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AQUATOX (RELEASE 2.2): MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS: Technical Documentation (addendum)

Background

Minor changes have been made to the AQUATOX model since Release 2.1 was publicly released. This document describes changes in the model that distinguish Release 2.2 from Release 2.1 and describes any changed equations.

What's New

- AQUATOX now outputs retention time of a waterbody:

$$Retention = Volume / Discharge \quad (1b)$$

where:

Retention	=	retention time for water body (d)
Volume	=	current volume of water (m3),
Discharge	=	discharge of water from waterbody (m3/d), and

- There has been a refinement in the way that the light extinction due to blue-greens is calculated that improves the calculation of self-shading and improves simulations of blue-greens overall.
    - When calculating self-shading for blue-greens, the model accounts for more intense self shading in the upper layer of the water column due to the floating concentration of blue-greens there.
    - The *Extinction* term for blue-greens (within equation (34) from the AQUATOX Release 2 Technical Documentation) is multiplied by the segment thickness and divided by the thickness over which blue-greens occur to account for the more intense self-shading effects of these blue greens concentrated at the top of the water.
- AQUATOX now calculates, as an additional index, blue-greens as a percentage of the total phytoplankton biomass
- AQUATOX now utilizes mean velocity rather than daily velocity when calculating "*Adaptation*" for sloughing velocity (see equation (3a) from the AQUATOX Release 2.1 Technical Documentation Addendum)
    - In Release 2.1, a unique *Adaptation* was calculated for each time-step depending on the mean velocity on that day.

  - In Release 2.2, a constant *Adaptation* is calculated using code that calculates the site's mean velocity on an annual basis.
  - Using a constant value was the original intent for the *Adaptation* factor and this change should improve the model's capabilities to simulate periphyton across sites.
- AQUATOX Release 2.1 (and previous versions) errantly under-calculated the effects of excess temperature in plants.
  - The mortality effects of excess temperature in plants should slowly increase up until 100% mortality is achieved at the maximum temperature (*TMax)* level. (see equation (59) and Figure 39 from the AQUATOX Release 2 Technical Documentation)
  - Release 2.1 (and previous versions) had a coding error in which excess temperature effects were not calculated until *TMax* was exceeded. That equation error has been fixed in Release 2.2.
  - This has had a negligible effect on existing AQUATOX calibrations as temperatures approaching and exceeding the *TMax* for various species were rarely encountered, and temperature limitations on photosynthesis adequately captured the majority of these effects.
- An error has been fixed in which initial conditions for phosphate and nitrate, when entered in units of Total P and Total N, were not calculated properly.
  - There was an error in the back-calculation of the amount that is available as freely dissolved nutrients by accounting for the nitrogen and phosphorus contributed by suspended and dissolved detritus and phytoplankton.
  - This had no effects on the existing set of calibrated study files.
- Release 2.2 contains an improved algal parameter set (Plant "Library") and the calibration of many of the enclosed study files has been improved.
- There have been small refinements made to the display of output graphs *(e.g. when examining output on a very small scale, Y1 and Y2 axis labels no longer disappear).*
- AQUATOX output units have been clarified with regard to wet or dry weight.
- There is an improved Graphical User Interface (GUI) to more easily assign toxicity data, by allowing a user to map links between chemicals and biota within a single entry screen (see the "*Edit All Toxicity Records*" button within animal and plants "underlying data").
- When adding a new animal or plant, a small "seed" loading is added by default to avoid extinctions (1E-5 mg/L or g/m^2).
- The help file has been updated to correct several light conversion factors (used when inputting light loadings to AQUATOX).
- Release 2.2 includes several minor interface refinements (e.g. units were clarified for loadings in the "Suspended and dissolved detritus" entry screen in terms of dry vs. wet weight as well as organic matter vs. organic carbon or BOD)

Other Changes to AQUATOX Technical Documentation

In the second printing of the Release 2 Technical Documentation (EPA-823-R-04-002, with a blue cover) two tables were missing entries due to a software conversion problem in the printing process. The following tables should be inserted on p. 4-1:

Table 3. **Significant Differentiating Processes for Plants**

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

Table 4. **Significant Differentiating Processes for Animals**

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

The following are citations missing from the References section of the Release 2 and 2.1 Technical Documentation:

Hanson, Paul C., Timothy B. Johnson, Daniel E. Schindler, and James F. Kitchell. 1997. Fish Bioenergetics 3.0. Madison: Center for Limnology, University of Wisconsin.

Sterner, Robert W., and Nicholas B. George. 2000. Carbon, Nitrogen, and Phosphorus Stoichiometry of Cyprinid Fishes. Ecology 81:127-140.

The Release 2.1 Technical Documentation Addendum omitted Appendix B (a list of AQUATOX parameters). The following is the complete and updated Appendix B:

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 m^3 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 OC
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	KAcid	pseudo-first-order acid-catalyzed rate constant for a given pH	L/mol · d

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Base catalyzed hydrolysis constant	KBase	KBase	pseudo-first-order rate constant for a given pH	L/mol · 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 (Internal Model)	parameter expressing variability in toxic response; default is 0.33	unitless
Weibull Slope Factor	WeibullSlopeFactor	Slope Factor (External Model)	slope at LC50 multiplied by LC50	unitless
Chemical is a Base	ChemIsBase	if the compound is a base	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.)	m^3
Surface Area	Area	Area	site area	m^2
Mean Depth	ZMean	ZMean	mean depth, (initial condition if mean depth is selected)	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
Annual Light Range	LightRange	LightRange	annual range in light intensity	Langleys/day
Total Alkalinity	*AlkCaCO3*	*N / A*	*Not utilized as a parameter by the code.*	*mg/L*
Hardness as CaCO3	*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	m^2
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
Total Length	TotalLength	TotLength	total river length for calculating phytoplankton retention	km
Watershed Area	WaterShedArea	WaterShed	watershed area for estimating total river length (above)	km^2

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.	$s / m^{1/3}$
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	TauScourSed	critical shear stress for scour of silt	kg/m^2
Silt: Critical Shear Stress for Deposition	tdep_silt	TauDepSed	critical shear stress for deposition of silt	kg/m^2
Silt: Fall Velocity	FallVel_silt	VTSed	terminal fall velocity of silt	m/s
Clay: Critical Shear Stress for Scour	ts_clay	TauScourSed	critical shear stress for scour of clay	kg/m^2
Clay: Critical Shear Stress for Deposition	tdep_clay	TauDepSed	critical shear stress for deposition of clay	kg/m^2
Clay: Fall Velocity	FallVel_clay	VTSed	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 (pertaining to organic matter)**	
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.*	
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
P to Organics, Labile	P2OrgLab	P2OrgLab	ratio of phosphate to labile organic matter	fraction dry weight
N to Organics, Labile	N2OrgLab	N2OrgLab	ratio of nitrate to labile organic matter	fraction dry weight
P to Organics, Refractory	P2OrgRefr	P2OrgRefr	ratio of phosphate to refractory organic matter	fraction dry weight
N to Organics, Refractory	N2OrgRefr	N2OrgRefr	ratio of nitrate to refractory organic matter	fraction dry weight
P to Organics, Diss. Labile	P2OrgDissLab	P2OrgDissLab	ratio of phosphate to dissolved labile organic matter	fraction dry weight
N to Organics, Diss. Labile	N2OrgDissLab	N2OrgDissLab	ratio of nitrate to dissolved labile organic matter	fraction dry weight
P to Organics, Diss. Refr.	P2OrgDissRefr	P2OrgDissRefr	ratio of phosphate to dissolved refractory organic matter	fraction dry weight
N to Organics, Diss. Refr.	N2OrgDissRefr	N2OrgDissRefr	ratio of nitrate to dissolved refractory organic matter	fraction dry weight
O2 : Biomass, Respiration	O2Biomass	O2Biomass	ratio of oxygen to organic matter	unitless ratio
O2: N, Nitrification	O2N	O2N	ratio of oxygen to nitrogen	unitless ratio
Detrital Sed Rate (KSed)	KSed	KSed	intrinsic sedimentation rate	m/d
PO4, Anaerobic Sed.	*PSedRelease*	*N / A*	*Not utilized as a parameter by the code.*	$g/m^2 \cdot d$
NH4, Aerobic Sed.	*NSedRelease*	*N / A*	*Not utilized as a parameter by the code.*	$g/m^2 \cdot d$

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Wet to Dry Susp. Labile	Wet2DrySLab	Wet2DrySLab	wet weight to dry weight ratio for suspended labile detritus	ratio
Wet to Dry Susp. Refr.	Wet2DrySRefr	Wet2DrySRefr	wet weight to dry weight ratio for suspended refractory detritus	ratio
Wet to Dry Sed. Labile	Wet2DryPLab	Wet2DryPLab	wet weight to dry weight ratio for particulate labile detritus	ratio
Wet to Dry Sed. Refr.	Wet2DryPRefr	Wet2DryPRefr	wet weight to dry weight ratio for particulate refractory detritus	ratio

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/m^3
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/m^3 or g/m^2
Temp Response Slope	Q10	Q10	slope or rate of change in 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
Endogenous Respiration	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
N to Organics	N2Org	N2Org	ratio of nitrate to organic matter for given species	fraction dry weight
P to Organics	P2Org	P2Org	ratio of phosphate to organic matter for given species	fraction dry weight
Wet to Dry	Wet2Dry	Wet2Dry	ratio of wet weight to dry weight for given species	ratio
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^2

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 org. wet
Mean Weight	MeanWeight	WetWt	mean wet weight of organism	g
Percent in Riffle	PrefRiffle	PreferenceHabitat	percentage of biomass of animal that is in riffle, as opposed to run or pool	%
Percent in Pool	PrefPool	PreferenceHabitat	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 sates	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		allometric consumption parameter	real number
Slope for weight dependence	CB		allometric consumption parameter	real number
Use Allometric Equation to Calculate Respiration	UseAllom_R		use allometric consumption respiration	true/false
RA	RA		intercept for species specific metabolism	real number
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		intercept of swimming speed vs. temperature and weight	real number
Preference (ratio)	TrophInt.Pref[ ]	Prefprey,pred	initial preference value from the animal parameter screen	unitless
Egestion (frac.)	TrophInt.Egest[ ]	EgestCoeffprey,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/m^3
N Half-saturation	KN	KN	half-saturation constant for nitrogen	gN/m^3
Inorg C Half-saturation	KCarbon	KCO2	half-saturation constant for carbon	gC/m^3
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
Photorespiration Coefficient	KResp	KResp	coefficient of proportionality between. excretion and photosynthesis at optimal light levels	unitless
Resp. Rate at 20 deg. C	Resp20	Resp20	respiration rate at 20°C	g/g·d
Mortality Coefficient	KMort	KMort	intrinsic mortality rate	g/g
Exponential Mort Coeff	EMort	EMort	exponential factor for suboptimal conditions	g/g·d
P to Organics	P2Org	P2Org	ratio of phosphate to organic matter for given species	fraction dry weight
N to Organics	N2Org	N2Org	ratio of nitrate to organic matter for given species	fraction dry weight
Light Extinction	ECoeffPhyto	EcoeffPhyto	attenuation coefficient for given alga	$1/m\text{-}g/m^3w$
Wet to Dry	Wet2Dry	Wet2Dry	ratio of wet weight to dry weight for given species	ratio

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
Phytoplankton: Sedimentation Rate	KSed	KSed	intrinsic settling rate	m/d
Phytoplankton: Exp. Sedimentation Rate	ESed	ESed	exponential settling coefficient	unitless
Carrying Capacity	*N / A*	*N / A*	*Not utilized as a parameter by the code.*	g/m^2
Periphyton: 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
Periphyton: Critical Force (FCrit)	FCrit	FCrit	critical force necessary to dislodge given periphyton group	newtons (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	µg/L
LC50 exp time (h)	LC50_exp_time	ObsTElapsed	exposure time in toxicity determination	h
K2 Elim rate const	K2	K2	elimination rate constant	1/d
K1 Uptake const	K1	K1	uptake rate constant, only used if "Enter K1" option is selected	L / kg dry day
BCF	BCF	BCF	Bioconcentration factor, only used if "Enter BCF" option is selected	L / kg dry
Biotrnsfm rate	BioRateConst	BioRateConst	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	µg/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	µg/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	µg/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	µg/L
EC50 exp time (h)	EC50_exp_time	ObsTElapsed	exposure time in toxicity determination	h

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
EC50 dislodge	EC50_dislodge	EC50Dislodge	for periphyton only: external concentration of toxicant at which there is 50% dislodge of periphyton	µg/L
K2 Elim rate const	K2	K2	elimination rate constant	1/d
K1 Uptake const	K1	K1	uptake rate constant, only used if "Enter K1" option is selected	L / kg dry day
BCF	BCF	BCF	bioconcentration factor, only used if "Enter BCF" option is selected	L / kg dry
Biotrnsfm rate	BioRateConst	BioRateConst	percentage of chemical that is biotransformed to specific daughter products	1/d
LC50	LC50	LC50	concentration of toxicant in water that causes 50% mortality	µg/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 org. dry
	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	µg/L
Gas-phase conc.	Tox_Air	Toxicantair	gas-phase concentration of the pollutant	g/m3
Loadings from Inflow	Loadings	Inflow Loadings	Daily loading as a result of the inflow of water	µg/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 Load	Daily loading from direct precipitation	$g/m^2 \cdot d$
Nonpoint-source Loadings	Alt_Loadings[NonPointsource]	Non-Point Source Loading	Daily loading from non-point sources	g/dTox_AirGas-phase concentrationg/m3
Biotransformation	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 (TotP or TotN optional)	mg/L
	Loadings	Inflow Loadings	daily loading as a result of the inflow of water (TotP or TotN optional)	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	$g/m^2 \cdot d$
Non-point source loadings	Alt_Loadings[NonPointsource]	Non-Point Source Loading	daily loading from non-point sources	g/d
Fraction of Phosphate Available	FracAvail		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/m^2
Initial Condition	TToxicant.InitialCond	Toxicant Exposure	initial toxicant exposure of the state variable, for each chemical	µg/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	µg/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	$g_{\textbf{organic matter}}$ /d
Nonpoint-source Loadings (Associated with Organic Matter)	Alt_Loadings	Non-Point Source Loading	daily loading from non-point sources	$g_{\textbf{organic matter}}$ /d
(Toxicant) Initial Condition	TToxicant.InitialCond	Toxicant Exposure	initial toxicant exposure of the suspended and dissolved detritus	µg/kg
(Toxicant) Loadings (associated with Organic Matter)	TToxicant.Loads	Tox Exposure of Inflow Loading	daily parameter; toxicant exposure of each type of inflowing detritus, for each chemical	µg/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	Kg/cu. m
(Toxicant) Initial Condition	TToxicant.InitialCond	Toxicant Exposure	initial toxicant exposure of the labile and refractory buried detritus, for each chemical simulated	Kg/cu. m
	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 or g/m^2 dry
Loadings from Inflow	Loadings	Inflow Loadings	daily loading as a result of the inflow of water	mg/L or g/m^2 dry
(Toxicant) Initial Condition	TToxicant.InitialCond	Toxicant Exposure	initial toxicant exposure of the plant	µg/kg
(Toxicant) Loadings	TToxicant.Loads	Tox Exposure of Inflow L	daily parameter; toxicant exposure of the inflow loadings, for each chemical simulated	µg/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/m^2
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	µg/kg
(Toxicant) Loadings	TToxicant.Loads	Tox Exposure of Inflow L	daily parameter; toxic exposure of the inflow loadings, for each chemical simulated	µg/kg
Preference (ratio)	TrophIntArray.Pref	Prefprey, pred	for each prey-type ingested, a preference value within the matrix of preferences	unitless
Egestion (frac.)	TrophIntArray.ECoeff	EgestCoeff	for each prey-type ingested, the fraction of ingested prey that is egested	unitless

USER INTERFACE	INTERNAL	TECH DOC	DESCRIPTION	UNITS
	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 .	m^3
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	m^3 /d (cu.m/d)
Discharge of Water	DischargeLoad	Discharge of Water	discharge of water; daily parameter, can choose between constant and dynamic loadings	m^3 /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
Site Mean Depth	DynZMean	user entered mean depth	optional, time series of mean depth for site	m
	Temperature	**Temperature**	**Temperature Parameters Required**	
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
	Wind	**Wind**	**Wind parameters required**	
Initial Condition	InitalCond		initial wind velocity 10 m above the water	m/s
Mean Value	MeanValue		mean wind velocity	m/s

Wind Loading	Wind	Wind	daily parameter; wind velocity 10 m above the water; can choose default time series, constant or dynamic loadings	m/s
USER INTERFACE	**INTERNAL**	**TECH DOC**	**DESCRIPTION**	**UNITS**
	Light	**Light**	**Light Parameters Required**	
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	**pH**	**pH Parameters Required**	
Initial Condition	InitialCond		initial pH value	pH
State Variable Valuation	pH	pH	pH of the segment; can choose constant or daily value.	pH
Mean alkalinity	alkalinity	alkalinity	mean Gran alkalinity (if dynamic pH option selected)	µeq CaCO3/L
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	FracSed	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[Pointsource]	Point Source Loadings	daily loading from point sources	g/d
Loadings from Direct Precipitation	Alt_Loadings[Direct Precip]	Direct Precipitation Load	daily loading from direct precipitation	Kg ·d
Non-point source loadings	Alt_Loadings[NonPointsource]	Non-Point Source Loading	Daily loading from non-point sources	g/d