn &= KMDegrdn_{Phase} \cdot DOCorrection \cdot TCorr \cdot pHCorr \\ &\quad \cdot Toxicant_{Phase} \end{aligned} \tag{225}$$

where:

MicrobialDegrdn	=	loss due to microbial degradation ($g/m^3 \cdot d$);
KMDegrdn	=	maximum degradation rate, either in water column or sediments (1/d);
DOCorrection	=	effect of anaerobic conditions (unitless), see **(131)**;
TCorr	=	effect of suboptimal temperature (unitless), see **(24)**;
pHCorr	=	effect of suboptimal pH (unitless), see **(133)**; and
Toxicant	=	concentration of organic toxicant (g/m^3).

Microbial degradation proceeds more quickly if the material is associated with surficial sediments rather than suspended in the water column (Godshalk and Barko, 1985); thus, in calculating the loss due to microbial degradation in the sorbed phase, the maximum degradation rate is set to four times the maximum degradation rate in the water. The model assumes that reported maximum microbial degradation rates are for the dissolved phase; if the reported degradation value is from a study with additional organic matter, such as suspended slurry or wet soil samples, then the parameter value that is entered should be one-fourth that reported.

7.5 Volatilization

Volatilization is modeled using the "stagnant boundary theory", or two-film model, in which a pollutant molecule must diffuse across both a stagnant water layer and a stagnant air layer to volatilize out of a waterbody (Whitman, 1923; Liss and Slater, 1974). Diffusion rates of pollutants in these stagnant boundary layers can be related to the known diffusion rates of chemicals such as oxygen and water vapor. The thickness of the stagnant boundary layers must also be taken into account to estimate the volatile flux of a chemical out of (or into) the waterbody.

The time required for a pollutant to diffuse through the stagnant water layer in a waterbody is based on the well-established equations for the reaeration of oxygen, corrected for the difference in diffusivity as indicated by the respective molecular weights (Thomann and Mueller, 1987, p. 533). The diffusivity through the water film is greatly enhanced by the degree of ionization (Schwarzenbach et al., 1993, p. 243), and the depth-averaged reaeration coefficient is multiplied by the thickness of the well-mixed zone:

$$KLiq = KReaer \cdot Thick \cdot \left(\frac{MolWtO2}{MolWt} \right)^{0.25} \cdot \frac{1}{Nondissoc} \tag{226}$$

where:

KLiq	=	water-side transfer velocity (m/d);
KReaer	=	depth-averaged reaeration coefficient for oxygen (1/d), see **(155)**-**(162)**;
Thick	=	mean thickness of the water body segment if stratified or men depth if unstratified (m);
MolWtO2	=	molecular weight of oxygen (g/mol, =32);
MolWt	=	molecular weight of pollutant (g/mol); and
Nondissoc	=	nondissociated fraction (unitless), see **(210)**.

Likewise, the thickness of the air-side stagnant boundary layer is also affected by wind. Wind usually is measured at 10 m, and laboratory experiments are based on wind measured at 10 cm, so a conversion is necessary (Banks, 1975). To estimate the air-side transfer velocity of a pollutant, we used the following empirical equation based on the evaporation of water, corrected for the difference in diffusivity of water vapor compared to the toxicant (Thomann and Mueller, 1987, p. 534):

$$KGas = 168 \cdot \left(\frac{MolWtH2O}{MolWt} \right)^{0.25} \cdot Wind \cdot 0.5 \tag{227}$$

where:

KGas	=	air-side transfer velocity (m/d);
Wind	=	wind speed ten meters above the water surface (m/s);
0.5	=	conversion factor (wind at 10 cm/wind at 10 m); and
MolWtH2O	=	molecular weight of water (g/mol, =18).

The total resistance to the mass transfer of the pollutant through both the stagnant boundary layers can be expressed as the sum of the resistances—the reciprocals of the air- and water-phase mass transfer coefficients (Schwarzenbach et al., 1993), modified for the effects of ionization:

$$\frac{1}{KOVol} = \frac{1}{KLiq} + \frac{1}{KGas \cdot HenryLaw \cdot Nondissoc} \tag{228}$$

where:

KOVol	=	total mass transfer coefficient through both stagnant boundary layers (m/d);

$$HenryLaw = \frac{Henry}{R \cdot TKelvin} \tag{229}$$

and where:

HenryLaw	=	Henry's law constant (unitless);
Henry	=	Henry's law constant (atm m^3 mol^{-1});
R	=	gas constant (=8.206E-5 atm m^3 $(mol\ K)^{-1}$); and
TKelvin	=	temperature in °K.

The Henry's law constant is applicable only to the fraction that is nondissociated because the ionized species will not be present in the gas phase (Schwarzenbach et al., 1993, p. 179).

The atmospheric exchange of the pollutant can be expressed as the depth-averaged total mass transfer coefficient times the difference between the concentration of the chemical and the saturation concentration:

$$Volatilization = \frac{KOVol}{Thick} \cdot \left(ToxSat - Toxicant_{water} \right) \tag{230}$$

where:

Volatilization	=	interchange with atmosphere (μg/L·d);
Thick	=	depth of water or thickness of surface layer (m);
ToxSat	=	saturation concentration of pollutant in equilibrium with the gas phase (μg/L); and
$Toxicant_{water}$	=	concentration of pollutant in water (μg/L).

Because theoretically toxicants can be transferred in either direction across the water-air interface, Eq. 209 is formulated so that volatilization takes a negative sign when it is a loss term.

The saturation concentration depends on the concentration of the pollutant in the air, ignoring temperature effects (Thomann and Mueller, 1987, p. 532; see also Schnoor, 1996), but adjusting for ionization and units:

$$ToxSat = \frac{Toxicant_{air}}{HenryLaw \cdot Nondissoc} \cdot 1000 \tag{231}$$

where:

$Toxicant_{air}$	=	user-supplied gas-phase concentration of the pollutant (g/m^3); and
Nondissoc	=	nondissociated fraction (unitless).

Often the pollutant can be assumed to have a negligible concentration in the air and *ToxSat* is zero. However, this general construct can represent the transferral of volatile pollutants into water bodies. Because ionized species do not volatilize, the saturation level increases if ionization is occurring.

The nondimensional Henry's law constant, which relates the concentration of a compound in the air phase to its concentration in the water phase, strongly affects the air-phase resistance. Depending on the value of the Henry's law constant, the water phase, the air phase or both may control volatilization. For example, with a depth of 1 m and a wind of 1 m/s, the gas phase is 100,000 times as important as the water phase for atrazine (Henry's law constant = 3.0E-9), but the water phase is 50 times as important as the air phase for benzene (Henry's law constant = 5.5E-3). Volatilization of atrazine exhibits a linear relationship with wind (**Figure 76**) in contrast to the exponential relationship exhibited by benzene (**Figure 77**).

Figure 76
Atrazine *KOVol* as a Function of Wind

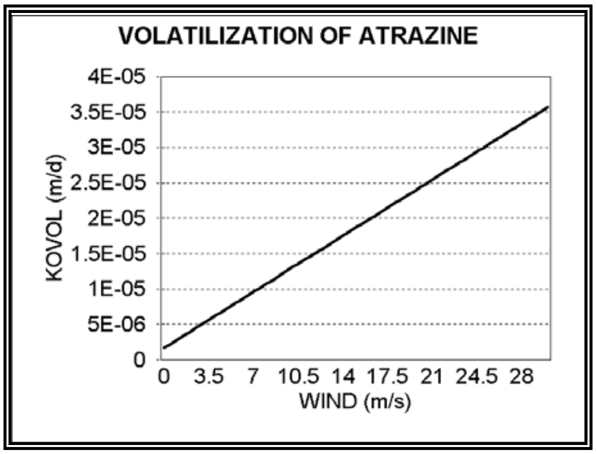
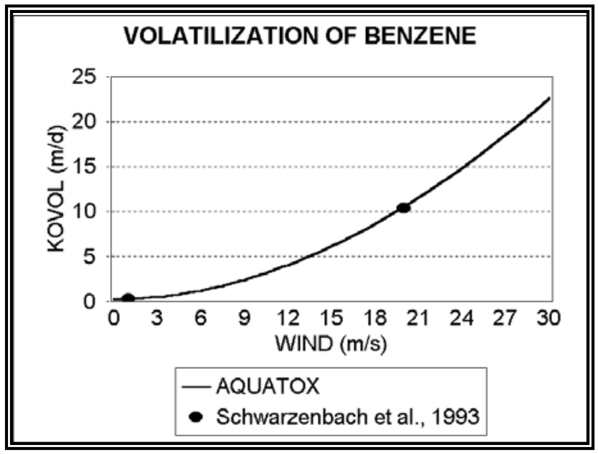


Figure 77
Benzene *KOVol* as a Function of Wind



7.6 Partition Coefficients

Although AQUATOX is a kinetic model, steady-state partition coefficients for organic pollutants are computed in order to constrain sorption to detritus and algae **(252)**, and to compute internal toxicities **(279)**. They are estimated from empirical regression equations and the pollutant's octanol-water partition coefficient.

Detritus

Natural organic matter is the primary sorbent for neutral organic pollutants. Hydrophobic chemicals partition primarily in nonpolar organic matter (Abbott et al. 1995). Refractory detritus is relatively nonpolar; its partition coefficient (in the non-dissolved phase) is a function of the octanol-water partition coefficient (N = 34, r^2 = 0.93; Schwarzenbach et al. 1993):

$$KOM_{RefrDetr} = 1.38 \cdot KOW^{0.82} \quad \textbf{(232)}$$

where:

$KOM_{RefrDetr}$	=	detritus-water partition coefficient (L/kg); and
KOW	=	octanol-water partition coefficient (L/kg).

Detritus in sediments is simulated separately from inorganic sediments, rather than as a fraction of the sediments as in other models. At this time AQUATOX does not simulate sorption to inorganic sediments. Therefore, refractory detritus is used as a surrogate for sediments in general; and the sediment partition coefficient *KPSed*, which can be entered manually by the user, is the same as $KOM_{RefrDetr}$.

Equation (232) and the equations that follow are extended to polar compounds, following the approach of Smejtek and Wang (1993):

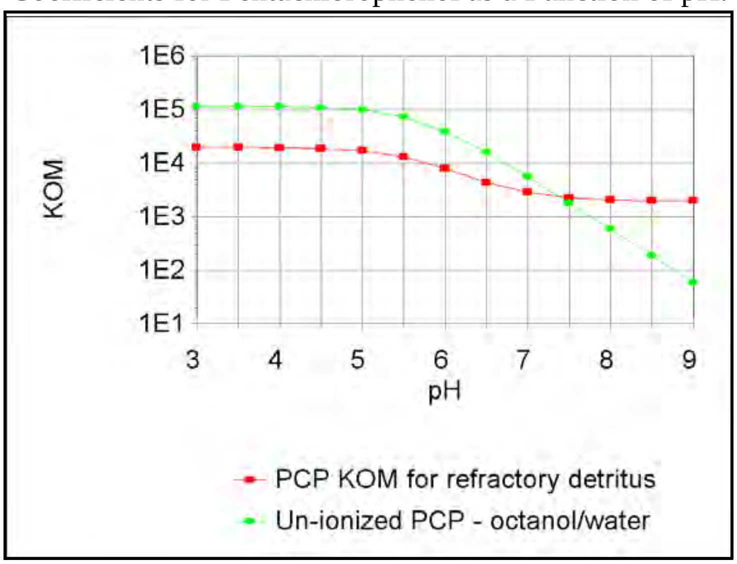
$$KOM_{RefrDetr} = 1.38 \cdot KOW^{0.82} \cdot Nondissoc + (1 - Nondissoc) \cdot IonCorr \cdot 1.38 \cdot KOW^{0.82} \quad (233)$$

where:

$Nondissoc$	=	un-ionized fraction (unitless); and
$IonCorr$	=	correction factor for decreased sorption, 0.01 for chemicals that are bases and 0.1 for acids. (unitless).

Using pentachlorophenol as a test compound, and comparing it to octanol, the influence of pH-mediated dissociation is seen in Figure 78. This relationship is verified by comparison with the results of Smejtek and Wang (1993) using egg membrane. However, in the general model Eq. (233) is used for refractory detrital sediments as well.

Figure 78
Refractory Detritus-water and Octanol-water Partition Coefficients for Pentachlorophenol as a Function of pH.



There appears to be a dichotomy in partitioning; data in the literature suggest that labile detritus does not take up hydrophobic compounds as rapidly as refractory detritus. Algal cell membranes contain polar lipids, and it is likely that this polarity is retained in the early stages of decomposition. KOC does not remain the same upon aging, death, and decomposition, probably because of polarity changes. In an experiment using fresh and aged algal detritus, there was a 100% increase in KOC with aging (Koelmans et al., 1995). KOC increased as the C/N ratio increased, indicating that the material was becoming more refractory. In another study, KOC doubled between day 2 and day 34, probably due to deeper penetration into the organic matrix and lower polarity (Cornelissen et al., 1997).

Polar substrates increase the pKa of the compound (Smejtek and Wang, 1993). This is represented in the model by lowering the pH of polar particulate material by one pH unit, which changes the dissociation accordingly.

The partition equation for labile detritus (non-dissolved) is based on a study by Koelmans et al. (1995) using fresh algal detritus (N = 3, r^2 = 1.0):

$$KOC_{LabPart} = 23.44 \cdot KOW^{0.61} \tag{234}$$

The equation is generalized to polar compounds and transformed to an organic matter partition coefficient:

$$\begin{aligned} KOM_{LabDetr} = {} & (23.44 \cdot KOW^{0.61} \cdot Nondissoc \\ & + (1 - Nondissoc) \cdot IonCorr \cdot 23.44 \cdot KOW^{0.61}) \cdot 0.526 \end{aligned} \tag{235}$$

where:

$KOC_{LabPart}$	=	partition coefficient for labile particulate organic carbon (L/kg);
$KOM_{LabDetr}$	=	partition coefficient for labile detritus (L/kg);
$IonCorr$	=	correction factor for decreased sorption, 0.01 for chemicals that are bases and 0.1 for acids. (unitless); and
0.526	=	conversion from KOC to KOM (g OC/g OM).

O'Connor and Connolly (1980; see also Ambrose et al., 1991) found that the sediment partition coefficient is the inverse of the mass of suspended sediment, and Di Toro (1985) developed a construct to represent the relationship. However, AQUATOX models partitioning directly to organic detritus and ignores inorganic sediments, which are seldom involved directly in sorption of neutral organic pollutants. Therefore, the partition coefficient is not corrected for mass of sediment.

Association of hydrophobic compounds with colloidal and dissolved organic matter (DOM) reduces bioavailability; such contaminants are unavailable for uptake by organisms (Stange and Swackhamer 1994, Gilek et al. 1996). Therefore, it is imperative that complexation of organic chemicals with DOM be modeled correctly. In particular, contradictory research results can be reconciled by considering that DOM is not homogeneous. For instance, refractory humic acids, derived from decomposition of terrestrial and wetland organic material, are quite different from labile exudates from algae and other indigenous organisms.

Humic acids exhibit high polarity and do not readily complex neutral compounds. Natural humic acids from a Finnish lake with extensive marshes were spiked with a PCB, but a PCB-humic acid complex could not be demonstrated (Maaret et al. 1992). In another study, Freidig et al. (1998) used artificially prepared Aldrich humic acid to determine a humic acid-DOC partition coefficient (n = 5, r^2, = 0.80), although they cautioned about extrapolation to the field:

$$KOC_{RefrDOM} = 28.84 \cdot KOW^{0.67} \tag{236}$$

where:

$KOC_{RefrDOM}$ = refractory dissolved organic carbon partition coefficient (L/kg).

Until a better relationship is found, we are using a generalization of their equation to include polar compounds, transformed from organic carbon to organic matter, in AQUATOX:

$$\begin{aligned} KOM_{RefrDOM} = {} & (28.84 \cdot KOW^{0.67} \cdot Nondissoc \\ & + (1 - Nondissoc) \cdot IonCorr \cdot 28.84 \cdot KOW^{0.67}) \cdot 0.526 \end{aligned} \tag{237}$$

where:

$KOM_{RefrDOM}$ = refractory dissolved organic matter partition coefficient (L/kg).

Nonpolar lipids in algae occur in the cell contents, and it is likely that they constitute part of the labile dissolved exudate, which may be both excreted and lysed material. Therefore, the stronger relationship reported by Koelmans and Heugens (1998) for partitioning to algal exudate (n = 6, r^2 = 0.926) is:

$$KOC_{LabDOC} = 0.88 \cdot KOW \tag{238}$$

which we also generalized for polar compounds and transformed:

$$\begin{aligned} KOM_{LabDOM} = {} & (0.88 \cdot KOW \cdot Nondissoc \\ & + (1 - Nondissoc) \cdot IonCorr \cdot 0.88 \cdot KOW) \cdot 0.526 \end{aligned} \tag{239}$$

where:

KOC_{LabDOC} = partition coefficient for labile dissolved organic carbon (L/kg); and
KOM_{LabDOM} = partition coefficient for labile dissolved organic matter (L/kg).

Unfortunately, older data and modeling efforts failed to distinguish between hydrophobic compounds that were truly dissolved and those that were complexed with DOM. For example, the PCB water concentrations for Lake Ontario, reported by Oliver and Niimi (1988) and used by many subsequent researchers, included both dissolved and DOC-complexed PCBs (a fact which they recognized). In their steady-state model of PCBs in the Great Lakes, Thomann and Mueller (1983) defined “dissolved” as that which is not particulate (passing a 0.45 micron filter). In their Hudson River PCB model, Thomann et al. (1991) again used an operational definition of dissolved PCBs.

AQUATOX distinguishes between truly dissolved and complexed compounds; therefore, the partition coefficients calculated by AQUATOX may be larger than those used in older studies.

Algae

Bioaccumulation of PCBs in algae depends on solubility, hydrophobicity and molecular configuration of the compound, and growth rate, surface area and type, and content and type of lipid in the alga (Stange and Swackhamer 1994). Phytoplankton may double or triple in one day and periphyton turnover may be so rapid that some PCBs will not reach equilibrium (cf. Hill and Napolitano 1997); therefore, one should use the term "bioaccumulation factor" (BAF) rather than "bioconcentration factor," which implies equilibrium (Stange and Swackhamer 1994).

Hydrophobic compounds partition to lipids in algae, but the relationship is not a simple one. Phytoplankton lipids can range from 3 to 30% by weight (Swackhamer and Skoglund 1991), and not all lipids are the same. Polar phospholipids occur on the surface. Hydrophobic compounds preferentially partition to internal neutral lipids, but those are usually a minor fraction of the total lipids, and they vary depending on growth conditions and species (Stange and Swackhamer 1994). Algal lipids have a much stronger affinity for hydrophobic compounds than does octanol, so that the algal $BAF_{lipid} > K_{OW}$ (Stange and Swackhamer 1994, Koelmans et al. 1995, Sijm et al. 1998).

For algae, the approximation to estimate the dry-weight bioaccumulation factor ($r^2 = 0.87$), computed from Swackhamer and Skoglund's (1993) study of numerous PCB congeners, is:

$$\log(BAF_{Alga}) = 0.41 + 0.91 \cdot LogKOW \qquad \textbf{(240)}$$

where:

BAF_{Alga} = partition coefficient between algae and water (L/kg).

Rearranging and extending to hydrophilic and ionized compounds:

$$\begin{aligned} BAF_{Alga} = {} & 2.57 \cdot KOW^{0.93} \cdot Nondissoc \\ & + (1 - Nondissoc) \cdot 0.257 \cdot KOW^{0.93} \end{aligned} \qquad \textbf{(241)}$$

Comparing the results of using these coefficients, we see that they are consistent with the relative importance of the various substrates in binding organic chemicals (**Figure 79**). Binding capacity of detritus is greater than dissolved organic matter in Great Lakes waters (Stange and Swackhamer 1994, Gilek et al. 1996). In a study using Baltic Sea water, less than 7% PCBs were associated with dissolved organic matter and most were associated with algae (Björk and Gilek 1999). In contrast, in a study using algal exudate and a PCB, 98% of the dissolved concentration was as a dissolved organic matter complex and only 2% was bioavailable (Koelmans and Heugens 1998).

The influence of substrate polarity is evident in **Figure 80**, which shows the effect of ionization on binding of pentachlorophenol to various types of organic matter. The polar substrates, such as algal detritus, have an inflection point which is one pH unit higher than that of nonpolar substrates, such as refractory detritus. The relative importance of the substrates for binding is also demonstrated quite clearly.

Macrophytes

For macrophytes, an empirical relationship reported by Gobas et al. (1991) for 9 chemicals with *LogKOW*s of 4 to 8.3 ($r^2 = 0.97$) is used:

$$\log(KB_{Macro}) = 0.98 \cdot LogKOW - 2.24 \tag{242}$$

Again, rearranging and extending to hydrophilic and ionized compounds:

$$KB_{Macro} = 0.00575 \cdot KOW^{0.98} \cdot (Nondissoc + 0.2) \tag{243}$$

Invertebrates

For the invertebrate bioconcentration factor, the following empirical equation is used for nondetritivores, based on 7 chemicals with *LogKOW*s ranging from 3.3 to 6.2 and bioconcentration factors for *Daphnia pulex* ($r^2 = 0.85$; Southworth et al., 1978; see also Lyman et al., 1982), converted to dry weight :

$$\log(KB_{Invertebrate}) = (0.7520 \cdot LogKOW - 0.4362) \cdot WetToDry \tag{244}$$

where:

$KB_{Invertebrate}$	=	partition coefficient between invertebrates and water (L/kg); and
$WetToDry$	=	wet to dry conversion factor (unitless, default = 5).

Extending and generalizing to ionized compounds:

$$KB_{Invertebrate} = 0.3663 \cdot KOW^{0.7520} \cdot (Nondissoc + 0.01) \tag{245}$$

For invertebrates that are detritivores the following equation is used, based on Gobas 1993:

$$KB_{Invertebrate} = \frac{FracLipid}{FracOC_{Detritus}} \cdot KOM_{RefrDetr} \cdot (Nondissoc + 0.01) \tag{246}$$

where:

$KB_{Invertebrate}$	=	partition coefficient between invertebrates and water (L/kg);
$FracLipid$	=	fraction of lipid within the organism;
$FracOC_{Detritus}$	=	fraction of organic carbon in detritus (= 0.526);
$KOM_{RefrDetr}$	=	partition coefficient for refractory sediment detritus (L/kg), see **(233)**.

Figure 79
Partitioning to Various Types of Organic Matter as a Function of KOW

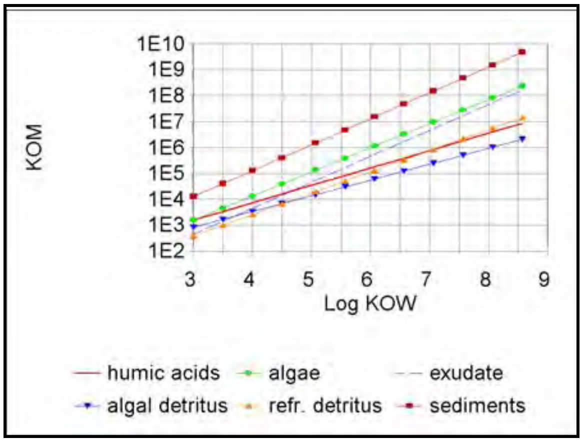
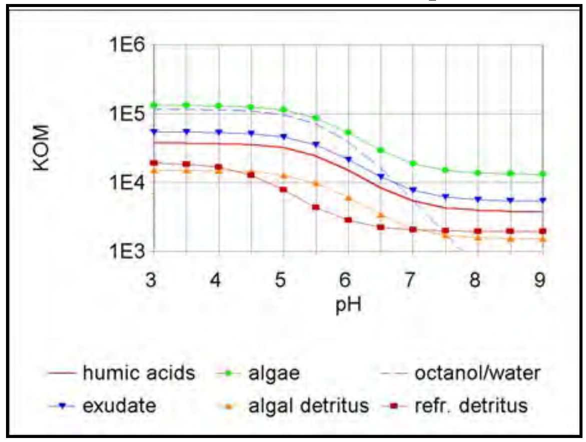


Figure 80
Partitioning to Various Types of Organic Matter as a Function of pH



Fish

Fish take longer to reach equilibrium with the surrounding water; therefore, a nonequilibrium bioconcentration factor is used. For each pollutant, a whole-fish bioconcentration factor is based on the lipid content of the fish extended to hydrophilic chemicals (McCarty et al., 1992), with provision for ionization:

$$KB_{Fish} = Lipid \cdot WetToDry \cdot KOW \cdot (Nondissoc + 0.01) \qquad \textbf{(247)}$$

where:

KB_{Fish}	=	partition coefficient between whole fish and water (L/kg);
$Lipid$	=	fraction of fish that is lipid (g lipid/g fish); and
$WetToDry$	=	wet to dry conversion factor (unitless, default = 5).

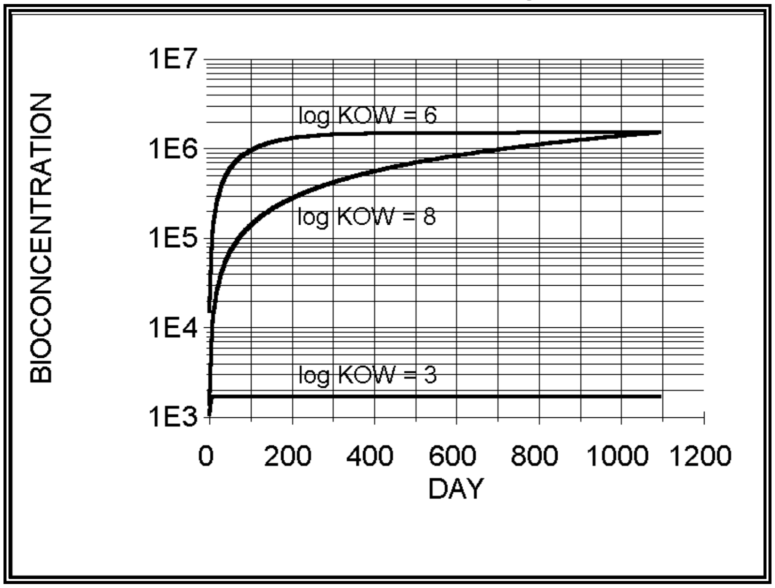
Lipid content of fish is either held constant or is computed depending on the potential for growth as predicted by the bioenergetics equations; the initial lipid values for the species are entered by the user. The bioconcentration factor is adjusted for the time to reach equilibrium as a function of the clearance or elimination rate and the time of exposure (Hawker and Connell, 1985; Connell and Hawker, 1988; **Figure 81**):

$$BCF_{Fish} = KB_{Fish} \cdot \left(1 - e^{(-Depuration \cdot TElapsed)}\right) \qquad \textbf{(248)}$$

where:

BCF_{Fish}	=	quasi-equilibrium bioconcentration factor for fish (L/kg);
$TElapsed$	=	time elapsed since fish was first exposed (d); and
$Depuration$	=	clearance, which may include biotransformation, see **(269)** (1/d).

Figure 81
Bioconcentration Factor for Fish
as a Function of Time and log KOW



7.7 Nonequilibrium Kinetics

Although partition coefficients are computed in AQUATOX in order to provide constraints on sorption and to compute internal toxicities, the model is basically a kinetic model. In nature there is often an absence of equilibrium due to growth or insufficient exposure time, metabolic biotransformation, dietary exposure, and nonlinear relationships for very large and/or superhydrophobic compounds (Bertelsen et al. 1998). It is important to have a knowledge of equilibrium partitioning because it is an indication of the condition toward which systems tend (Bertelsen et al. 1998), but steady-state potential is often not achieved due to changes in bioavailability and physiology (Landrum 1998). For example, PCBs may not be at steady state even in large systems such as Lake Ontario that have been polluted over a long period of time. In fact, PCBs in Lake Ontario exhibit a 25-fold disequilibrium (Cook and Burkhard 1998). The challenge is to obtain sufficient data for a kinetic model (Gobas et al. 1995).

Sorption and Desorption to Detritus

Partitioning to detritus appears to involve rapid sorption to particle surfaces, followed by slow movement into, and out of, organic matter and porous aggregates (Karickhoff and Morris, 1985). Therefore attainment of equilibrium may be slow. Because of the need to represent sorption and desorption separately in detritus, kinetic formulations are used (Thomann and Mueller, 1987), with provision for ionization:

$$\begin{aligned} Sorption = {} & k1_{Detr} \cdot Toxicant_{Water} \cdot Diff_{Carrier} \cdot (Nondissoc + 0.01) \\ & \cdot Org2C \cdot Detr \cdot UptakeLimit \cdot 1e{-6} \end{aligned} \tag{249}$$

$$Desorption = k2_{Detr} \cdot Toxicant_{Detr} \tag{250}$$

where:

Sorption	=	rate of sorption to given detritus compartment (μg/L·d);
$k1_{Detr}$	=	sorption rate constant (1.39 L/kg·d);
Nondissoc	=	fraction not ionized (unitless);
$Toxicant_{Water}$	=	concentration of toxicant in water (μg/L);
Diff	=	factor to normalize rate constant based on all competing uptake rates (unitless), see (251);
Org2C	=	conversion factor for organic matter to carbon (= 0.526 g C/g organic matter);
Detr	=	mass of each of the detritus compartments per unit volume (mg/L);
1e -6	=	units conversion (kg/mg);
Desorption	=	rate of desorption from given sediment detritus compartment (μg/L·d);
$k2_{Detr}$	=	desorption rate constant (1/d), see (254);
UptakeLimit	=	factor to limit uptake as equilibrium is reached (unitless); see (252) and
$Toxicant_{Detr}$	=	mass of toxicant in each of the detritus compartments (μg/L).

Because there are several processes competing for the dissolved toxicant, the rate constants for these processes are normalized in order to preserve mass balance. The *Diff* factor is computed considering all direct uptake processes, including sorption to detritus and algae, uptake by macrophytes, and uptake across animal gills. If the sum of the competing processes per day is less than the mass available in the water then *Diff* = 1, otherwise:

$$Diff = \frac{Toxicant_{Water}}{\left(\sum Sorption_{Detritus} + \sum PlantUptake_{Plant} + \sum GillUptake_{Animal}\right) \cdot dt} \tag{251}$$

where:

$Sorption_{Detritus}$	=	rate of sorption to given detrital group (μg/L·d), see (249);
$PlantUptake_{Plant}$	=	rate of uptake by given plant group (μg/L·d), see (256), (260);
$GillUptake_{Animal}$	=	rate of uptake by given animal group (μg/L·d), see (265); and
dt	=	time step (d).

In order to limit sorption to detritus and algae as equilibrium is reached, *UptakeLimit* is computed as:

$$UptakeLimit_{Carrier} = \frac{Toxicant_{Water} \cdot kp_{Carrier} - PPB_{Carrier}}{Toxicant_{Water} \cdot kp_{Carrier}} \tag{252}$$

where:

$UptakeLimit_{Carrier}$ = factor to limit uptake as equilibrium is reached (unitless);
$kp_{Carrier}$ = partition coefficient or bioconcentration factor for each carrier (L/kg), see (233) to (241);
$PPB_{Carrier}$ = concentration of toxicant in each carrier (μg/kg), see (209).

Desorption of the detrital compartments is the reciprocal of the reaction time, which Karickhoff and Morris (1985) found to be a linear function of the partition coefficient over three orders of magnitude (r^2 = 0.87):

$$\frac{1}{k2} \approx 0.72 \cdot KOM \tag{253}$$

So $k2$ is taken to be:

$$k2 = \frac{1.39}{KOM_{RefrDetr}} \tag{254}$$

where:

$KOM_{RefrDetr}$ = detritus-water partition coefficient (L/kg OM, see section 7.1); and

Because the kinetic definition of the detrital partition coefficient KOM is:

$$KOM = \frac{k1}{k2} \tag{255}$$

the sorption rate constant $k1$ is set to 1.39 L/kg·d.

Bioaccumulation in Macrophytes and Algae

Macrophytes—As Gobas et al. (1991) have shown, submerged aquatic macrophytes take up and release organic chemicals over a measurable period of time at rates related to the octanol-water partition coefficient. Uptake and elimination are modeled assuming that the chemical is transported through both aqueous and lipid phases in the plant, with rate constants using empirical equations fit to observed data (Gobas et al., 1991), modified to account for ionization effects (Figure 82, Figure 83):

$$MacroUptake = k1 \cdot Diff \cdot Toxicant_{Water} \cdot StVar_{Plant} \cdot 1e-6 \tag{256}$$

$$Depuration_{Plant} = k2 \cdot Toxicant_{Plant} \tag{257}$$

If the user selects to estimate the elimination rate constant based on KOW, the following equation is used:

$$k2 = \frac{1}{1.58 + 0.000015 \cdot KOW \cdot DissocFactor} \tag{258}$$

$$k1 = \frac{1}{0.0020 + \dfrac{500}{KOW \cdot DissocFactor}} \tag{259}$$

$$\text{if } Nondissoc < 0.01 \text{ then } DissocFactor = 0.01$$
$$\text{else } DissocFactor = Nondissoc$$

where:

MacroUptake	=	uptake of toxicant by plant (µg/L·d);
$Depuration_{Plant}$	=	clearance of toxicant from plant (µg/L·d);
$StVar_{Plant}$	=	biomass of given plant (mg/L);
1 e -6	=	units conversion (kg/mg);
$Toxicant_{Plant}$	=	mass of toxicant in plant (µg/L);
k1	=	sorption rate constant (L/kg·d);
k2	=	elimination rate constant (1/d).
Diff	=	factor to normalize uptake rates (unitless), see (251);
KOW	=	octanol-water partition coefficient (unitless);
Nondissoc	=	fraction of un-ionized toxicant (unitless): and
DissocFactor	=	constrained factor based on *Nondissoc* (unitless).

Figure 82
Uptake Rate Constant for Macrophytes
(after Gobas et al., 1991)

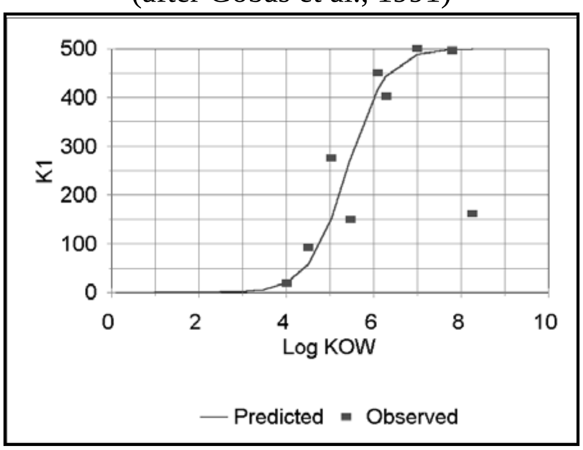
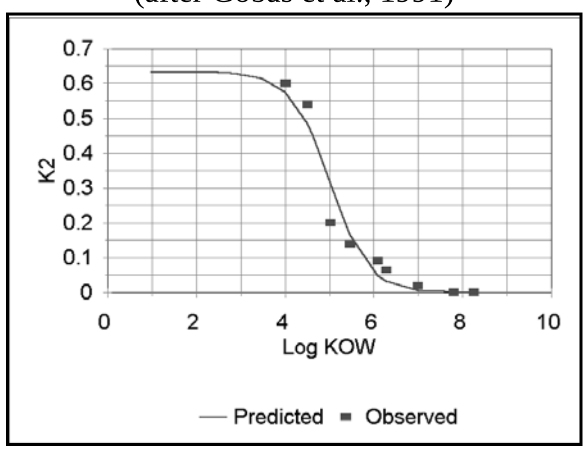


Figure 83
Elimination Rate Constant for Macrophytes
(after Gobas et al., 1991)



Algae—Aside from obvious structural differences, algae may have very high lipid content (20% for *Chlorella* sp. according to Jørgensen et al., 1979) and macrophytes have a very low lipid content (0.2% in *Myriophyllum spicatum* as observed by Gobas et al. (1991), which affect both uptake and elimination of toxicants. However, the approach used by Gobas et al. (1991) in modeling bioaccumulation in macrophytes provides a useful guide to modeling kinetic uptake in algae.

There is probably a two-step algal bioaccumulation mechanism for hydrophobic compounds, with rapid surface sorption of 40-90% within 24 hours and then a small, steady increase with transfer to interior lipids for the duration of the exposure (Swackhamer and Skoglund 1991). Uptake increases with increase in the surface area of algae (Wang et al. 1997). Therefore, the smaller the organism the larger the uptake rate constant (Sijm et al. 1998). However, in small phytoplankton, such as the nannoplankton that dominate the Great lakes, a high surface to volume ratio can increase sorption, but high growth rates can limit internal contaminant concentrations (Swackhamer and Skoglund 1991). The combination of lipid content, surface area, and growth rate results in species differences in bioaccumulation factors among algae (Wood et al. 1997). Uptake of toxicants is a function of the uptake rate constant and the concentration of toxicant truly dissolved in the water, and is constrained by competitive uptake by other compartments; also, because it is fast, it is limited as it approaches equilibrium, similar to sorption to detritus :

$$AlgalUptake = k1 \cdot UptakeLimit_{Alga} \cdot Diff \cdot ToxState \cdot Carrier \cdot 1e-6 \qquad \textbf{(260)}$$

where:

AlgalUptake	=	rate of sorption by algae (μg/L-d);
k1	=	uptake rate constant (L/kg-d), see **(261)**;
$UptakeLimit_{Alga}$	=	factor to limit uptake as equilibrium is reached (unitless), see **(252)**;
Diff	=	factor to normalize uptake rates (unitless), see **(251)**;
ToxState	=	concentration of dissolved toxicant (μg/L);
Carrier	=	biomass of algal compartment (mg/L); and
1e-6	=	conversion factor (kg/mg).

The kinetics of partitioning of toxicants to algae is based on studies on PCB congeners in The Netherlands by Koelmans, Sijm, and colleagues and at the University of Minnesota by Skoglund and Swackhamer. Both groups found uptake to be very rapid. Sijm et al. (1998) presented data on several congeners that were used in this study to develop the following relationship for phytoplankton (**Figure 84**):

$$k1 = \frac{1}{1.8E-6 + 1/(KOW \cdot DissocFactor)} \qquad \textbf{(261)}$$

Depuration is modeled as a linear function; it does not include loss due to excretion of photosynthate with associated toxicant, which is modeled separately:

$$Depuration = k2 \cdot State \qquad \textbf{(262)}$$

where:

Depuration	=	elimination of toxicant (:g/L-d);
State	=	concentration of toxicant associated with alga (:g/L); and
k2	=	elimination rate constant (1/d).

The elimination rate in plants may be input in the toxicity record by the user or it may be estimated using the following equation based in part on Skoglund et al. (1996). Unlike Skoglund, this equation ignores surface sorption and recognizes that growth dilution is explicit in AQUATOX (see **Figure 85**):

$$k2_{Algae} = \frac{2.4E+5}{(KOW \cdot DissocFactor \cdot LFrac \cdot WetToDry)} \tag{263}$$

where:

$k2_{Akgae}$	=	desorption rate constant (1/d);
LFrac	=	fraction lipid, as entered in the chemical toxicity screen; and
WetToDry	=	translation from wet to dry weight (5.0).

If more than 20% of the compound is ionized, the $k2_{Algae}$ is estimated from the $k1$ and *BCF* values:

$$k2 = \frac{k1}{BCF} \tag{264}$$

Figure 84
Algal Sorption Rate Constant as a Function of Octanol-water Partition Coefficient

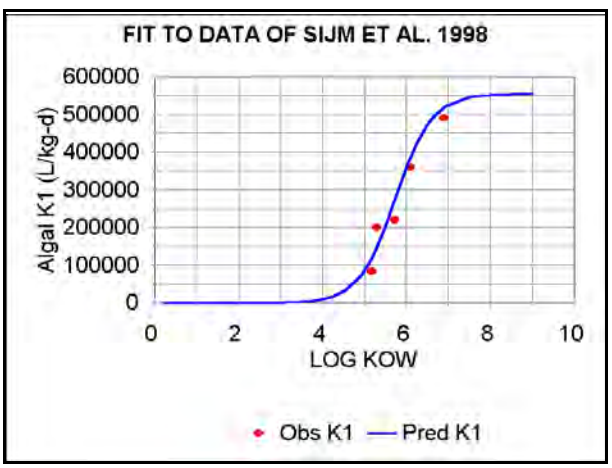
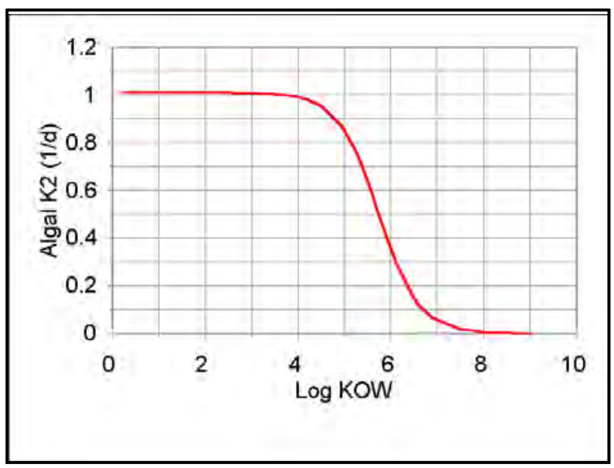


Figure 85
Rate of Elimination by Algae as a Function of Octanol-water Partition Coefficient



Bioaccumulation in Animals

Animals can absorb toxic organic chemicals directly from the water through their gills and from contaminated food through their guts, hence they *bioaccumulate*, and seldom is steady-state *bioconcentration* an important factor. Direct sorption onto the body is ignored as a simplifying assumption in this version of the model. Reduction of body burdens of organic chemicals is accomplished through excretion and biotransformation, which are often considered together as empirically determined elimination rates. “Growth dilution” occurs when growth of the organism is faster than accumulation of the toxicant. Gobas (1993) includes fecal egestion, but in AQUATOX egestion is merely the amount ingested but not assimilated; it is accounted for indirectly in *DietUptake*. However, fecal loss is important as an input to the detrital toxicant pool, and it is considered later in that context. Inclusion of mortality and promotion terms is necessary for mass balance, but emphasizes the fact that average concentrations are being modeled for any particular compartment.

Gill Sorption—An important route of exposure is by active transport through the gills (Macek et al., 1977). This is the route that has been measured so often in bioconcentration experiments with fish. As the organism respires, water is passed over the outer surface of the gill and blood is moved past the inner surface. The exchange of toxicant through the gill membrane is assumed to be facilitated by the same mechanism as the uptake of oxygen, following the approach of Fagerström and Åsell (1973, 1975), Weininger (1978), and Thomann and Mueller (1987; see also Thomann, 1989). Therefore, the uptake rate for each animal can be calculated as a function of respiration (Leung, 1978; Park et al., 1980):

$$GillUptake = KUptake \cdot Toxicant_{Water} \cdot Diff \tag{265}$$

$$KUptake = \frac{WEffTox \cdot Respiration \cdot O2Biomass}{Oxygen \cdot WEffO2} \tag{266}$$

where:

GillUptake	=	uptake of toxicant by gills (µg/L - d);
KUptake	=	uptake rate (1/d);
$Toxicant_{Water}$	=	concentration of toxicant in water (µg/L);
Diff	=	factor to normalize rate constant based on all competing uptake rates (unitless), see **(251)**;
WEffTox	=	withdrawal efficiency for toxicant by gills (unitless), see **(267)**;
Respiration	=	respiration rate (mg biomass/L·d), see **(87)**;
O2Biomass	=	ratio of oxygen to organic matter (mg oxygen/mg biomass; 0.575);
Oxygen	=	concentration of dissolved oxygen (mg oxygen/L), see **(150)**; and
WEffO2	=	withdrawal efficiency for oxygen (unitless, generally 0.62).

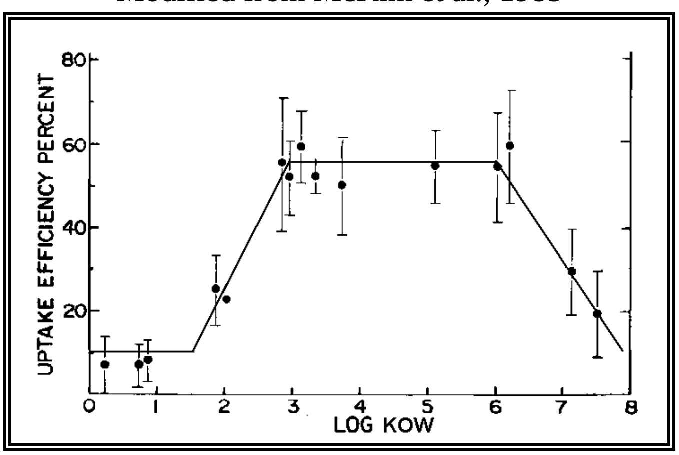
The oxygen uptake efficiency *WEffO2* is assigned a constant value of 0.62 based on observations of McKim et al. (1985). The toxicant uptake efficiency, *WEffTox*, can be expected to have a sigmoidal relationship to the log octanol-water partition coefficient based on aqueous and lipid transport (Spacie and Hamelink, 1982). This is represented by an inelegant but reasonable, piece-wise fit (**Figure 86**) to the data of McKim et al. (1985) using 750-g fish, corrected for ionization:

$$\begin{gathered}
\text{If } LogKOW < 1.5 \text{ then} \\
WEffTox = 0.1 \\[1em]
\text{If } 1.5 \leq LogKOW > 3.0 \text{ then} \\
WEffTox = 0.1 + Nondissoc \cdot (0.3 \cdot LogKOW - 0.45) \\[1em]
\text{If } 3.0 \leq LogKOW \leq 6.0 \text{ then} \\
WEffTox = 0.1 + Nondissoc \cdot 0.45 \\[1em]
\text{If } 6.0 < LogKOW < 8.0 \text{ then} \\
WEffTox = 0.1 + Nondissoc \cdot (0.45 - 0.23 \cdot (LogKOW - 6.0)) \\[1em]
\text{If } LogKOW \geq 8.0 \text{ then} \\
WEffTox = 0.1
\end{gathered} \tag{267}$$

where:

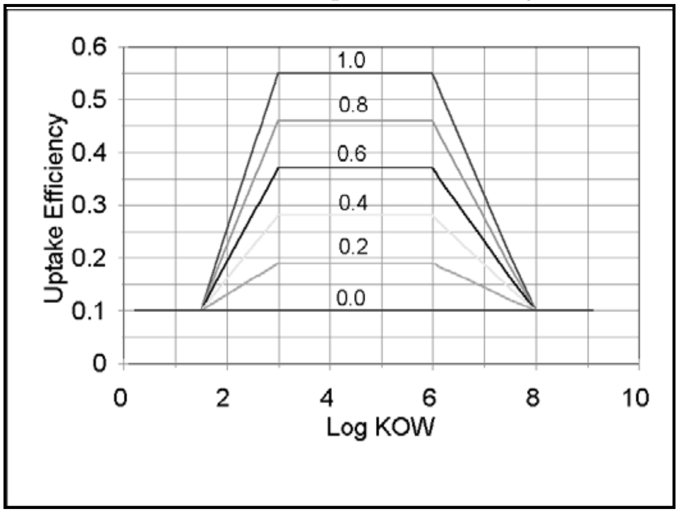
LogKOW	=	log octanol-water partition coefficient (unitless); and
Nondissoc	=	fraction of toxicant that is un-ionized (unitless), see (210).

Figure 86
Piece-wise Fit to Observed Toxicant Uptake Data;
Modified from McKim et al., 1985



Ionization decreases the uptake efficiency (Figure 87). This same algorithm is used for invertebrates. Thomann (1989) has proposed a similar construct for these same data and a slightly different construct for small organisms, but the scatter in the data do not seem to justify using two different constructs.

Figure 87
The Effect of Differing Fractions of Un-ionized Chemical on Uptake Efficiency



Dietary Uptake—Hydrophobic chemicals usually bioaccumulate in larger animals primarily through absorption from contaminated food. Persistent, highly hydrophobic chemicals demonstrate biomagnification or increasing concentrations as they are passed up the food chain from one trophic level to another; therefore, dietary exposure can be quite important (Gobas et al., 1993). Uptake from contaminated prey can be computed as (Thomann and Mueller, 1987; Gobas, 1993):

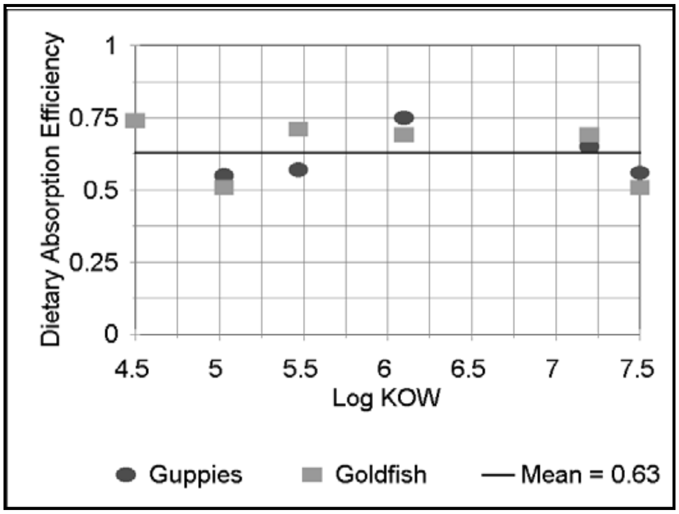
$$DietUptake_{Prey} = GutEffTox \cdot PPB_{Prey} \cdot Ingestion_{Prey} \cdot 1e-6 \qquad \textbf{(268)}$$

where:

$DietUptake_{Prey}$	=	uptake of toxicant from given prey (μg toxicant/L·d);
$GutEffTox$	=	efficiency of sorption of toxicant from gut (unitless); and
PPB_{Prey}	=	concentration of toxicant in given prey (μg toxicant/kg prey), see (209);
$Ingestion_{Prey}$	=	ingestion of given prey (mg prey/L·d), see (78).
1 e-6	=	units conversion (kg/mg);

Gobas (1993) presents an empirical equation for estimating *GutEffTox* as a function of the octanol-water partition coefficient. However, data published by Gobas et al. (1993) suggest that there is no trend in efficiency between *LogKOW* 4.5 and 7.5 (**Figure 88**); this is to be expected because the digestive system has evolved to assimilate a wide variety of organic molecules. Therefore, the mean value of 0.62 is used in AQUATOX as a constant for small fish. Nichols et al. (1998) demonstrated that uptake is more efficient in larger fish; therefore, a value of 0.92 is used for large game fish because of their size. Invertebrates generally exhibit lower efficiencies; Landrum and Robbins (1990) showed that values ranged from 0.42 to 0.24 for chemicals with log KOWs from 4.4 to 6.7; the mean value of 0.35 is used for invertebrates in AQUATOX. These values cannot be edited at this time.

Figure 88
GutEffTox Constant Based on Mean Value for Data from Gobas et al., 1993



Elimination—Elimination or clearance includes both excretion (depuration) and biotransformation of a toxicant by organisms. Biotransformation may cause underestimation of elimination (McCarty et al., 1992). An overall elimination rate constant is estimated and reported in the toxicity record. The user may then modify the value based on observed data; that value is used in subsequent simulations. If known, biotransformation also can be explicitly modeled.

For any given time the clearance rate is:

$$Depuration_{Animal} = k2 \cdot Toxicant_{Animal} \cdot TCorr \tag{269}$$

where:

$Depuration_{Animal}$	=	clearance rate (:g/L"d);
$k2$	=	elimination rate constant (1/d);
$Toxicant_{Animal}$	=	mass of toxicant in given animal (:g/L); and
$TCorr$	=	correction for suboptimal temperature (unitless), see (51).

Because much animal depuration is across the gills, estimation of the elimination rate constant *k2* is based on a slope related to log *KOW* and an intercept that is a direct function of respiration, assuming an allometric relationship between respiration and the weight of the animal (**Figure 89**, Thomann, 1989), and an inverse function of the lipid content:

If *WetWt* < 5 g then

$$Log\ k2 = -0.536 \cdot Log\ KOW - Log\ DissocFactor + 0.065 \cdot \frac{WetWt^{RB}}{LipidFrac} \tag{270}$$

else

$$Log\ k2 = -0.536 \cdot Log\ KOW - Log\ DissocFactor + 0.116 \cdot \frac{WetWt^{RB}}{LipidFrac} \quad \mathbf{(271)}$$

where

KOW	=	octanol-water partition coefficient (unitless);
LipidFrac	=	fraction of lipid in organism (g lipid/g organism);
WetWt	=	mean wet weight of organism (g);
RB	=	allometric exponent for respiration (unitless);
DissocFactor	=	constrained factor for *Nondissoc*, see **(259)**.

The other gain and loss terms in equation **(208)** (*TurbDiff*, *Predation, Mortality, Migration, Recruit*, GameteLoss, *Promotion, Drift*, *Migration, and EmergeInsect)* are all simply multiplied by the appropriate toxicant concentration to complete the computation of the overall toxicant concentration in the animal.

Biotransformation

Biotransformation can cause the conversion of a toxicant to another toxicant or to a harmless daughter product through a variety of pathways. Internal biotransformation to given daughter products by plants and animals is modeled by means of empirical rate constants provided by the user in the Chemical Biotransformation screen:

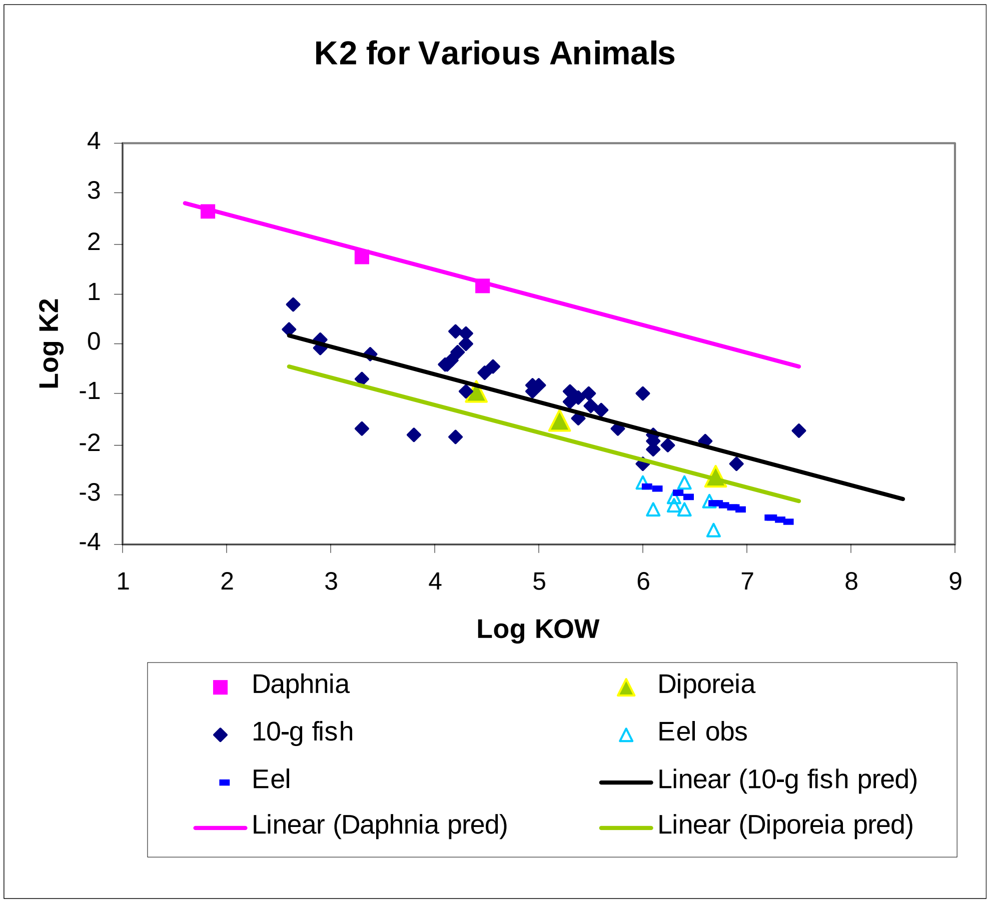
$$Biotransformation = Toxicant_{organism} \cdot BioRateConst_{organism,tox} \quad \mathbf{(272)}$$

where

Biotransformation	=	rate of conversion of chemical by given organism (μg/L d),
BioRateConst	=	biotransformation rate constant to a given toxicant, provided by user (1/day)

with the model keeping track of both the loss and the gains to various daughter compartments.

Figure 89
Depuration Rate Constants for Invertebrates and Fish



Biotransformation also can take place as a consequence of microbial decomposition. The percentage of microbial biotransformation from and into each of the organic chemicals in a simulation can be specified, with different values for aerobic and anaerobic decomposition. The amount of biotransformation into a given chemical can then be calculated as follows for aerobic conditions:

$$Biotransform_{MicrobIn} = \sum_{OrgTox} MicrobialDegradn_{OrgTox} \cdot FracAerobic \cdot Frac_{OrgTox} \quad \textbf{(273)}$$

and for anaerobic conditions:

$$Biotransform_{MicrobIn} = \sum_{OrgTox} MicrobialDegradn_{OrgTox} \cdot (1 - FracAerobic) \cdot Frac_{OrgTox} \quad \textbf{(274)}$$

where

$Biotransform_{MicrobIn}$ = Biotransformation to a given organic chemical in a given detrital compartment due to microbial decomposition (:g/L d);

MicrobialDegradn	=	total microbial degradation of a different toxicant in this detrital compartment (:g/L d) see (225);
FracAerobic	=	fraction of the microbial degradation that is aerobic (unitless), see (275); and
$Frac_{OrgTox}$	=	user input fraction of the organic toxicant that is transformed to the current organic toxicant (inputs can differ depending on whether the degradation is aerobic or anaerobic).

To calculate the fraction of microbial decomposition that is aerobic, the following equation is used:

$$FracAerobic = \frac{Factor}{DoCorr} \tag{275}$$

where

Factor	=	Michaelis-Menten factor (unitless) see (132);
DoCorr	=	effect of oxygen on microbial decomposition (unitless) see (131).

Linkages to Detrital Compartments

Toxicants are transferred from organismal to detrital compartments through defecation and mortality. The amount transferred due to defecation is the unassimilated portion of the toxicant that is ingested:

$$DefecationTox = \sum (KEgest_{Pred,\ Prey} \cdot PPB_{Prey} \cdot 1\,e-6) \tag{276}$$

$$KEgest_{Pred,\ Prey} = (1 - GutEffTox) \cdot Ingestion_{Pred,\ Prey} \tag{277}$$

where:

DefecationTox	=	rate of transfer of toxicant due to defecation (:g/L"d);
$KEgest_{Pred,\ Prey}$	=	fecal egestion rate for given prey by given predator (mg prey/L"d);
PPB_{Prey}	=	concentration of toxicant in given prey (:g/kg), see (209);
1 e-6	=	units conversion (kg/mg);
GutEffTox	=	efficiency of sorption of toxicant from gut (unitless), see **page 7-31**; and
$Ingestion_{Pred,\ Prey}$	=	rate of ingestion of given prey by given predator (mg/L"d), see (78).

The amount of toxicant transferred due to mortality may be large; it is a function of the concentrations of toxicant in the dying organisms and the mortality rates. The general equation is:

$$MortTox_{Detr} = \sum (Mortality_{Org} \cdot PPB_{Org} \cdot 1e-6) \tag{278}$$

where:

$MortTox_{Detr}$	=	rate of transfer of toxicant to a given detrital compartment due to mortality (µg/L·d);
$Mortality_{Org}$	=	rate of mortality of given organism (mg/L·d), see **(58)**, **(74)** and **(98)**;
PPB_{Org}	=	concentration of toxicant in given organism (µg/kg), see **(209)**; and
1 e-6	=	units conversion (kg/mg).

8 ECOTOXICOLOGY

Unlike most models, AQUATOX contains an ecotoxicology submodel that computes acute and chronic toxic effects from the concentration of a toxicant in a given organism, using the critical body residue approach (McCarty 1986, McCarty and Mackay 1993). Because the model simulates toxicity based on internal concentrations as a consequence of bioaccumulation, both water and dietary exposure pathways are represented equally well. Furthermore, as an ecosystem model, AQUATOX can simulate indirect effects such as loss of forage base, reduction in predation, and anoxia due to decomposition following a fish kill.

User-supplied values for *LC50*, the concentration of a toxicant in water that causes 50% mortality, form the basis for a sequence of computations that lead to estimates of the biomass of a given organism lost through acute toxicity each day. The sequence, which is documented in this chapter, is to compute:

- the internal concentration causing 50% mortality for a given period of exposure;
- the internal concentration causing 50% mortality after an infinite period of time based on an asymptotic concentration-response relationship;
- the time-varying lethal internal concentration of a chemical;
- the cumulative mortality for a given internal concentration;
- the biomass lost per day as an increment to the cumulative mortality.

The user-supplied *EC50*s, the concentrations in water eliciting chronic toxicity responses in 50% of the population, are used to obtain application factors relating the chronic toxicities to the acute toxicity. Because AQUATOX can simulate as many as twenty toxic organic chemicals simultaneously, the simplifying assumption is made that the toxic effects are additive.

8.1 Acute Toxicity of Compounds

Toxicity is based on the internal concentration of the toxicant in the specified organism. Many compounds, especially those with higher octanol-water partition coefficients, take appreciable time to accumulate in the tissue. Therefore, length of exposure is critical in determining toxicity. Although AQUATOX cannot currently model mercury, mercury is used as an example in the following discussion because of the availability of excellent data. The same principles apply to organic toxicants and to both plants and animals.

$$InternalLC50 = BCF \cdot LC50 \tag{279}$$

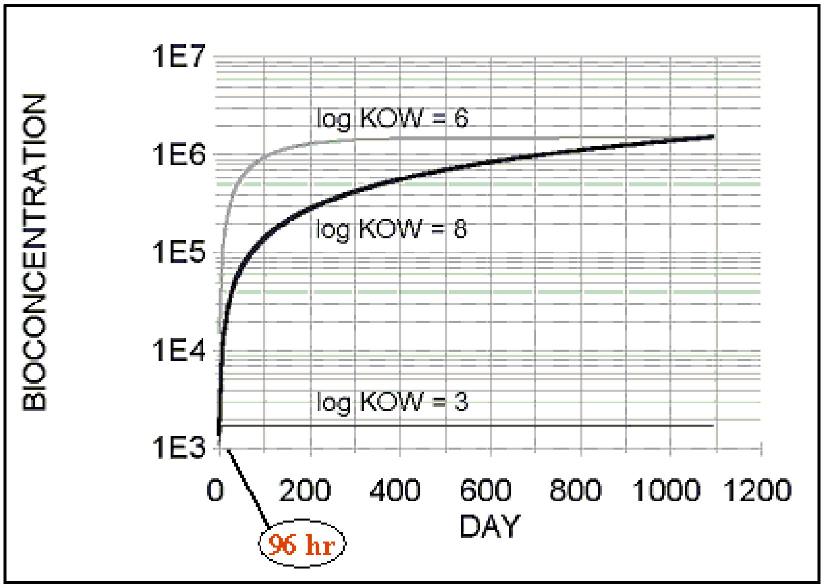
The internal lethal concentration or lethal body residue can be computed from reported acute toxicity data for the reported period of exposure based on the simple relationship suggested by an algorithm in the FGETS model (Suárez and Barber, 1992):
where:

InternalLC50 = internal concentration that causes 50% mortality for a given period of exposure (μg/kg);

BCF	=	time-dependent bioconcentration factor (L/kg), see **(241)**, **(248)**; and
LC50	=	concentration of toxicant in water that causes 50% mortality for a given period of exposure (µg/L).

Note that time is implicit in the toxicity parameters. For compounds with a *LogKOW* in excess of 5 the usual 96-hr toxicity exposure does not reach steady state, so a time-dependent *BCF* is used to account for the actual internal concentration at the end of the toxicity determination. This is applicable no matter what the length of exposure (**Figure 85**, based on **Figure 81**).

Figure 85
Bioconcentration Factor as a Function of Time and *KOW*



A given *LC50* can be provided by the user, or the user may choose to have the model estimate the *LC50* from other species or groups for which there are data based on linear regressions (Mayer and Ellersieck, 1986) and maximum likelihood estimators (Suter et al., 1986). In this way the model can be parameterized to represent a complete food web (Table 7).

$$\text{Log } CalcLC50 = Intercept + Slope \cdot \text{Log } LC50 \qquad \textbf{(280)}$$

where:

CalcLC50	=	estimated *LC50* (µg/L);
Intercept	=	intercept for regression (µg/L);
Slope	=	slope of the regression equation;
LC50	=	external concentration of toxicant at which 50% of population is killed (µg/L).

Table 7. Interspecies regression parameters.

From	**To**	**Intercept**	**Slope**	**Correl. r**	
minnow	trout	-0.09	0.947	0.95	Mayer and Ellersieck, 1986
minnow	bass	-0.433	0.972	0.93	Mayer and Ellersieck, 1986
minnow	catfish	0.954	0.832	0.88	Mayer and Ellersieck, 1986
minnow	bluegill	0.018	0.954	0.93	Mayer and Ellersieck, 1986
bluegill	trout	0.44	0.898	0.96	Mayer and Ellersieck, 1986
bluegill	bass	0.051	1.003	0.98	Mayer and Ellersieck, 1986
bluegill	catfish	1.918	0.713	0.78	Mayer and Ellersieck, 1986
bluegill	minnow	0.947	0.883	0.92	Mayer and Ellersieck, 1986
trout	bass	0.258	0.983	0.96	Mayer and Ellersieck, 1986
trout	catfish	1.391	0.802	0.82	Mayer and Ellersieck, 1986
trout	bluegill	0.135	1.005	0.96	Mayer and Ellersieck, 1986
trout	minnow	0.796	0.928	0.94	Mayer and Ellersieck, 1986
Daphnia	chironomid	0.802	0.846	0.86	Mayer and Ellersieck, 1986
Daphnia	stonefly	1.475	0.667	0.65	Mayer and Ellersieck, 1986
Daphnia	ostracod	0.79	0.62		Suter et al., 1986
Daphnia	amphipod	-0.462	1.01	0.82	Mayer and Ellersieck, 1986

A constant toxicity parameter independent of time is obtained by determining the asymptotic toxicity relationship, which is a rearrangement of **(283)** for the special case of observed toxicity data:

$$LCInfinite = InternalLC50 \cdot (1 - e^{-k2 \cdot ObsTElapsed}) \qquad \textbf{(281)}$$

where:

LCInfinite	=	internal concentration causing 50% mortality after an infinite period of exposure (:g/kg);
k2	=	elimination rate constant (1/d); and
ObsTElapsed	=	exposure time in toxicity determination (h converted to d).

The model estimates *k2*, see **(258)**, **(263)**, **(270)** and **(271)**, assuming that this *k2* is the same as that measured in bioconcentration tests; good agreement has been reported between the two (Mackay et al., 1992). The user may then override that estimate by entering an observed value. The *k2* can be calculated off-line by the user based on the observed half-life:

$$k2 = \frac{0.693}{t_{1/2}} \qquad \textbf{(282)}$$

where:

$t_{½}$	=	observed half-life.

Based on the Mancini (1983) model, the lethal internal concentration of a toxicant for a given exposure period can be expressed as (Crommentuijn et al. (1994):

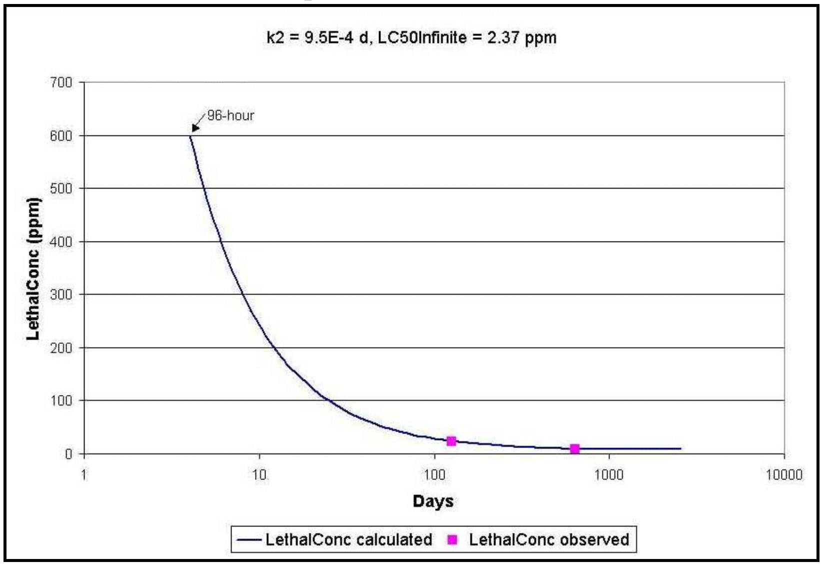
$$LethalConc = \frac{LCInfinite}{1 - e^{-k2 \cdot TElapsed}} \qquad \textbf{(283)}$$

where:

LethalConc	=	time-varying tissue-based concentration of toxicant that causes 50% mortality (ppb or :g/kg), used in **(286)** to compute fraction killed;
LCInfinite	=	ultimate internal lethal toxicant concentration after an infinitely long exposure time (:g/kg);
TElapsed	=	time elapsed since beginning of exposure to toxicant (d).

The longer the exposure the lower the internal concentration required for lethality (**Figure 86**).

Figure 86
Lethal concentration of MeHg in brook trout as a function of time; two data points from McKim et al., 1976



Exposure is limited to the lifetime of the organism:

$$\text{If } TElapsed > LifeSpan \text{ Then } TElapsed = LifeSpan \qquad \textbf{(284)}$$

where:

LifeSpan = user-defined mean lifetime for given organism (d).

Based on an estimate of time to reach equilibrium (Connell and Hawker, 1988),

$$\begin{gathered}\text{if } TElapsed > \frac{4.605}{k2} \text{ then} \\ LethalConc = LCInfinite\end{gathered} \qquad \textbf{(285)}$$

The fraction killed by a given internal concentration of toxicant is best estimated using the time-dependent *LethalConc* in the cumulative form of the Weibull distribution (Mackay et al., 1992; see also Christensen and Nyholm, 1984):

$$CumFracKilled = 1 - e^{-\left(\frac{PPB}{LethalConc}\right)^{\frac{1}{Shape}}} \qquad \textbf{(286)}$$

where:

CumFracKilled = cumulative fraction of organisms killed for a given period of exposure (fraction/d),

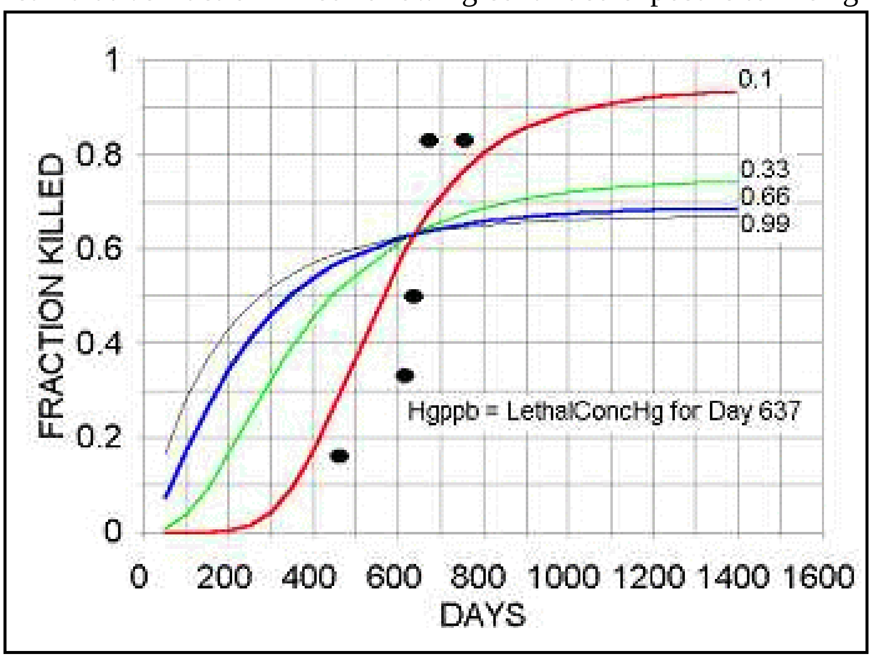
PPB = internal concentration of toxicant (:g/kg), see **(209)**; and

Shape	=	parameter expressing variability or spread in toxic response (unitless, default = 0.33).

As a practical matter, if *CumFracKilled* exceeds 95%, then it is set to 100% to avoid complex computations with small numbers. By setting organismal loadings to very small numbers, seed values can be maintained in the simulation.

The probit, logit, and Weibull equations yield similar results over most of the range of distributions, but the Weibull formulation is preferable because it is algebraically simple and yet based on mechanistic relationships (Mackay et al., 1992), and it is most sensitive to the tails of the distribution–the EC_{10} and EC_{90} values (Christensen and Nyholm, 1984). The *Shape* parameter is important because it controls the spread of mortality, providing a probabilistic response. The larger the value, the greater the spread of mortality over toxicant concentrations and time. For example, methyl mercury toxicity exhibits a rapid response over a short time period with most of the fish dying when a threshold internal concentration is reached, so *Shape* has a value of less than 0.1 (**Figure 87**). However, Mackay et al. (1992) found that a value of 0.33 gave the best fit to data on toxicity of 21 narcotic chemicals to fathead minnows. This value is used as a default in AQUATOX, but it can be changed by the user.

Figure 87
The effect of *Shape* in fitting the observed (McKim et al., 1976) cumulative fraction killed following continued exposure to MeHg



The biomass killed per day is computed by disaggregating the cumulative mortality. Think of the biomass at any given time as consisting of two types: biomass that has already been exposed to the toxicant previously, which is called *Resistant* because it represents the fraction that was not killed; and new biomass that has formed through growth, reproduction, and migration and has not been exposed to a given level of toxicant and therefore is referred to as *Nonresistant*. Then think of the cumulative distribution as being the total *CumFracKilled*, which includes the *FracKilled* that is in excess of the cumulative amount on the previous day if the internal concentration of toxicant increases. A conservative estimate of the biomass killed at a given time, ignoring the possibility of inherited tolerance, is computed as:

$$Poisoned = Resistant \cdot FracKill + Nonresistant \cdot CumFracKill \tag{287}$$

$$Resistant = Biomass_{t-1} - Poisoned_{t-1} \tag{288}$$

$$\begin{gathered}\text{If } Resistant < Biomass \quad \text{then} \\ Nonresident = Biomass - Resistant\end{gathered} \tag{289}$$

$$\begin{gathered}\text{If } FracKill_{t-1} \geq CumFracKill \text{ then } \quad FracKill = 0 \\ \text{else} \quad FracKill = CumFracKill - FracKill_{t-1}\end{gathered} \tag{290}$$

where:

Poisoned	=	biomass of given organisms killed by exposure to toxicant at given time (g/m^3 d);
Resistant	=	biomass not killed by previous exposure (g/m^3);
FracKill	=	fraction killed per day in excess of the previous fraction (fraction/d);
$FracKill_{t-1}$	=	fraction killed previous day (fraction/d);
Nonresistant	=	biomass not previously exposed; the biomass in excess of the resistant biomass (g/m^3).

Poisoned then becomes a term in the mortality equations **(58)**, **(74)**, and **(98)**.

8.2 Chronic Toxicity

Organisms usually have adverse reactions to toxicants at levels significantly below those that cause death. In fact, the acute to chronic ratio is commonly used to quantify this relationship. Application factors (*AF*s), which are the inverse of the acute to chronic ratio, are employed in the model to predict chronic effect responses for both plants and animals. The user can supply observed *EC50* and *LC50* values, which are used to compute AFs. For example:

$$AFGrowth = \frac{EC50Growth}{LC50} \tag{291}$$

where:

EC50Growth	=	external concentration of toxicant at which there is a 50% reduction in growth in animals (:g/L);
AFGrowth	=	chronic to acute ratio for growth (unitless); and

LC50 = external concentration of toxicant at which 50% of population is killed (:g/L).

If the user enters observed *EC50* and *LC50* values for a given species, the model provides the option of applying the resulting *AF* to estimate *EC50*s for other animals. One is more likely to have *LC50* data for animals and *EC50* data for plants, so the model will estimate *LC50*s for plants given *EC50*s and a computed *AF*.

The computations for *AFRepro* and *AFPhoto* are similar:

$$AFRepro = \frac{EC50Repro}{LC50} \tag{292}$$

$$AFPhoto = \frac{EC50Photo}{LC50} \tag{293}$$

where:

EC50Repro = external concentration of toxicant at which there is a 50% reduction in reproduction in animals (:g/L);
AFRepro = chronic to acute ratio for reproduction (unitless);
EC50Photo = external concentration of toxicant at which there is a 50% reduction in photosynthesis (:g/L); and
AFPhoto = chronic to acute ratio for photosynthesis (unitless).

Similar to computation of acute toxicity in the model, chronic toxicity is based on internal concentrations of a toxicant. Often chronic effects form a continuum with acute effects and the difference is merely one of degree (Mackay et al., 1992). Regardless of whether or not the mode of action is the same, the computed application factors relate the observed effect to the acute effect and permit efficient computation of chronic effects factors in conjunction with computation of acute effects. Because AQUATOX simulates biomass, no distinction is made between reduction in a process in an individual and the fraction of the population exhibiting that response. The commonly measured reduction in photosynthesis is a good example: the data only indicate that a given reduction takes place at a given concentration, not whether all individuals are affected. The application factor enters into the Weibull equation to estimate reduction factors for photosynthesis, growth, and reproduction:

$$FracPhoto = e^{-\frac{PPB}{LethalConc \cdot AFPhoto}^{1/Shape}} \tag{294}$$

$$RedGrowth = 1 - e^{-\frac{PPB}{LethalConc \cdot AFGrowth}^{1/Shape}} \tag{295}$$

$$RedRepro = 1 - e^{-\left(\frac{PPB}{LethalConc \cdot AFRepro}\right)^{1/Shape}} \qquad \textbf{(296)}$$

where:

FracPhoto	=	reduction factor for effect of toxicant on photosynthesis (unitless);
RedGrowth	=	factor for reduced growth in animals (unitless);
RedRepro	=	factor for reduced reproduction in animals (unitless);
PPB	=	internal concentration of toxicant (:g/kg), see **(209)**;
LethalConc	=	time-varying tissue-based concentration of toxicant that causes 50% mortality (ppb or :g/kg), see **(283)**;
AFPhoto	=	chronic to acute ratio for photosynthesis (unitless, default of 0.10);
AFGrowth	=	chronic to acute ratio for growth in animals (unitless, default of 0.10);
AFRepro	=	chronic to acute ratio for reproduction in animals (unitless, default of 0.05); and
Shape	=	parameter expressing variability in toxic response (unitless, default of 0.33).

The reduction factor for photosynthesis, *FracPhoto*, enters into the photosynthesis equation **(31)**, and it also appears in the equation for the acceleration of sinking of phytoplankton due to stress **(62)**.

The variable for reduced growth, *RedGrowth*, is arbitrarily split, based on calibration, between two processes, ingestion **(78)**, where it reduces consumption by 20%:

$$ToxReduction = 1 - (0.2 \cdot RedGrowth) \qquad \textbf{(297)}$$

and egestion **(84)**, where it increases the amount of food that is not assimilated by 80%:

$$IncrEgest = (1 - EgestCoeff_{prey,\, pred}) \cdot 0.8 \cdot RedGrowth \qquad \textbf{(298)}$$

These have indirect effects on the rest of the ecosystem through reduced predation and increased production of detritus in the form of feces.

Embryos are often more sensitive to toxicants, although reproductive failure may occur for various reasons. As a simplification, the factor for reduced reproduction, *RedRepro*, is used only to increase gamete mortality **(102)** beyond what would occur otherwise:

$$IncrMort = (1 - GMort) \cdot RedRepro \qquad \textbf{(299)}$$

where:

IncrMort	=	increased gamete and embryo mortality due to toxicant (1/d).

Sloughing of periphyton and drift of invertebrates also can be elicited by toxicants. For example, sloughing can be caused by a surfactant that disrupts the adhesion of the periphyton, or an invertebrate may release its hold on the substrate when irritated by a toxicant. Often the response is immediate so that these responses can be modeled as dependent on dissolved concentrations of toxicants with an available chronic toxicity parameter, as in the equation for periphyton sloughing:

$$Dislodge_{Peri,Tox} = MaxToxSlough \cdot \frac{Toxicant_{Water}}{Toxicant_{Water} + EC50_{Dislodge}} \cdot Biomass_{Peri} \tag{300}$$

where:

$Dislodge_{Peri,\ Tox}$	=	periphyton sloughing due to given toxicant (g/m^3 d);
$MaxToxSlough$	=	maximum fraction of periphyton biomass lost by sloughing due to given toxicant (fraction/d, 0.1);
$Toxicant_{Water}$	=	concentration of toxicant dissolved in water (:g/L); see **(199)**;
$EC50\_Dislodge$	=	external concentration of toxicant at which there is 50% sloughing (:g/L); and
$Biomass_{Peri}$	=	biomass of given periphyton (g/m^3); see **(30)**.

Likewise, drift is greatly increased when zoobenthos are subjected to stress by sublethal doses of toxic chemicals (Muirhead-Thomson, 1987), and that is represented by a saturation-kinetic formulation that utilizes an analogous chronic toxicity parameter :

$$Dislodge_{Tox} = \sum_{tox} \frac{Toxicant_{Water} - DriftThreshold}{Toxicant_{Water} - DriftThreshold + EC50Growth} \tag{301}$$

where:

$Toxicant_{Water}$	=	concentration of toxicant in water (:g/L);
$DriftThreshold$	=	the concentration of toxicant that initiates drift (:g/L); and
$EC50Growth$	=	concentration at which half the population is affected (:g/L).

These terms are incorporated in the respective sloughing **(64)** and drift **(106)** equations.

By modeling chronic and acute effects, AQUATOX makes the link between chemical fate and the functioning of the aquatic ecosystem—a pioneering approach that has been refined over the past fifteen years, following the first publications (Park et al., 1988; Park, 1990).

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APPENDIX A. GLOSSARY OF TERMS

Taken in large part from: The Institute of Ecology. 1974. *An Ecological Glossary for Engineers and Resource Managers*. TIE Publication #3, 50 pp.

Abiotic	nonliving, pertaining to physico-chemical factors only
Adsorption	the adherence of substances to the surfaces of bodies with which they are in contact
Aerobic	living, acting, or occurring in the presence of oxygen
Algae	any of a group of chlorophyll-bearing aquatic plants with no true leaves, stems, or roots
Allochthonous	material derived from outside a habitat or environment under consideration
Algal bloom	rapid and flourishing growth of algae
Alluvial	of alluvium
Alluvium	sediments deposited by running water
Ambient	surrounding on all sides
Anaerobic	capable of living or acting in the absence of oxygen
Anoxic	pertaining to conditions of oxygen deficiency
Aphotic	below the level of light penetration in water
Assimilation	transformation of absorbed nutrients into living matter
Autochthonous	material derived from within a habitat, such as through plant growth
Benthic	pertaining to the bottom of a water body; pertaining to organisms that live on the bottom
Benthos	those organisms that live on the bottom of a body of water
Biodegradable	can be broken down into simple inorganic substances by the action of decomposers (bacteria and fungi)
Biochemical oxygen demand (BOD)	the amount of oxygen required to decompose a given amount of organic matter
Bioaccumulation	the uptake of contaminants from all sources including direct sorption to the body, transport across gill membranes, and through ingestion of prey and sediments
Bioavailability	the existence of a chemical in a form that it can be readily integrated into an organism by means of any form of intake or attachment
Biodegradation	the process of breaking down into simple organic substances by decomposers (bacteria and fungi)
Biomagnification	the step by step concentration of chemicals in successive levels of a food chain or food web
Biomass	the total weight of matter incorporated into (living and/or dead) organisms
Biota	the fauna and flora of a habitat or region
Biotransformation	the permanent changing of a substance from one chemical identity to another by means of biotically driven processes
Chlorophyll	the green, photosynthetic pigments of plants

Colloid	a dispersion of particles larger than small molecules and that do not settle out of suspension
Consumer	an organism that consumes another
Copepods	a large subclass of usually minute, mostly free-swimming aquatic crustaceans
Crustacean	a large class of arthropods that bear a horny shell
Decomposers	bacteria and fungi that break down organic detritus
Depuration	excretion of contaminant by an organism
Desorption	the process by which chemicals are detached and released from solid surfaces; the opposite of adsorption
Detritus	dead organic matter
Diatom	any of class of minute algae with cases of silica
Diurnal	pertaining to daily occurrence
Dynamic equilibrium	a state of relative balance between processes having opposite effects
Ecology	the study of the interrelationships of organisms with and within their environment
Ecosystem	a biotic community and its (living and nonliving) environment considered together
Emergent	aquatic plants, usually rooted, which have portions above water for part of their life cycle
Environment	the sum total of all the external conditions that act on an organism
Epilimnion	the well mixed surficial layer of a lake; above the hypolimnion
Epiphytes	plants that grow on other plants, but are not parasitic
Equilibrium	a steady state in a dynamic system, with outflow balancing inflow
Euphotic	pertaining to the upper layers of water in which sufficient light penetrates to permit growth of plants
Eutrophic	aquatic systems with high nutrient input and high plant growth
Fauna	the animals of a habitat or region
Flood plain	that part of a river valley that is covered in periods of high (flood) water
Flora	plants of a habitat or region
Fluvial	pertaining to a stream
Food chain	animals linked by linear predator-prey relationships with plants or detritus at the base
Food web	similar to food chain, but implies cross connections
Forage fish	fish eaten by other fish
Habitat	the environment in which a population of plants or animals occurs
Humic	pertaining to the partial decomposition of leaves and other plant material
Hydrodynamics	the study of the movement of water
Hypolimnion	the lower layer of a stratified water body, below the well mixed zone
Influent	anything flowing into a water body
Inorganic	pertaining to matter that is neither living nor immediately derived from living matter
Invertebrate	animals lacking a backbone

Kinetic processes	description of the dynamic rate and mode of change in the transformation or degradation of a substance in an ecosystem
Kinetic reaction	a physical, chemical or biological transformation/reaction that is best represented using a formulation that is time-dependent
Limiting factor	an environmental factor that limits the growth of an organism; the factor that is closest to the physiological limits of tolerance of that organism
Limnetic zone	the open water zone of a lake or pond from the surface to the depth of effective light penetration
Limnology	the study of inland waters
Lipids	structural components of the cell that are fatty or waxy
Littoral zone	the shoreward zone of a water body in which the light penetrates to the bottom, thus usually supporting rooted aquatic plants
Macrofauna	animals visible to the naked eye
Macrophytes	large (non-microscopic), usually rooted, aquatic plants
Mass balance	an equation that accounts for the flux of mass going into a defined area and the flux of mass leaving the defined area; the flux in must equal the flux out
Migration	movement of an organism from one location to another
Nutrients	chemical elements essential to life
Omnivorous	feeding on a variety of organisms and organic detritus
Organic chemical	compounds containing carbon;
Overturn	the complete circulation or mixing of the upper and lower waters of a lake when temperatures (and densities) are similar
Oxygen depletion	exhaustion of oxygen by chemical or biological use
Parameter	a measurable, variable quantity as distinct from a statistic
Pelagic zone	open water with no association with the bottom
Periphyton	community of algae and associated organisms, usually small but densely set, closely attached to surfaces on or projecting above the bottom
Oxidation	a reaction between molecules, ordinarily involves gain of oxygen
Photic zone	the region of aquatic environments in which the intensity of light is sufficient for photosynthesis
Phytoplankton	small, mostly microscopic algae floating in the water column
Plankton	small organisms floating in the water
Pond	a small, shallow lake
Population	a group of organisms of the same species
Predator	an organism, usually an animal, that kills and consumes other organisms
Prey	an organism killed and at least partially consumed by a predator
Producer	an organism that can synthesize organic matter using inorganic materials and an external energy source (light or chemical)
Production	the amount of organic material produced by biological activity
Productivity	the rate of production of organic matter
Productivity, primary	the rate of production by plants

Productivity, secondary	the rate of production by consumers
Reservoir	an artificially impounded body of water
Riverine	pertaining to rivers
Rough fish	a non-sport fish, usually omnivorous in food habits
Sediment	any mineral and/or organic matter deposited by water or air
Siltation	the deposition of silt-sized and clay-sized (smaller than sand-sized) particles
Stratification	division of a water body into two or more depth zones due to temperature or density
Substrate	the layer on which organisms grow; the organic substance attacked by decomposers
Succession	the replacement of one plant assemblage with another through time
Tolerance	an organism's capacity to endure or adapt to unfavorable conditions
Trophic level	all organisms that secure their food at a common step in the food chain
Turbidity	condition of water resulting from suspended matter, including inorganic and organic material and plankton
Volatilization	the act of passing into a gaseous state at ordinary temperatures and pressures
Wastewater	water derived from a municipal or industrial waste treatment plant
Wetlands	land saturated or nearly saturated with water for most of the year; usually vegetated
Zooplankton	small aquatic animals, floating, usually with limited swimming capability

APPENDIX B. USER-SUPPLIED PARAMETERS AND DATA

The model has many parameters and internal variables. Most of these are linked to data structures such as ChemicalRecord, SiteRecord, and ReminRecord, which in turn may be linked to input forms that the user accesses through the Windows environment. Although consistency has been a goal, some names may differ between the code, the user interface, and the technical documentation

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	ChemicalRecord	**Chemical Underlying Data**	**For each chemical simulated, the following parameters are required**	
Chemical	ChemName	N / A	Chemical's Name. Used for Reference only.	N / A
CAS Registry No.	CASRegNo	N / A	CAS Registry Number. Used for Reference only.	N / A
Molecular Weight	MolWt	MolWt	molecular weight of pollutant	(g/mol)
Dissociation Constant	pka	pKa	acid dissociation constant	negative log
Solubility	Solubility	N / A	Not utilized as a parameter by the code.	(ppm)
Henry's Law Constant	Henry	Henry	Henry's law constant	(atm m3 mol-1)
Vapor Pressure	VPress	N / A	Not utilized as a parameter by the code.	mm Hg
Octanol-water partition coefficient	LogP	LogKow	log octanol-water partition coefficient	(unitless)
KPSED	KPSed	KPSed	detritus-water partition coefficient	(L/kg)
Activation Energy for Temperature	En	En	Arrhenius activation energy	(cal/mol)
Rate of Anaerobic Microbial Degradation	KMDegrAnaerobic	KAnaerobic	decomposition rate at 0 g/m3 oxygen	(1/d)
Max. Rate of Aerobic Microbial Degradation	KMDegrdn	KMDegrdn	Maximum (microbial) degradation rate	(1/ d)
Uncatalyzed hydrolysis constant	KUnCat	KUncat	the measured first-order reaction rate at pH 7	(1/d)
Acid catalyzed hydrolysis constant	KAcid	KAcidExp	pseudo-first-order acid-catalyzed rate constant for a given pH	(1/d)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Base catalyzed hydrolysis constant	KBase	KBaseExp	pseudo-first-order rate constant for a given pH	(1/d)
Photolysis Rate	PhotolysisRate	KPhot	direct photolysis first-order rate constant	(1/d)
Oxidation Rate Constant	OxRateConst	N / A	Not utilized as a parameter by the code.	(L/ mol d)
Weibull Shape Parameter	Weibull_Shape	Shape	parameter expressing variability in toxic response; default is 0.33	(unitless)
Chemical is a Base	ChemIsBase	if the compound is a base	if the compound is a base	(True/False)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	SiteRecord	**Site Underlying Data**	**For each water body simulated, the following parameters are required**	
Site Name	SiteName	N / A	Site's Name. Used for Reference only.	N / A
Max Length (or reach)	SiteLength	Length	maximum effective length for wave setup	(km)
Vol.	Volume	Volume	initial volume of site (must be copied into state var.)	(m3)
Surface Area	Area	Area	site area	(m2)
Mean Depth	ZMean	ZMean	mean depth	(m)
Maximum Depth	ZMax	ZMax	maximum depth	(m)
Ave. Temp. (epilimnetic or hypolimnetic)	TempMean	TempMean	mean annual temperature of epilimnion (or hypolimnion)	(°C)
Epilimnetic Temp. Range (or hypolimnetic)	TempRange	TempRange	annual temperature range of epilimnion (or hypolimnion)	(°C)
Latitude	Latitude	Latitude	latitude	(Deg, decimal)
Average Light	LightMean	LightMean	mean annual light intensity	Langleys/day (ly/d)
Annual Light Range	LightRange	LightRange	annual range in light intensity	Langleys/day (ly/d)
Total Alkalinity	AlkCaCO3	N / A	Not utilized as a parameter by the code.	mg/L
Hardness as $CaCO_3$	HardCaCO3	N / A	Not utilized as a parameter by the code.	mg CaCO3 / L
Sulfate Ion Conc	SO4Conc	N / A	Not utilized as a parameter by the code.	mg/L
Total Dissolved Solids	TotalDissSolids	N / A	Not utilized as a parameter by the code.	mg/L
Limnocorral Wall Area	LimnoWallArea	LimnoWallArea	area of limnocorral walls; only relevant to limnocorral	(m2)
Mean Evaporation	MeanEvap	MeanEvap	mean annual evaporation	inches / year
Extinct. Coeff Water	ECoeffWater	ExtinctH2O	light extinction of wavelength 312.5 nm in pure water	(1/m)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	SiteRecord (Stream-Specific)	**Site Underlying Data**	**For each stream simulated, the following parameters are required**	
Channel Slope	Channel_Slope	Slope	slope of channel	(m/m)
Maximum Channel Depth Before Flooding	Max_Chan_Depth	Max_Chan_Depth	depth at which flooding occurs	(m)
Sediment Depth	SedDepth	SedDepth	maximum sediment depth	(m)
Stream Type	StreamType	Stream Type	concrete channel, dredged channel, natural channel	Choice from List
use the below value	UseEnteredManning		do not determine Manning coefficient from streamtype	(true/false)
Mannings Coefficient	EnteredManning	Manning	manually entered Manning coefficient.	s / m1$^{/3}$
Percent Riffle	PctRiffle	Riffle	percent riffle in stream reach	%
Percent Pool	PctPool	Pool	percent pool in stream reach	%
	SiteRecord (Sand-Silt-Clay Specific)	**Site Underlying Data**	**For each stream with the inorganic sediments model included, the following parameters are required**	
Silt: Critical Shear Stress for Scour	ts_silt	$TauScour_{Sed}$	critical shear stress for scour of silt	(kg/m3)
Silt: Critical Shear Stress for Deposition	tdep_silt	$TauDep_{Sed}$	critical shear stress for deposition of silt	(kg/m3)
Silt: Fall Velocity	FallVel_silt	VT_{Sed}	terminal fall velocity of silt	(m/s)
Clay: Critical Shear Stress for Scour	ts_clay	$TauScour_{Sed}$	critical shear stress for scour of clay	(kg/m3)
Clay: Critical Shear Stress for Deposition	tdep_clay	$TauDep_{Sed}$	critical shear stress for deposition of clay	(kg/m3)
Clay: Fall Velocity	FallVel_clay	VT_{Sed}	terminal fall velocity of clay	(m/s)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	ReminRecord	**Remineralization Data**	**For each simulation, the following parameters are required**	
Max. Degrdn Rate, labile	DecayMax_Lab	DecayMax	maximum decomposition rate	(g/g·d)
Max Degrdn Rate, Refrac	DecayMax_Refr	ColonizeMax	maximum colonization rate under ideal conditions	(g/g·d)
Temp. Response Slope	Q10	Q10	Not utilized as a parameter by the code.	(unitless)
Optimum Temperature	TOpt	TOpt	optimum temperature for degredation to occur	(°C)
Maximum Temperature	TMax	TMax	maximum temperature at which degradation will occur	(°C)
Min. Adaptation Temp	TRef	TRef	Not utilized as a parameter by the code.	(°C)
Min pH for Degradation	pHMin	pHMin	minimum pH below which limitation on biodegradation rate occurs.	pH
Max pH for Degradation	pHMax	pHMax	maximum pH above which limitation on biodegradation rate occurs.	pH
Organics to Phosphate	Org2Phosphate	Org2Phosphate	ratio of phosphate to organic matter (unitless)	(unitless)
Organics to Ammonia	Org2Ammonia	Org2Ammonia	ratio of ammonia to organic matter	(unitless)
O2 : Biomass, Respiration	O2Biomass	O2Biomass	ratio of oxygen to organic matter	(unitless)
O2: N, Nitrification	O2N	O2N	ratio of oxygen to nitrogen	(unitless)
Detrital Sed Rate	KSed	KSed	intrinsic sedimentation rate	(m/d)
PO4, Anaerobic Sed.	PSedRelease	N / A	Not utilized as a parameter by the code.	(g/m2·d)
NH4, Aerobic Sed.	NSedRelease	N / A	Not utilized as a parameter by the code.	(g/m2·d)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	ZooRecord	**Animal Underlying Data**	**For each animal in the simulation, the following parameters are required**	
Animal	AnimalName	N / A	Animal's Name. Used for Reference only.	N / A
Animal Type	Animal_Type	Animal Type	Animal Type (Fish, Pelagic Invert, Benthic Invert, Benthic Insect)	Choice from List
Taxonomic Type or Guild	Guild_Taxa	Taxonomic type or guild	Taxonomic type or trophic guild	Choice from List
Toxicity Record	ToxicityRecord	N / A	associates animal with appropriate toxicity data	Choice from List
Half Saturation Feeding	FHalfSat	FHalfSat	half-saturation constant for feeding by a predator	(g/m3)
Maximum Consumption	CMax	CMax	maximum feeding rate for predator	(g/g·d)
Min Prey for Feeding	BMin	BMin	minimum prey biomass needed to begin feeding	(g/m3) (or g/m2)
Temp Response Slope	Q10	Q10	slope or rate of change in given process per 10°C temperature change	(unitless)
Optimum Temperature	TOpt	TOpt	optimum temperature for given process	(°C)
Maximum Temperature	TMax	TMax	maximum temperature tolerated	(°C)
Min Adaptation Temp	TRef	TRef	adaptation temperature below which there is no acclimation	(°C)
Respiration Rate	EndogResp	EndogResp	basal respiration rate at 0° C for given predator	(1/day)
Specific Dynamic Action	KResp	KResp	proportion assimilated energy lost to specific dynamic action	(unitless)
Excretion:Respiration	KExcr	KExcr	proportionality constant for excretion:respiration	(unitless)
Gamete : Biomass	PctGamete	PctGamete	fraction of adult predator biomass that is in gametes	(unitless)
Gamete Mortality	GMort	GMort	gamete mortality	(1/d)
Mortality Coefficient	KMort	KMort	intrinsic mortality rate	(1/d)
Carrying Capacity	KCap	KCap	carrying capacity	g/m^3

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Average Drift	AveDrift	Dislodge	fraction of biomass subject to drift per day	fraction / day
VelMax	VelMax	VelMax	maximum water velocity tolerated	(cm/s)
Mean lifespan	LifeSpan	LifeSpan	mean lifespan in days	days
Initial fraction that is lipid	FishFracLipid	LipidFrac	fraction of lipid in organism	(g lipid/g organism)
Mean Weight	MeanWeight	WetWt	mean wet weight of organism	(g)
Percent in Riffle	PrefRiffle	$Preference_{Habitat}$	Percentage of biomass of animal that is in riffle, as opposed to run or pool	%
Percent in Pool	PrefPool	$Preference_{Habitat}$	percentage of biomass of animal that is in pool, as opposed to run or riffle	%
Fish spawn automatically, based on temperature range	AutoSpawn		Does AQUATOX calculate Spawn Dates	(true/false)
Fish spawn of the following dates each year	SpawnDate1..3		User Entered Spawn Dates	(date)
Fish can spawn an unlimited number of times...	UnlimitedSpawning		Allow fish to spawn unlimited times each year	(true/false)
Fish can only spawn...	SpawnLimit		Number of spawns allowed for this species this year	(integer)
Use Allometric Equation to Calculate Maximum Consumption	UseAllom_C		Use Allometric Consumption Equation	(true/false)
Intercept for weight dependence	CA	CA	Allometric Consumption Parameter	(real number)
Slope for weight dependence	CB	CB	Allometric Consumption Parameter	(real number)
Use Allometric Equation to Calculate Respiration	UseAllom_R		Use Allometric Consumption Respiration	(true/false)
RA	RA	RA	Intercept for species specific metabolism	(real number)
RB	RB	RB	Weight dependence coefficient	(real number)

USER INTERFACE	**INTERNAL**	**TECH DOC**	**DESCRIPTION**	**UNITS**
Use “Set 1" of Respiration Equations	UseSet1		Use "Set 1" of Allometric Respiration Parameters	(true/false)
RQ	RQ	RQ	Allometric Respiration Parameter	(real number)
RTL	RTL	RTL	temperature below which swimming activity is an exponential function of temperature	(°C)
ACT	ACT	ACT	intercept for swimming speed for a 1g fish	(cm/s)
RTO	RTO	RTO	coefficient for swimming speed dependence on metabolism	(s/cm)
RK1	RK1	RK1	intercept for swimming speed above the threshold temperature	(cm/s)
BACT	BACT	BACT	coefficient for swimming at low temperatures	(1/ °C)
RTM	RTM		not currently used as a parameter by the code	
RK4	RK4	RK4	weight-dependent coefficient for swimming speed	(real number)
ACT	ACT	ACT	intercept of swimming speed vs. temperature and weight	(real number)
Preference (ratio)	TrophInt.Pref[ ]	$Pref_{prey, pred}$	initial preference value from the animal parameter screen	(unitless)
Egestion (frac.)	TrophInt.Egest[ ]	$EgestCoeff_{prey, pred}$	fraction of ingested prey that is egested	(unitless)

USER INTERFACE	**INTERNAL**	**TECH DOC**	**DESCRIPTION**	**UNITS**
	PlantRecord	**Plant Underlying Data**	**For each Plant in the Simulation, the following parameters are required**	
Plant	PlantName		Plant's Name. Used for Reference only.	N / A
Plant Type	PlantType	Plant Type	Plant Type: (Phytoplankton, Periphyton, Macrophytes, Bryophytes)	Choice from List
Taxonomic Group	Taxonomic_Type	Taxonomic Group	Taxonomic group	Choice from List
Toxicity Record	ToxicityRecord	N / A	associates plant with appropriate toxicity data	Choice from List
Saturating Light	LightSat	LightSat	light saturation level for photosynthesis	(ly/d)
P Half-saturation	KPO4	KP	half-saturation constant for phosphorus	(gP/m3)
N Half-saturation	KN	KN	half-saturation constant for nitrogen	(gN/m3)
Inorg C Half-saturation	KCarbon	KCO2	half-saturation constant for carbon	(gC/m3)
Temp Response Slope	Q10	Q10	slope or rate of change per 10°C temperature change	(unitless)
Optimum Temperature	TOpt	TOpt	optimum temperature	(°C)
Maximum Temperature	TMax	TMax	maximum temperature tolerated	(°C)
Min. Adaptation Temp	TRef	TRef	adaptation temperature below which there is no acclimation	(°C)
Max. Photosynthesis Rate	PMax	PMax	maximum photosynthetic rate	(1/d)
Respiration Coefficient	KResp	KResp	coefficient of proportionality between. excretion and photosynthesis at optimal light levels	(unitless)
Mortality Coefficient	KMort	KMort	intrinsic mortality rate	(g/g·d)
Exponential Mort Coeff	EMort	EMort	exponential factor for suboptimal conditions	(unitless)
P : Photosynthate	UptakePO4	Uptake Phosphorus	fraction of photosynthate that is nutrient (P)	(unitless)
N: Photosynthate	UptakeN	Uptake Nitrogen	fraction of photosynthate that is nutrient (N)	(unitless)
Light Extinction	ECoeffPhyto	EcoeffPhyto	attenuation coefficient for given alga	(1/m-g/m3)vv

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Sedimentation Rate	KSed	KSed	intrinsic settling rate	(m/d)
Exp. Sedimentation Coefficient	ESed	ESed	exponential settling coefficient	(unitless)
Carrying Capacity	N A	N A	not used by the code	(g/m2)
Reduction in Still Water	Red_Still_Water	RedStillWater	reduction in photosynthesis in absence of current	(unitless)
VelMax for macrophytes	Macro_VelMax	VelMax	velocity at which total breakage occurs	(cm/s)
Critical Force (Fcrit for periphyton only)	FCrit	Fcrit	critical force necessary to dislodge given periphyton group	(kg m/s^2)
Percent in Riffle	PrefRiffle	PrefRiffle	Percentage of biomass of plant that is in riffle, as opposed to run or pool	(%)
Percent in Pool	PrefPool	PrefPool	Percentage of biomass of plant that is in pool, as opposed to run or riffle	(%)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	AnimalToxRecord	**Animal Toxicity Parameters**	**For each Chemical Simulated, the following parameters are required for each animal simulated**	
LC50	LC50	LC50	concentration of toxicant in water that causes 50% mortality	(:g/L)
LC50 exp time (h)	LC50_exp_time	ObsTElapsed	exposure time in toxicity determination	(h)
Elim rate const	K2	K2	elimination rate constant	(1/d)
Biotrnsfm rate	BioTrans[ ]	Biotransform	percentage of chemical that is biotransformed to specific daughter products	(1/d)
EC50 growth	EC50_growth	EC50Growth	external concentration of toxicant at which there is a 50% reduction in growth	(:g/L)
Growth exp (h)	Growth_exp_time	ObsTElapsed	exposure time in toxicity determination	(h)
EC50 repro	EC50_repro	EC50Repro	external concentration of toxicant at which there is a 50% reduction in reprod	(:g/L)
Repro exp time (h)	Repro_exp_time	ObsTElapsed	exposure time in toxicity determination	(h)
Ave. wet wt. (g)	Ave_wet_wt	WetWt	mean wet weight of organism	(g)
Lipid Frac	Lipid_frac	LipidFrac	fraction of lipid in organism	(g lipid/g organ)
Drift Threshold (ug/L)	Drift_Thresh	Drift Threshold	concentration at which drift is initiated	(:g/L)
	TPlantToxRecord	**Plant Toxicity Parameter**	**For each Chemical Simulated, the following parameters are required for each plant simulated**	
EC50 photo	EC50_photo	EC50Photo	external concentration of toxicant at which there is 50% reduction in photosynthesis	(:g/L)
EC50 exp time (h)	EC50_exp_time	ObsTElapsed	exposure time in toxicity determination	(h)
EC50 dislodge	EC50_dislodge	EC50Dislodge	for periphyton only: external concentration of toxicant at which there is 50% dislodge of periphyton	(:g/L)
Elim rate const	K2	K2	elimination rate constant	(1/d)

USER INTERFACE	**INTERNAL**	**TECH DOC**	**DESCRIPTION**	**UNITS**
LC50	LC50	LC50	concentration of toxicant in water that causes 50% mortality	(:g/L)
LC50 exp.time (h)	LC50_exp_time	ObsTElapsed	exposure time in toxicity determination	(h)
Lipid Frac	Lipid_frac	LipidFrac	fraction of lipid in organism	(g lipid/g organ
	TChemical	**Chemical Parameters**	**For each Chemical to be simulated, the following parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of the state variable	:g/L
Gas-phase conc.	Tox_Air	$Toxicant_{air}$	gas-phase concentration of the pollutant	g/m^3
Loadings from Inflow	Loadings	Inflow Loadings	Daily loading as a result of the inflow of water	:g/L
Loadings from Point Sources	Alt_Loadings[Pointsource]	Point Source Loadings	Daily loading from point sources	(g/d)
Loadings from Direct Precipitation	Alt_Loadings[DirectPrecip]	Direct Precipitation Load	Daily loading from direct precipitation	(g/m2 ·d)
Nonpoint-source Loadings	Alt_Loadings[NonPointsource]	Non-Point Source Loading	Daily loading from non-point sources	(g/d)Tox_AirGas-phase concentration(g/m3)
Biotrnsfm rate	BioTrans[ ]	Biotransform	percentage of chemical that is biotransformed to specific daughter products	%

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	TRemineralize	**Nutrient Parameters**	**For each Nutrient to be simulated, O2 and CO2, the following parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of the state variable	mg/L
	Loadings	Inflow Loadings	Daily loading as a result of the inflow of water	mg/L
Loadings from Point Sources	Alt_Loadings[Pointsource]	Point Source Loadings	Daily loading from point sources	(g/d)
Loadings from Direct Precipitation	Alt_Loadings[Direct Precip]	Direct Precipitation Loa	Daily loading from direct precipitation	(g/m2·d)
Non-point source loadings	Alt_Loadings[NonPointsource]	Non-Point Source Loading	Daily loading from non-point sources	(g/d)
Fraction of Phosphate Available	FracAvail	FracAvail	Fraction of phosphate loadings that is available versus that which is tied up in minerals	(unitless)
	TSedDetr	**Sed. Detritus Parameters**	**For the Labile and Refractory Sedimented Detritus compartments, the following parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of the labile or refractory sedimented detritus	(g/m2)
Initial Condition	TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant Exposure of the state variable, for each chemical simulated	:g/kg
Loadings from Inflow	Loadings	Inflow Loadings	Daily loading of the sedimented detritus as a result of the inflow of water	mg/L
(Toxicant) Loadings	TToxicant.Loads	Tox Exposure of Inflow L	Daily parameter; Toxicant Exposure of each type of inflowing detritus, for each chemical	:g/kg

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	TDetritus	**Susp & Dissolved Detritus**	**For the Suspended and Dissolved Detritus compartments, the following parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of suspended & dissolved detritus, as organic matter, organic carbon, or biochemical oxygen demand	mg/L
Initial Condition: % Particulate	Percent_Part_IC		Percent of Initial Condition that is particulate as opposed to dissolved detritus	percentage
Initial Condition: % Refractory	Percent_Refr_IC		Percent of Initial Condition that is refractory as opposed to labile detritus	percentage
Inflow Loadings	Loadings	Inflow Loadings	Daily loading as a result of the inflow of water	mg/L
All Loadings: % Particulate	Percent_Part	Percent Particulate Infl	Daily parameter; % of all loadings that are particulate as opposed to dissolved detritus	percentage
All Loadings: % Refractory	Percent_Refr	Percent Refractory Inflo	Daily parameter; % of loading that is refractory as opposed to labile detritus	percentage
Loadings from Point Sources	Alt_Loadings[Pointsource]	Point Source Loadings	Daily loading from point sources	(g/d)
Nonpoint-source Loadings (Associated with Organic Matter)	Alt_Loadings [NonPointsource]	Non-Point Source Loading	Daily loading from non-point sources	(g/d)
(Toxicant) Initial Condition	TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant Exposure of the suspended and dissolved detritus	:g/kg
(Toxicant) Loadings (associated with Organic Matter)	TToxicant.Loads	Tox Exposure of Inflow L	Daily parameter; Toxicant Exposure of each type of inflowing detritus, for each chemical	:g/kg

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	TBuried Detritus	**Buried Detritus**	**For Each Type of Buried Detritus, the following parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of the labile and refractory buried detruitus	(g/m2) Kg/cu.m (on screen)
(Toxicant) Initial Condition	TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant Exposure of the labile and refractory buried detritus , for each chemical simulated	:g/kg (Kg/cu. m on screen)
	TPlant	**Plant Parameters**	**For each plant type simulated, the following parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of the plant	mg/L
Loadings from Inflow	Loadings	Inflow Loadings	Daily loading as a result of the inflow of water	mg/L
(Toxicant) Initial Condition	TToxicant.InitialCond	Toxicant Exposure	Initial Toxicant Exposure of the plant	:g/kg
(Toxicant) Loadings	TToxicant.Loads	Tox Exposure of Inflow L	Daily parameter; Tox.icant exposure of the Inflow Loadings, for each chemical simulated	:g/kg
	TAnimal	**Animal Parameters**	**For each animal type simulated, the following parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of the animal	mg/L or g/sq m) also expressed as g/m2)
Loadings from Inflow	Loadings	Inflow Loadings	Daily loading as a result of the inflow of water	mg/L or g/sq. m
(Toxicant) Initial Condition	Ttoxicant.InitialCond	Toxicant Exposure	Initial Toxicant Exposure of the animal	:g/kg
(Toxicant) Loadings	TToxicant.Loads	Tox Exposure of Inflow L	Daily parameter; toxic exposure of the Inflow Loadings, for each chemical simulated	:g/kg
Preference (ratio)	TrophIntArray.Pref	Prefprey, pred	for each prey-type ingested, a preference value within the matrix of preferences	(unitless)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Egestion (frac.)	TrophIntArray.ECoeff	EgestCoeff	for each prey-type ingested, the fraction of ingested prey that is egested	(unitless)
	TVolume	**Volume Parameters**	**For each segment simulated, the following water flow parameters are required**	
Initial Condition	InitialCond	Initial Condition	Initial Condition of the water volume .	(m3)
Water volume	Volume	Volume	Choose method of calculating volume; choose between Manning’s equation, constant volume, variable depending upon inflow and discharge, or use known values	cu. m
Inflow of Water	InflowLoad	Inflow of Water	Inflow of water; daily parameter, can choose between constant and dynamic loadings	(m3 /d) (cu m/d)
Discharge of Water	DischargeLoad	Discharge of Water	Discharge of water; daily parameter, can choose between constant and dynamic loadings	(m3 /d)
	Site Characteristics	**Site Characteristics**	**The following parameters are required**	
Site Type	SiteType	Site Type	Site type affects many portions of the model.	Pond, Lake, Stream, Reservoir, Limnocorral
Temperature				
Initial Condition	InitialCond	Initial condition	Initial temperature of the segment or layer (if vertically stratified	(°C)
Could this system stratify			could system vertically stratify	true/false
Valuation or loading			Temperature of the segment. Can use annual means for each stratum and constant or dynamic values	(°C)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Wind				
Initial Condition	InitalCond		Initial wind velocity 10 m above the water	(m/s)
Mean Value	Wind(MeanValue)	$CosCoeff_0$	Mean wind velocity	(m/s)
Wind Loading	Wind	Wind	Daily parameter; wind velocity 10 m above the water; l, can choose default time series, constant or dynamic loadings	(m/s)
Light				
Initial Condition	Light	Light		(ly/d)
Loading	Loadsrec		Daily parameter; avg. light intensity at segrment top; can choose annual mean, constant loading or dynamic loadings	
Photoperiod	Photoperiod	Photoperiod	Fraction of day with daylight; optional, can be calculated from latitude	(hr/d)
pH				
Initial Condition	InitialCond		Initial pH value	(pH)
State Variable Valuation	pH	pH	pH of the segment; can choose constant or daily value.	(pH)

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Sand / Silt / Clay	**TSediment**	**Inorganic Sediment Parameters**	**If the inorganic sediments model is included in AQUATOX, the following parameters are required for sand, silt, and clay**	
Initial Susp. Sed.	InitialCond	Initial Condition	Initial Condition of the sand, silt, or clay	(mg/L)
Frac in Bed Seds	FracInBed	$Frac_{Sed}$	Fraction of the bed that is composed of this inorganic sediment. Fractions of sand, silt, and clay must add to 1.0	(fraction)
Loadings from Inflow	Loadings	Inflow Loadings	Daily sediment loading as a result of the inflow of water	mg/L
Loadings from Point Sources	Alt_Loadings[Point source]	Point Source Loadings	Daily loading from point sources	(g/d)
Loadings from Direct Precipitation	Alt_Loadings[Direct Precip]	Direct Precipitation Loa	Daily loading from direct precipitation	(Kg Ad)
Non-point source loadings	Alt_Loadings[Non Pointsource]	Non-Point Source Loading	Daily loading from non-point sources	(g/d)