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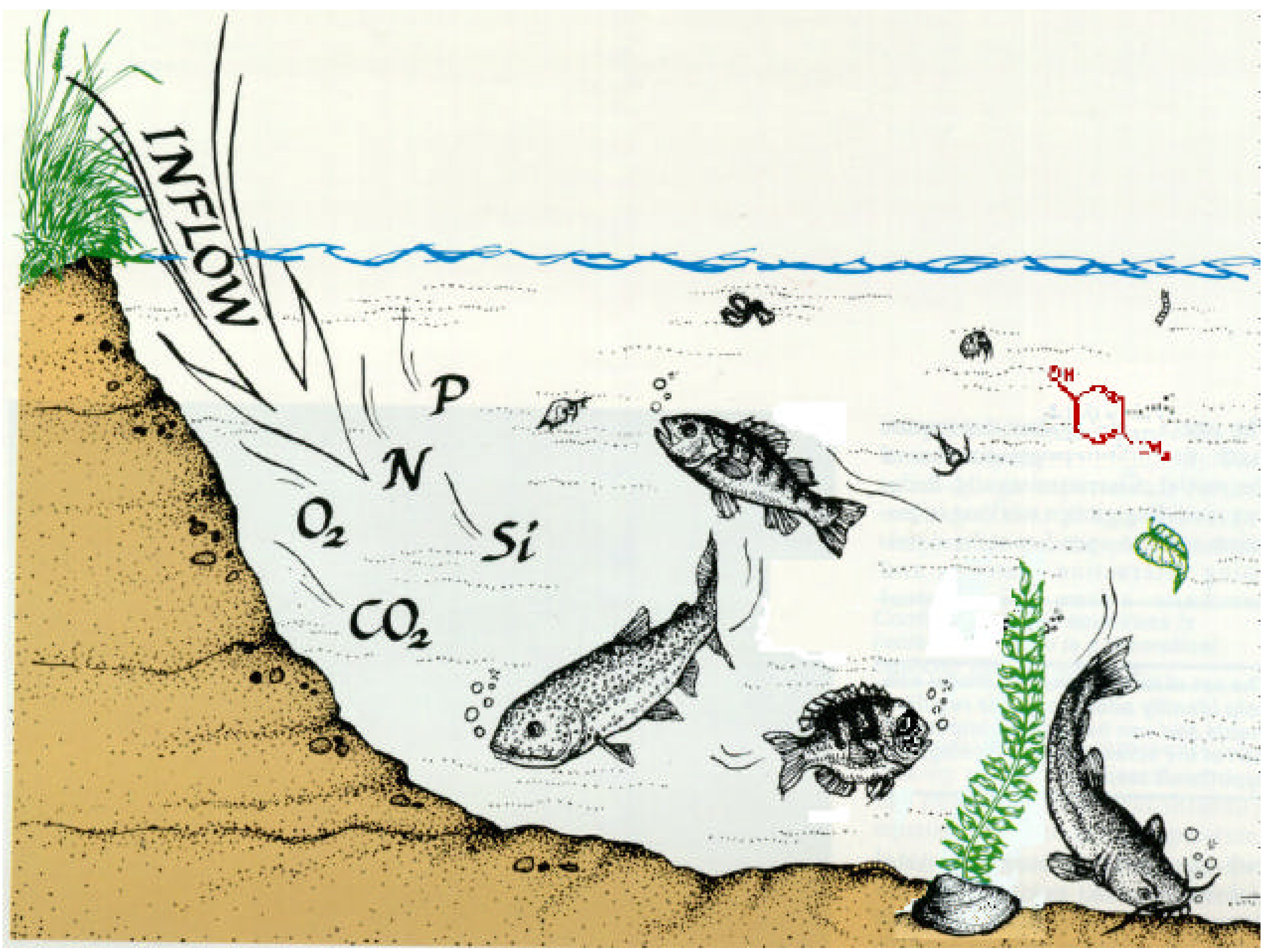
AQUATOX FOR WINDOWS

A MODULAR FATE AND EFFECTS MODEL FOR AQUATIC ECOSYSTEMS

RELEASE 1.1

VOLUME 3: MODEL VALIDATION REPORTS ADDENDUM



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VOLUME 3: MODEL VALIDATION REPORTS

ADDENDUM: FORMULATION, CALIBRATION, AND VALIDATION OF A PERIPHYTON SUBMODEL FOR AQUATOX RELEASE 1.1

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This document presents a calibration and validation for a new application for AQUATOX, an aquatic ecosystem simulation model which was originally released in September 2000. 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

Daily flow data for Walker Branch were collected as part of the Walker Branch Watershed research project supported by the Environmental Sciences Division, Office of Biological and Environmental Research, U.S. Department of Energy and were provided by Patrick Mulholland, Oak Ridge National Laboratory. This calibration and validation would not have been possible without the remarkable factorial experiments and the rigorous data set compiled by Amy Rosemond for her dissertation. Access to Dr. Rosemond's raw data is especially appreciated.

AQUATOX has been developed and documented by Dr. Richard A. Park of Eco Modeling; most of the programming has been by Jonathan S. Clough under subcontract to Eco Modeling. It was funded with Federal funds from the U.S. Environmental Protection Agency, Office of Science and Technology. This validation study was funded under contract numbers 68-C-98-010 and 68-C-01-0037 to AQUA TERRA Consultants, Anthony Donigian, Work Assignment Manager. AQUATOX programming and other support was provided by Jonathan Clough, and his help is gratefully acknowledged. Marjorie Coombs Wellman, as the EPA work assignment manager, provided technical direction, encouragement, and editorial insights that were very helpful.

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: 1996 Report to Congress, 36 percent of assessed river lengths and 39 percent of assessed lake areas were impaired for one or more of their designated uses (US EPA 1998). The most commonly reported causes of impairment in rivers and streams were siltation, nutrients, bacteria, oxygen-depleting substances, and pesticides; in lakes and reservoirs the causes also included metals and noxious aquatic plants. The most commonly reported sources of impairment were agriculture, nonpoint sources, municipal point sources, atmospheric deposition, hydrologic modification, habitat alteration and resource extraction. There were 2196 fish consumption advisories, which may include outright bans, in 47 States, the District of Columbia and American Samoa. Seventy-six percent of the advisories were due to mercury, with the rest due to PCBs, chlordane, dioxin, and DDT (US EPA 1998). 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 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.

The AQUATOX model is described in these documents. Volume 1: User's Manual describes the usage of the model. 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: Model Validation Reports presents three model validation studies performed for different environmental stressors and in different waterbody types. The validations were performed using test versions of the model which had only very minor differences from Release Version 1; the specific test version is noted in the title of each report. This **Addendum to Volume 3** presents a calibration and validation study for the use of AQUATOX to simulate periphyton in streams. Constructs were added to AQUATOX in order to better represent periphyton dynamics; these are described in the text. Readers should visit the AQUATOX website (http://www.epa.gov/ost/models/aquatox/) to download the new executable program that contains the new constructs.

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Abstract

The AQUATOX periphyton submodel was successfully calibrated and validated with data from Walker Branch, Tennessee. A single parameter set for diatoms, green algae, and gastropods was developed to fit all twenty treatments in a factorial experiment involving low and high nutrient levels, low and high light levels, and grazing and no grazing in stream-side channels and stream enclosures. A two-year data set for periphyton on cobbles in the stream bed was used to validate the model for continuous ambient conditions in this woodland stream. Nitrogen, phosphorus, light, and grazing were all limiting, both singly and in combination. Inclusion of a sloughing term based on senescence due to deteriorating environmental conditions and the drag force of currents on exposed periphyton biomass provided a realistic response to limiting environmental factors and was especially useful in modeling the effects of variable flow rates on diatoms and filamentous algae. The model was shown to be calibrated and validated based on the weight of evidence of reproduction of observed patterns of biomass change, concordance of maxima between predicted and observed biomass, and equivalence in predicted and observed means and variances as confirmed by relative bias and F tests.

FORMULATION, CALIBRATION, AND VALIDATION OF A PERIPHYTON SUBMODEL FOR AQUATOX RELEASE 1

Introduction

Periphyton are benthic algae and associated organic detritus that are attached to hard substrates and macrophytes and that carpet stabilized sands. They are an important constituent of the aquatic community, especially in shallow lakes, ponds, streams, and rivers (Stevenson, 1996). They also are an important link for bioaccumulation of organic contaminants (Wang et al., 1999). Periphyton have been shown to be sensitive to eutrophication of streams (Marcus, 1980; Bothwell, 1985; Hart and Robinson, 1990; Van Nieuwenhuyse and Jones, 1996; Biggs, 2000). Although they are nominally included in several ecosystem models, periphyton have been difficult to model. The purpose of this study is to test alternate formulations, calibrate for several different combinations of environmental factors, and validate with data from a woodland stream.

Modifications to Formulations in AQUATOX

Originally periphyton were modeled in AQUATOX Release 1 as if they were merely non-sinking phytoplankton subject to current-induced scour. However, two processes distinguish periphyton from their free-living counterparts. First, as periphyton die, detritus accumulates and remains a part of the operational biomass (best characterized as ash-free dry weight). Second, as environmental conditions deteriorate or water velocity increases, sloughing occurs and large proportions of biomass are lost instantaneously. AQUATOX has been modified to account for both these processes.

Sloughing

Earlier attempts at calibration were unsuccessful because they were unable to reproduce the buildup and then decline in biomass in 1989 at Walker Branch. As a result, the formulation for scour was reexamined and the more complex sloughing formulation, extending the approach of Asaeda and Son (2000), was implemented. This function was able to represent a wide range of conditions better. 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:

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

where:

DragForce	=	drag force (kg m/s^2);
Rho	=	density (kg/m^3);
DragCoeff	=	drag coefficient (2.53E-4, unitless);
Vel	=	velocity (m/s);
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):

$$Biovol_{Dia} = \frac{Biomass}{2.08E-9}$$
$$Biovol_{Fil} = \frac{Biomass}{8.57E-9}$$

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 and nutrients 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 suboptimal nutrients and light on photosynthesis, and which is multiplied by 5 to desensitize its effect on sloughing. *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, then sloughing occurs:

$$\text{If } DragForce > Suboptimal_{Org} \cdot FCrit_{Org} \text{ then } Slough = Biomass \cdot FracSloughed$$
$$\text{else } Slough = 0$$

where:

$Suboptimal_{Org}$	=	factor for suboptimal nutrient and light effect on senescence of given periphyton group (unitless);
$FCrit_{Org}$	=	critical force necessary to dislodge given periphyton group ($kg\ m/s^2$);
Slough	=	biomass lost by sloughing (g/m^3);
FracSloughed	=	fraction of biomass lost at one time (90%, unitless).

$$Suboptimal_{Org} = NutrLimit_{Org} \cdot LtLimit_{Org} \cdot 5$$
$$\text{If } Suboptimal_{Org} > 1 \text{ then } Suboptimal_{Org} = 1$$

where:

NutrLimit	=	nutrient limitation for given algal group (unitless) computed by AQUATOX;
$LtLimit_{Org}$	=	light limitation for given algal group (unitless) computed by AQUATOX.

Detrital Accumulation

In phytoplankton, mortality results in immediate production of detritus, and that transfer is modeled. However, 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 model 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, with compensation through the high internal extinction rate constant.

Calibration Strategy

One of the difficulties with modeling periphyton is that there are few parameter values that are based on laboratory or field studies. Many studies have been conducted, but not with the goal of obtaining process-level estimates that can be used in modeling. Therefore, an additional burden is placed on the calibration effort.

The strategy for calibration involving several poorly defined parameters has been to use the results of field experiments on Walker Branch, Tennessee, conducted by Rosemond (1993) involving a factorial design (see also Mulholland and Rosemond, 1992; Rosemond, 1994; Rosemond, 1995; Rosemond et al., 1996; Rosemond et al., 2000). Walker Branch is a small woodland stream with naturally low discharge, nutrient-poor conditions, intense grazing, and low light levels (Rosemond, 1993). Nutrients were increased and grazers (gastropods) were removed in Spring, 1989, and nutrients were increased, grazers were removed, and light levels were increased in Summer, 1989, in stream-side channels; nutrients were increased and grazers were removed in Spring, 1990, in stream enclosures (**Tables 1-3**). Poorly defined parameters such as light saturation levels, maximum photosynthetic rates, and light extinction due to self-shading were calibrated for diatoms and green algae; and the maximum consumption rate, minimum biomass for feeding, and carrying capacity were calibrated for gastropods (see **Appendix**). The calibrations were then validated with a two-year data set from Walker Branch (Rosemond, 1993).

All simulations were conducted with exactly the same set of parameter values so that only the site characteristics (such as channel morphometry) and loadings (such as discharge, light, and nutrient loadings) were changed among simulations. Calibrations were conducted on each successive parameter in an iterative approach.

Table 1. Loadings and Initial Conditions Used in Spring, 1989, Simulations of Walker Br.

Spring, 1989 (March 15 to May 3)					
	Treatment	Control	High Nutrients	High N	High P
Initial gastropod biomass (g/m^2)*	Grazed	2.5	2.5	2.5	2.5
	Ungrazed	0	0	0	0
Nutrients (mg/L)	NH_4-N	0.006	0.0338	0.0338	0.006
	NO_3-N	0.0183	0.2078	0.2078	0.0183
	PO_4-P	0.00194	0.0366	0.00194	0.0366
Light (Ly/d)$^+$		57.5 to 10.5	57.5 to 10.5	57.5 to 10.5	57.5 to 10.5
Velocity (cm/s)		9.44	9.44	9.44	9.44
Initial algal biomass (g/m^2)*	Diatoms	0.0236	0.019	0.0324	0.0324
	Greens	0.0118	0.0096	0.0162	0.0162

$^+$ Light was reported by Rosemond (1993) as photosynthetic active radiation, which was multiplied by 2 to provide total radiation values used by AQUATOX *All biomass is ash-free dry weight

Table 2. Loadings and Initial Conditions Used in Spring, 1990, Simulations of Walker Br.

Spring, 1990 (March 5 to April 24)			
	Treatment	Control	High Nutrients
Initial gastropod biomass (g/m^2)*	Grazed	2.5	2.5
	Ungrazed	0.25	0.25
Nutrients (mg/L)	NH_4-N	0.002	0.0441
	NO_3-N	0.0101	0.2233
	PO_4-P	0.0024	0.0441
Light (Ly/d)$^+$		45 to 20	45 to 20
Velocity (cm/s)		9.44	9.44
Initial algal biomass (g/m^2)* differed between treatments	Diatoms	0.0116, 0.0178	0.019, 0.02
	Greens	0.0058, 0.0089	0.01, 0.01

$^+$ Light was reported by Rosemond (1993) as photosynthetic active radiation, which was multiplied by 2 to provide total radiation values used by AQUATOX *All biomass is ash-free dry weight

Table 3. Loadings and Initial Conditions Used in Summer, 1989, Simulations of Walker Br.

Summer, 1989 (July 21 to September 8)					
	Treatment	Control	High Nutrients	High Light, Control	High Light & Nutrients
Initial gastropod biomass (g/m^2)	Grazed	2.5	2.5	2.5	2.5
	Ungrazed	0	0	0	0
Nutrients (mg/L)	NH_4-N	0.006	0.05338	0-0.0076	0.05338
	NO_3-N	0.0183	0.2078	0.0296-0.0392	0.2078
	PO_4-P	0.00194	0.04366	0.0027-0.0049	0.04366
Light (Ly/d)$^+$		15.2 to 20	15.2 to 20	204	204
Velocity (cm/s)		9.44	9.44	9.44	9.44
Initial algal biomass (g/m^2)*	Diatoms	0.024, 0.019	0.02	0.027	0.024
	Greens	0.012, 0.009	0.01	0.014	0.012

$^+$ Light was reported by Rosemond (1993) as photosynthetic active radiation, which was multiplied by 2 to provide total radiation values used by AQUATOX *All biomass is ash-free dry weight

Calibration Results

Altogether, twenty treatments were simulated, including controls and manipulated grazing, nutrient, and light experiments. These are named, described, and keyed to the figures in **Table 4**.

Comparison of Maximum Values

Data from twenty factorial treatments were used in the calibration. Initially the objective was to minimize the squared deviations of the observed and predicted maxima. A close fit was obtained across almost all treatments; however, observed temporal patterns were not well represented (see next section). Therefore, the criteria were relaxed so that the temporal patterns could be matched as well. Because grazing usually prevents a buildup of biomass (ash-free dry weight or AFDW), the maxima of the grazed treatments were fairly uniform (**Figure 1**). The observed grazed maximum values were all higher than the predicted values, but often only one point exceeded the predicted. The ungrazed treatments exhibit the opposite relationship: almost all predicted maxima exceed the observed (**Figure 2**). However, the data were taken approximately every two weeks, and it is likely that observed maxima would miss peak biomass buildup that was followed by sloughing (Rosemond, pers. comm.). Therefore, it is to be expected that the predicted maxima often would exceed the observed biomass for treatments where there was stimulation in the absence of grazing. Note the difference in scale between the two graphs, which emphasizes the magnitude of the grazing pressure.

Table 4. Summary of Treatments Simulated

File Name	Description	Figure No.
WBCtlSpr89	control, Spring 1989	22
WBCtlSpr90	control, Spring 1990	23
WBCtlSmr89	control, Summer 1989	24
WBNSpr89	N-enriched, Spring 1989	16
WBPSpr89	P-enriched, Spring 1989	17
WBN&PSpr89	N- and P-enriched, Spring 1989	3, 4, 5,6,11
WBN&PSpr90	N- and P-enriched, Spring 1990	7
WBN&PSmr90	N- and P-enriched, Summer 1989	8
WBHiLtSmr89	High light, Summer 1989	28
WBN&PHiLtSmr89	N- and P-enriched, high light, Summer 1989	29
WBCtlwoGrzSpr89	Control, without grazers, Spring 1989	18, 19
WBCtl10%GrzSpr90	Control, 10% grazers, Spring 1990	20
WBCtlwoGrzSmr89	Control, without grazers, Summer 1989	21
WBNwoGrzSpr89	N-enriched, without grazers, Spring 1989	14
WBPwoGrzSpr89	P-enriched, without grazers, Spring 1989	15
WBN&PwoGrzSpr89	N- and P-enriched, without grazers, Spring 1989	9, 10,11,19
WBN&P10%GrzSpr90	N- and P-enriched, 10% grazers, Spring 1990	12
WBN&PwoGrzSmr89	N- and P-enriched, without grazers, Summer 1989	13, 27
WBHiLtwoGrzSmr89	High light, without grazers, summer, 1989	25
WBN&PHiLtwoGrzSmr89	N- and P-enriched, high light, without grazers, Summer 1989	26, 27

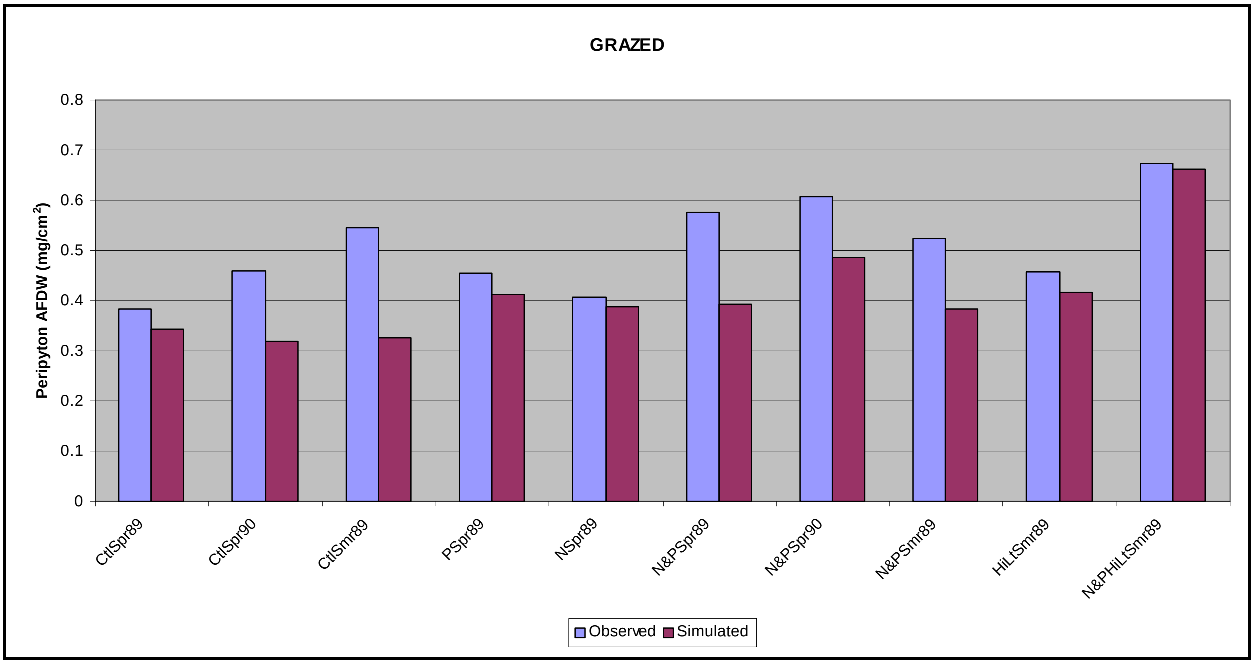

Figure 4. Comparison of observed (Rosemond, 1993) and predicted maxima for periphyton in Walker Branch, Tennessee, for various grazed treatments.

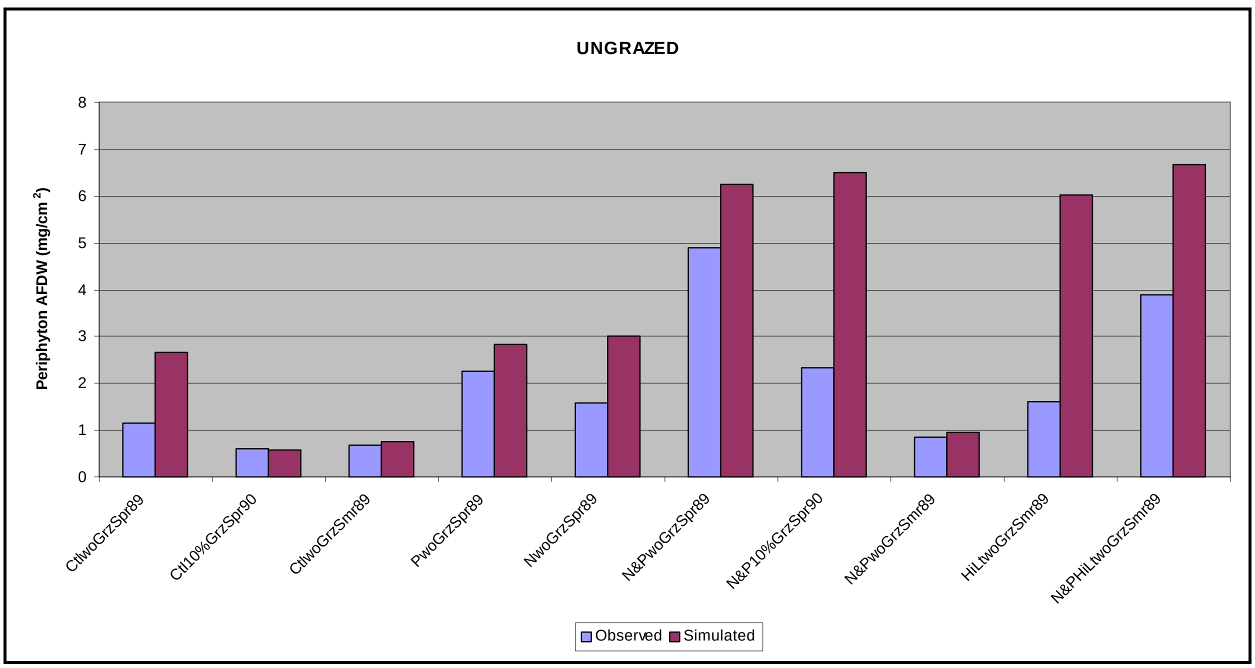

Figure 5. Comparison of observed (Rosemond, 1993) and predicted maxima for periphyton in Walker Branch, Tennessee, for various ungrazed treatments.

Statistical Tests

Two measures help answer the question: how much overlap is there between data and model distributions? Relative bias is a robust measure of how well central tendencies of predicted and observed results correspond; a value of 0 indicates that the means are the same (Bartell et al. 1992):

$$rB = \frac{(\overline{Pred} - \overline{Obs})}{S_{obs}}$$

where:

rB	=	relative bias (standard deviation units);
$\overline{Pred}$	=	mean predicted value;
$\overline{Obs}$	=	mean observed value; and
S_{obs}	=	standard deviation of observations.

The F test is the ratio of the variance of the model and the variance of the data. A value of 1 indicates that the variances are the same:

$$F = \frac{S^2_{pred}}{S^2_{obs}}$$

Very small F values suggest that the observed data may be too variable to determine the goodness of fit; very large F values indicate that the predictions are imprecise (Bartell et al., 1992). Large F values also may indicate that the model is predicting greater fluctuations than can be supported by sparse data. Assuming normal distributions, the probability that the observed and predicted distributions are the same can be evaluated. Putting the two tests together, if a comparison has rB = 0 and F = 1, then the predicted and observed results are identical.

Table 5 provides statistics for the simulations. For purposes of computing the variances and standard deviations, all observations were pooled, which tended to emphasize the sample variability. Six out of the twenty simulations exhibited similar predicted and observed means and variances at the 95% confidence level. Twelve other treatments had similar means, but the distributions were indeterminate and could not be compared because the observed data were considerably more variable than predicted. In one treatment, with high light and no grazing, the predictions and observations were significantly different. In the remaining treatment the variances were similar but the means were significantly different. In the following graphs, presented for visual inspection, the standard deviations are plotted for each sample mean, aiding in the evaluation.

Table 5. Statistics of Overlap Between Predicted and Observed Distributions

Fig.	Simulation	Mean predicted	Mean observed	rB	F
3	N & P, Spr, 1989	0.366	0.415	-0.348^{+}	0.00601$^{?}$
7	N & P, Spr, 1990	0.411	0.415	-0.0313^{+}	0.0259$^{?}$
8	N & P, Smr, 1989	0.369	0.386	-0.137^{+}	0.00271$^{?}$
9	N & P, no Grz, Spr, 1989	1.94	1.77	0.0978^{+}	0.121*
12	N & P, 10% Grz, Spr, 1990	1.91	1.14	0.880^{+}	0.591*
13	N & P, no Grz, Smr, 1989	0.520	0.687	-0.992^{+}	0.579*
14	N, no Grz, Spr, 1989	1.12	0.742	0.810^{+}	0.550*
15	P, no Grz, Spr, 1989	1.05	0.801	0.268^{+}	0.0956$^{?}$
16	N, Spr, 1989	0.385	0.384	0.0124^{+}	-0.0121$^{?}$
17	P, Spr, 1989	0.404	0.388	0.147^{+}	0.00647$^{?}$
18	Ctl, No grz, Spr, 1989	1.18	0.623	1.80	1.03*
20	Ctl, 10% grz, Spr, 1990	0.326	0.349	-0.0856^{+}	0.0354$^{?}$
21	Ctl, no Grz, Smr, 1989	0.475	0.372	0.871^{+}	0.290*
22	Ctl, Spr, 1989	0.336	0.320	0.172^{+}	0.0008$^{?}$
23	Ctl, Spr, 1990	0.312	0.348	-0.299^{+}	0.00215$^{?}$
24	Ctl, Smr, 1989	0.327	0.389	-0.570^{+}	0.0009 $^{?}$
25	Ctl, Hi Lt, no Grz, Smr, 1989	1.85	1.07	2.41	19.3
26	N & P, Hi Lt, no Grz, Smr, 1989	2.40	1.68	0.609^{+}	1.28*
28	Ctl, Hi Lt, Smr, 1989	0.395	0.400	-0.0255^{+}	0.00207$^{?}$
29	Nut, Hi Lt, Smr, 1989	0.499	0.404	0.580^{+}	0.0967$^{?}$

N - nitrogen enriched, P - phosphorus enriched, Grz - grazers, Ctl - control, $^{+}$ predicted mean = observed (95% CL), * predicted variance = observed (95% CL), $^{?}$ = indeterminate due to high observed variance

Visual Inspection

Visual inspections of fits of predictions to observed data are useful in evaluating how well patterns are represented, with allowance for the vagaries of widely spaced data points. Although not qualitative, they contribute considerably to the weight of evidence that the model is representing the periphyton dynamics realistically. In the graphs that follow, predictions are shown for diatoms and other periphyton (nominally greens), and the sum of these is presented for comparison with the observed data, which are shown with ± 1 standard deviation.

Simulation of the stream-side channel experiment in Spring, 1989, with both nitrogen (N) and phosphorus (P) enrichment and with normal density of grazers represented a mean response similar to the five periphyton observations, including the given initial condition (**Figure 3**). The gastropod biomass is stable at 2.5 g/m^2, compared to observed biomass of 1 to 3.3 (Rosemond, pers. comm.). Examination of the process rates for diatoms shows that photosynthesis is balanced with grazing (**Figure 4**). Although the parameter set was derived to give the best fit to all the treatments, it is instructive to examine the sensitivity of the simulations to key parameters. There was little response of diatoms to a normal distribution of values for the maximum photosynthetic rate (0.8 ± 0.24 g/g d) as shown in **Figure 5**; this is almost certainly due to suppression by grazing (*cf.* Hill, 1992). In another sensitivity analysis, gastropods exhibited only a 10% change in biomass by the end of the seven weeks, but diatoms exhibited a large and varied response to a normal distribution of values for the maximum consumption rate of gastropods (0.05 ± 0.015 g/g d) as shown in **Figure 6**.

Simulation of the comparable stream enclosure experiment in Spring, 1990, exhibited a very similar response with a mean that was very close to the mean of the observations (**Figure 7**). Simulation of the comparable stream-side channel experiment in Summer, 1989, also was close to the mean for the five observed points (**Figure 8**).

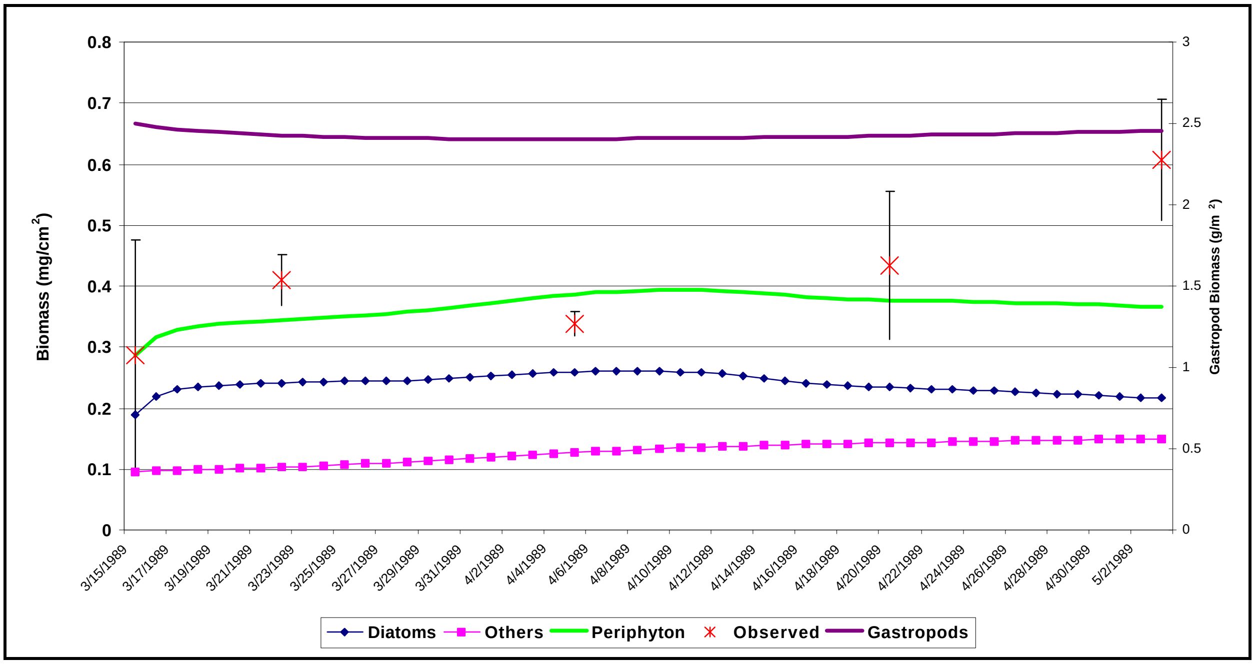

Figure 6. Comparison of predicted biomass of periphyton, constituent algae, observed biomass of periphyton ± 1 standard deviation (Rosemond, 1993, pers. comm.), and gastropods in Walker Branch, Tennessee, with addition of both N and P in Spring, 1989.

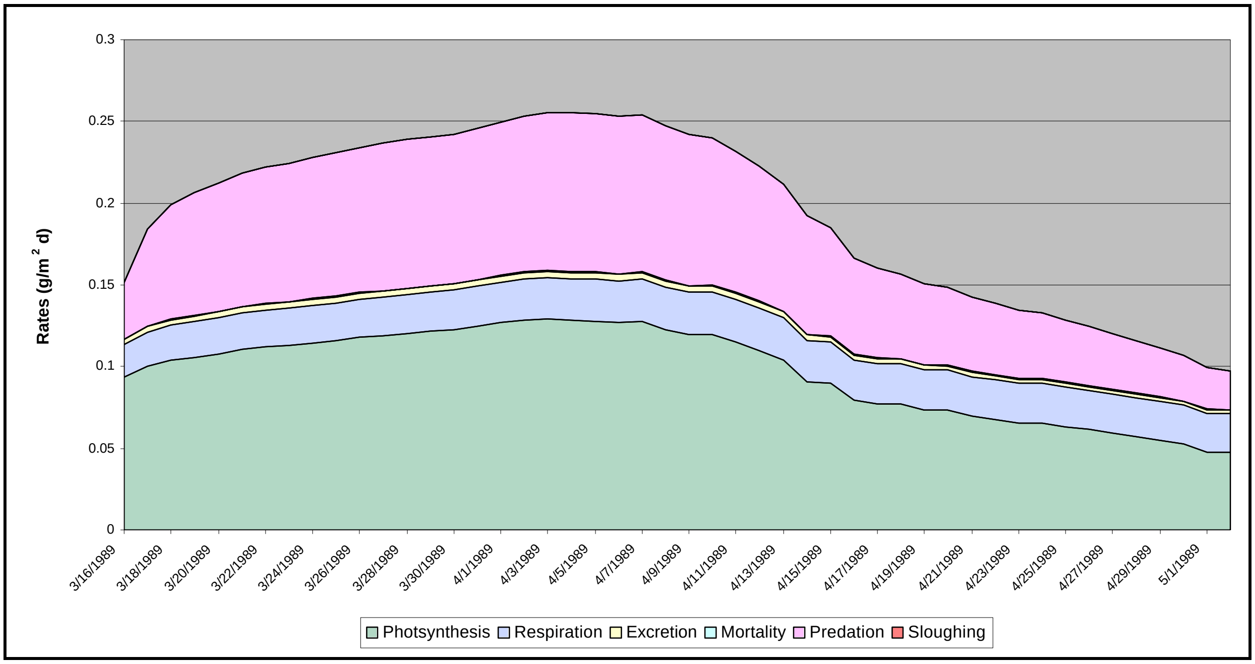

Figure 7. Predicted rates for diatoms in Walker Branch, Tennessee, with addition of both N and P in Spring, 1989. Note the importance of photosynthesis and grazing.

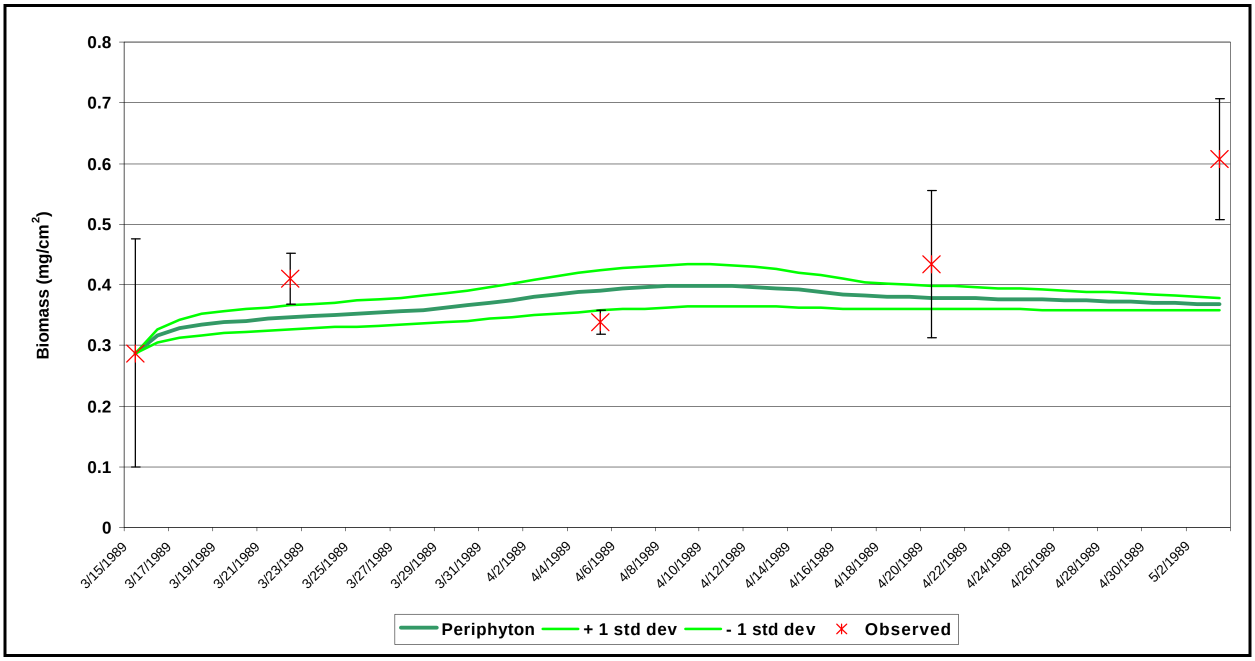

Figure 8. Sensitivity of periphyton predictions to ± 30% change in maximum photosynthetic rate for diatoms with addition of N and P in Spring, 1989. Observed data from Rosemond (1993, pers. comm.).

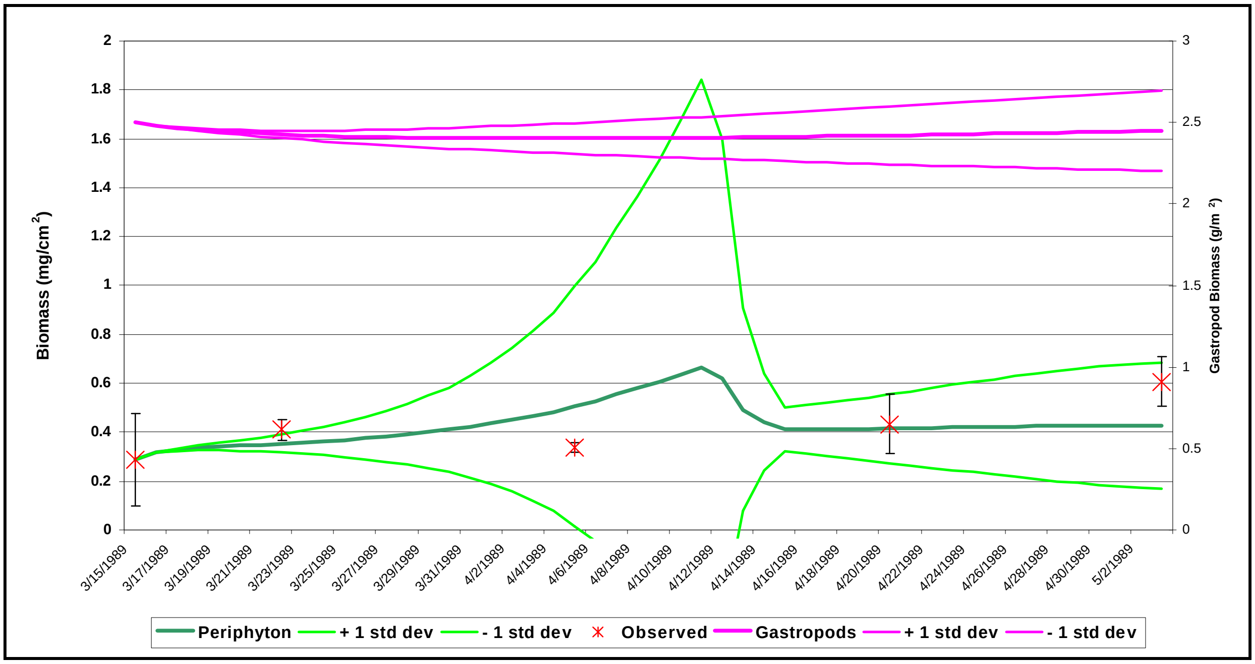

Figure 9. Sensitivity of periphyton and gastropod predictions to ± 30% change in maximum consumption rate for gastropods with addition of N and P in Spring, 1989. Observed data from Rosemond (1993, pers. comm.).

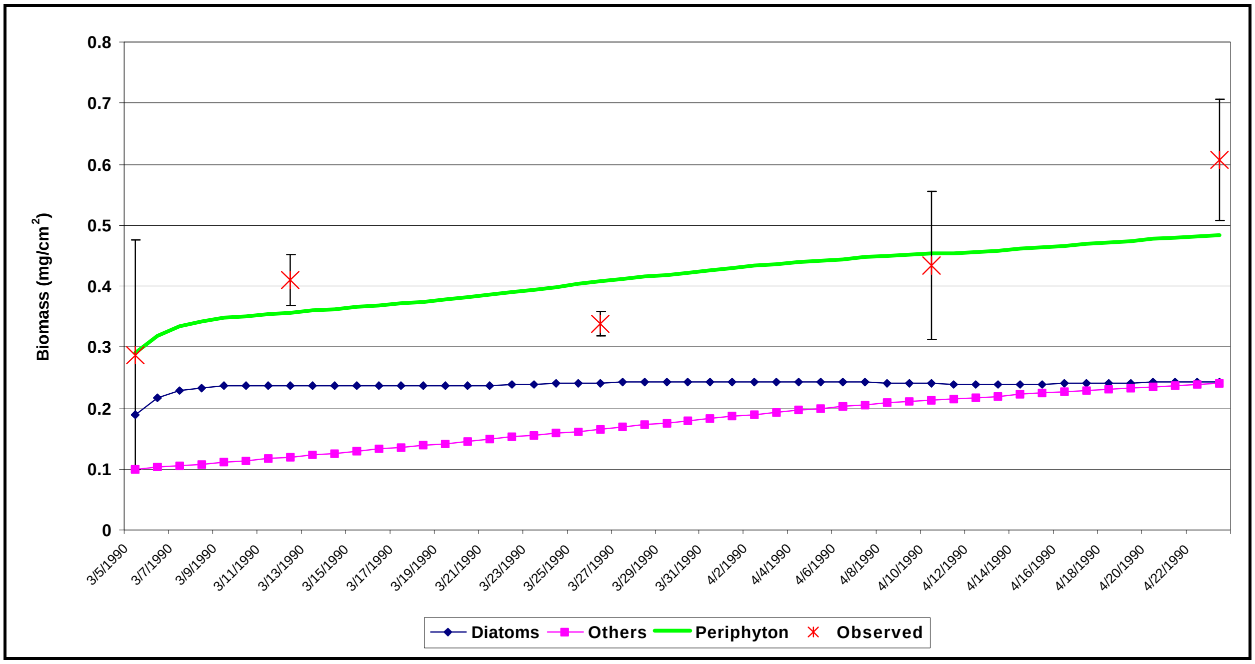

Figure 10. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993, pers. comm.) in Walker Branch, Tennessee, with addition of both N and P in Spring, 1990.

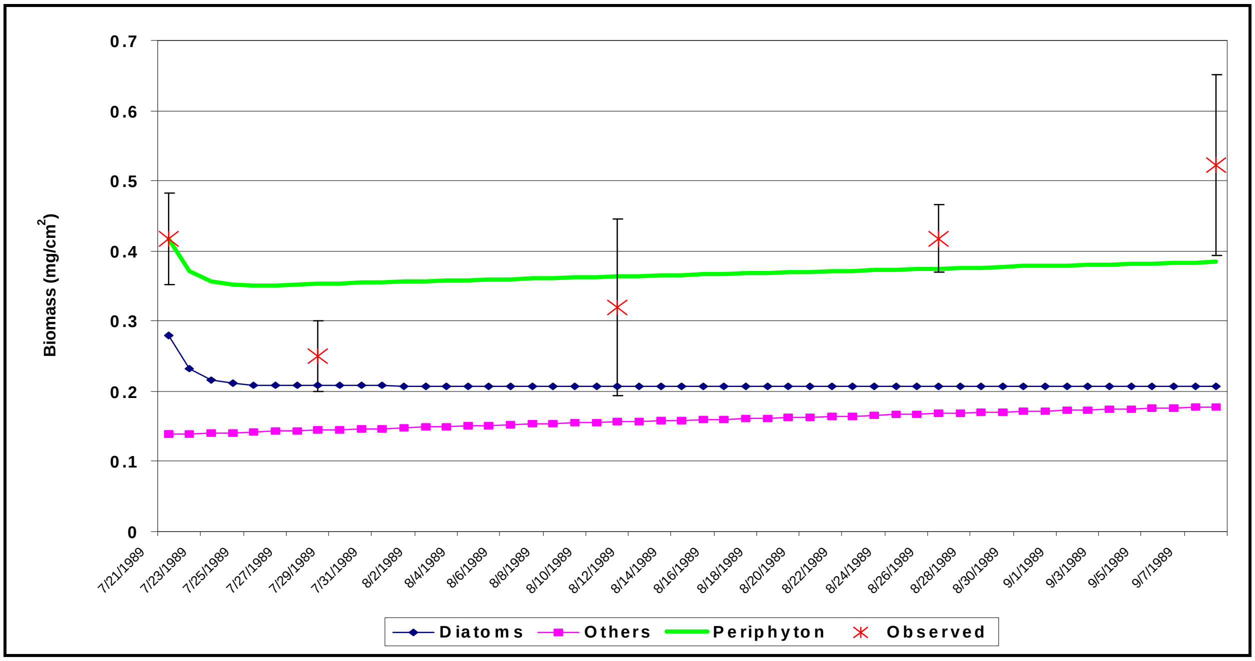

Figure 11. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of both N and P in Summer, 1989.

Without grazers, the Spring, 1989, stream-side, N- and P-enriched experiment exhibited an exponential buildup of biomass, followed by a decline due to sloughing (Rosemond, 1993). Given the sampling interval, it is difficult to be sure that the model simulated the dynamics properly; however, all five data points are matched quite well, and the predicted maximum is within one standard deviation of the nearest observation (**Figure 9**). Examination of the constituent rates for diatoms (?) reveals that sloughing occurs as a threshold biomass is reached or as photosynthesis starts to decline; in the latter case, seen near the end of the experiment, deteriorating environmental conditions caused senescence and sloughing. Comparison of grazed and ungrazed treatments confirms the importance of grazing in depressing periphyton biomass even with nutrient enrichment (?).

The fit to the Spring, 1990, channel enclosure, N- and P-enriched experiment with about 90% grazers removed is equally as good, with a similar prediction of greater biomass buildup and sloughing than can be confirmed with the data (**Figure 12**). Simulation of the comparable channel experiment in Summer, 1989, with severe light limitation, did not exhibit the rapid buildup suggested by the observations in Week 1, but statistically it was a good fit to the observed mean and variance (**Figure 13**). However, the model indicates that the growth is almost entirely diatoms, while Rosemond (1993) showed that much of the buildup is green algae.

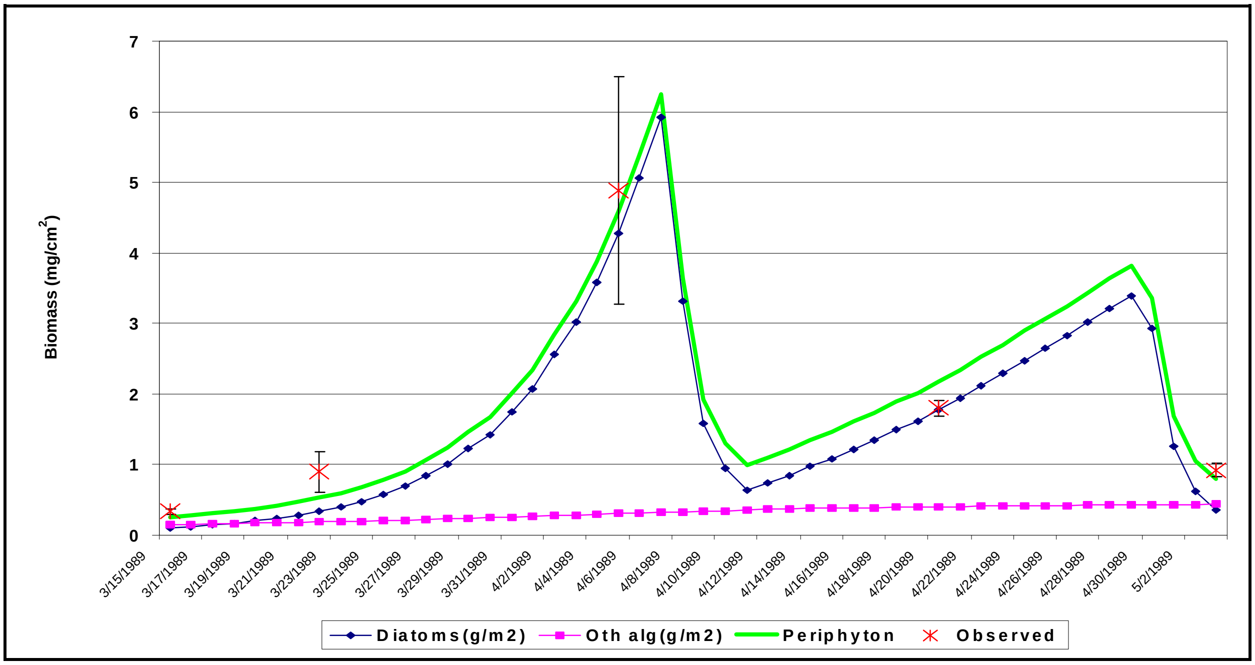

Figure 12. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of both N and P and removal of grazers in Spring, 1989.

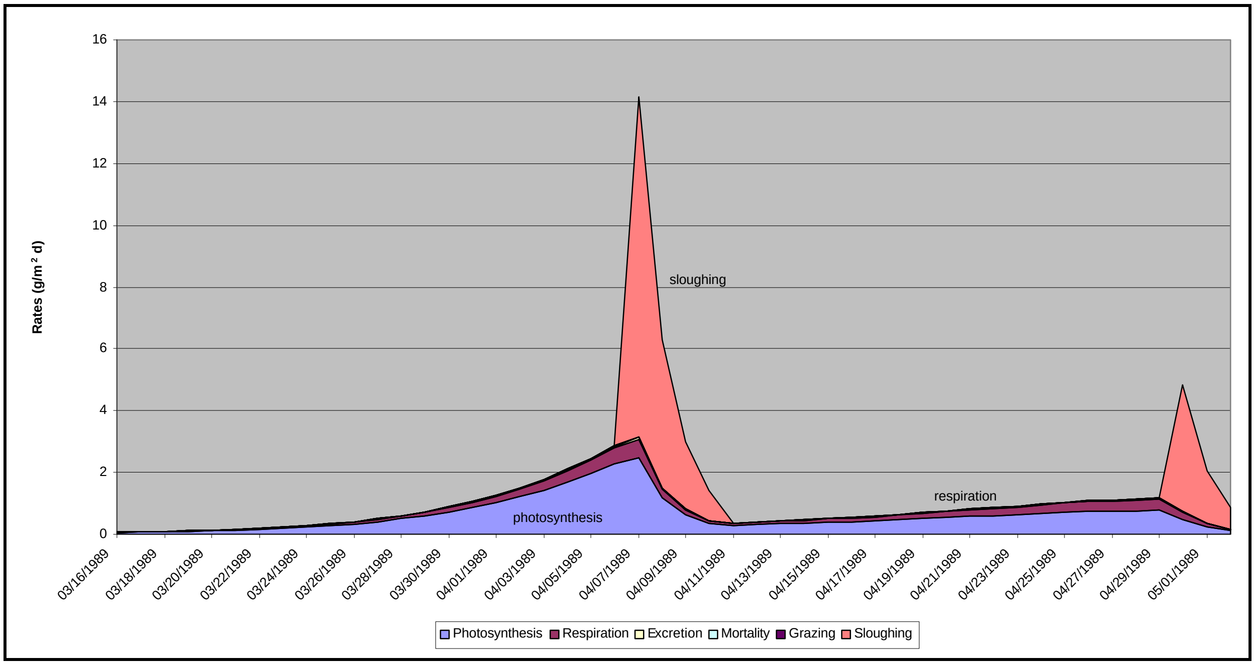

Figure 13: Predicted rates for diatoms in Walker Branch, Tennessee, with addition of both N and P and removal of grazers in Spring, 1989. Note the importance of periodic sloughing.

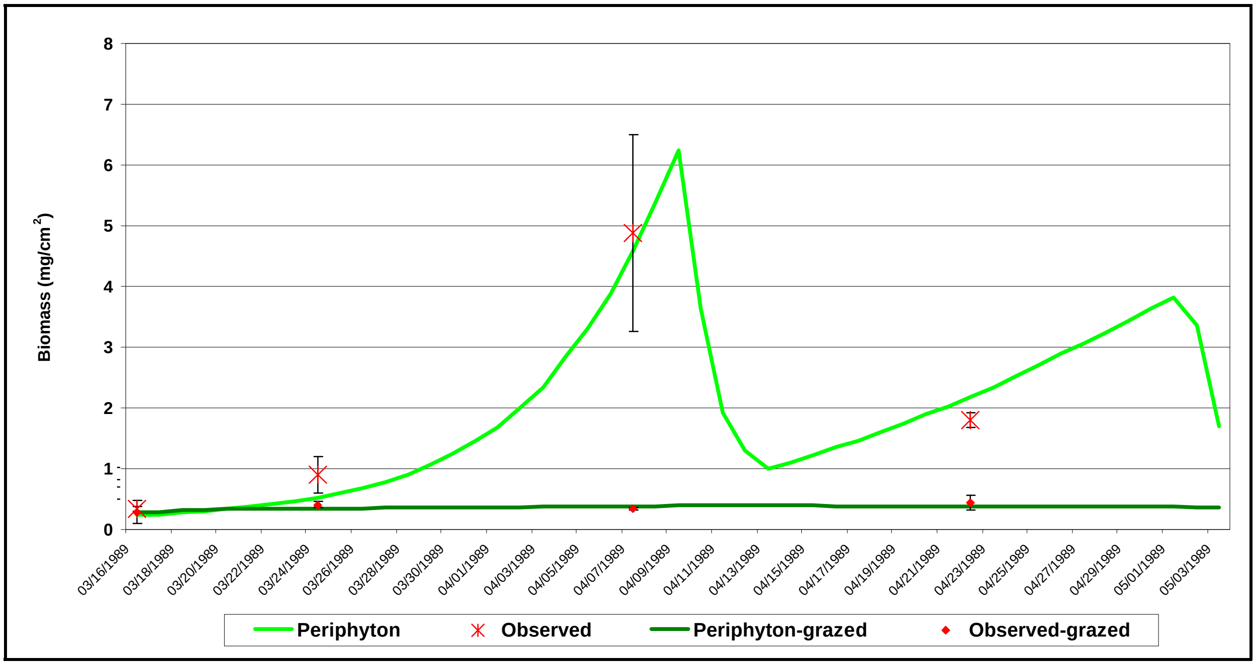

Figure 14. Grazed and ungrazed predicted and observed biomasses of periphyton in Walker Branch, Tennessee, with addition of N and P in Spring, 1989. This figure combines **Figure 3** and **Figure 9** for purposes of comparison.

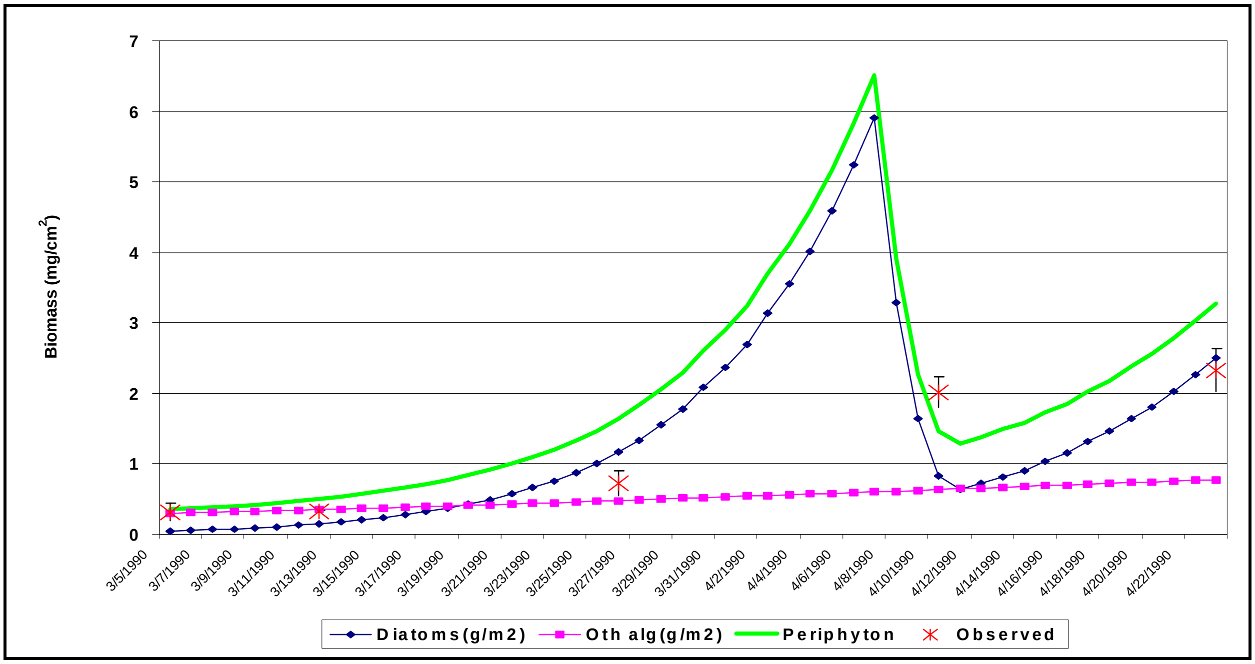

Figure 15. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of both N and P and removal of 90% of grazers in Spring, 1990.

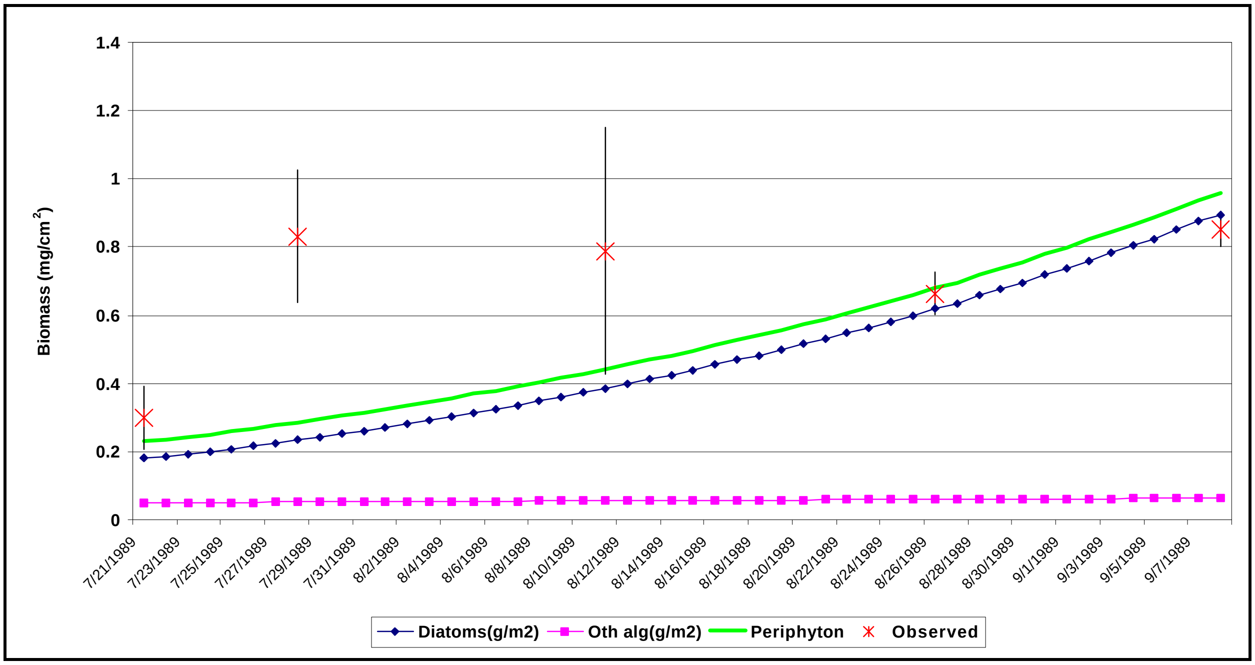

Figure 16. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of both N and P and removal of grazers but with low light in Summer, 1989.

Fits to data from enrichment studies involving the addition of either N or P, but not both, and with removal of grazers are interesting because both the observed data and the simulations suggest that addition of either nutrient led to moderate stimulation (**Figure 14** and **Figure 15**). Simulations of both the N-enrichment treatment and the P-enrichment seem to fit to the observed data well. With grazers included, the simulations bound the higher observed results but do not exhibit the 0.1-0.2 g/m^2 fluctuations that were observed temporally and within samples (**Figure 16** and **Figure 17**). Perhaps grazing is variable from one tile to another—a detail that is not simulated by a spatially aggregated model such as AQUATOX.

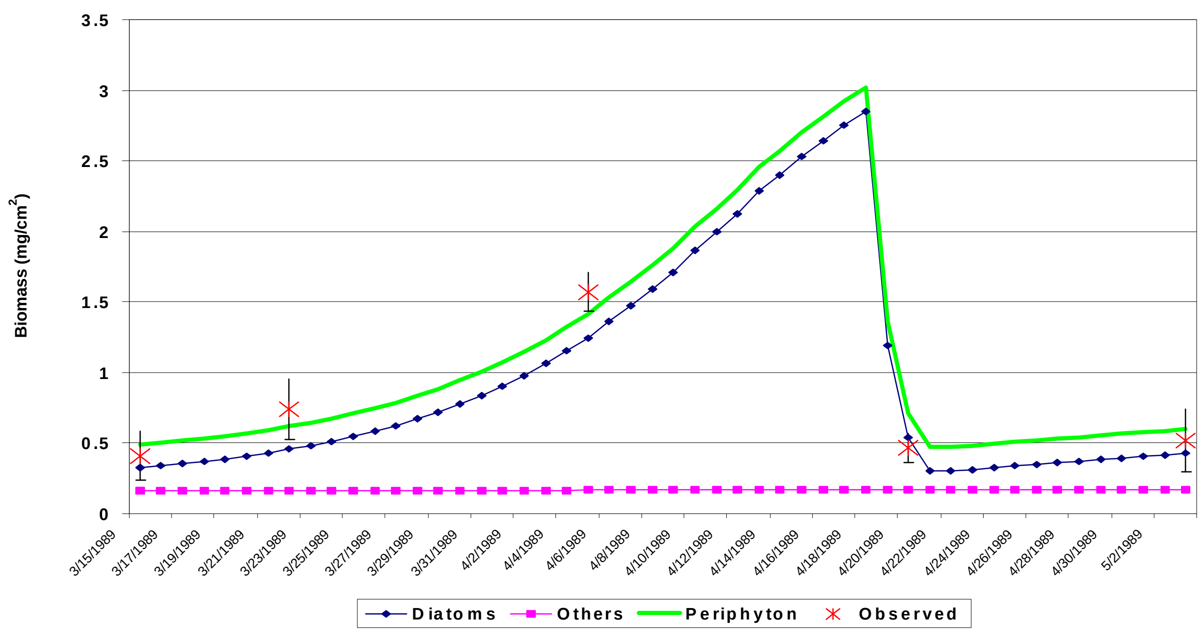

Figure 17. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of N and removal of grazers in Spring, 1989

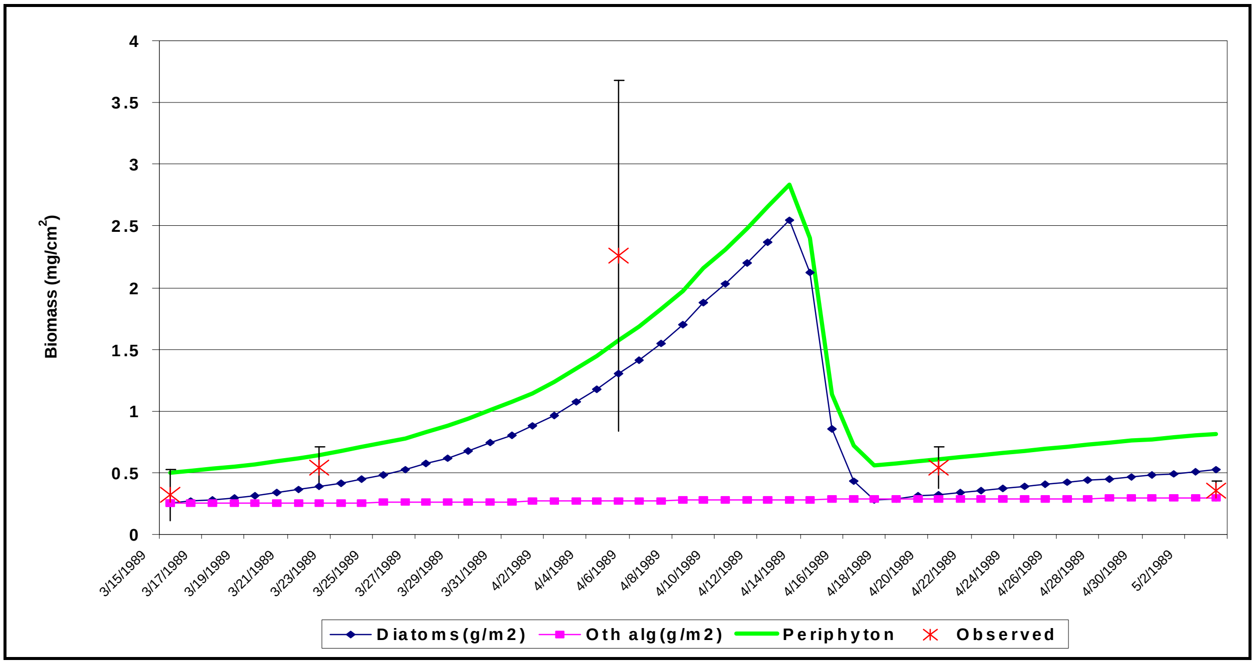

Figure 18. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of P and removal of grazers in Spring, 1989.

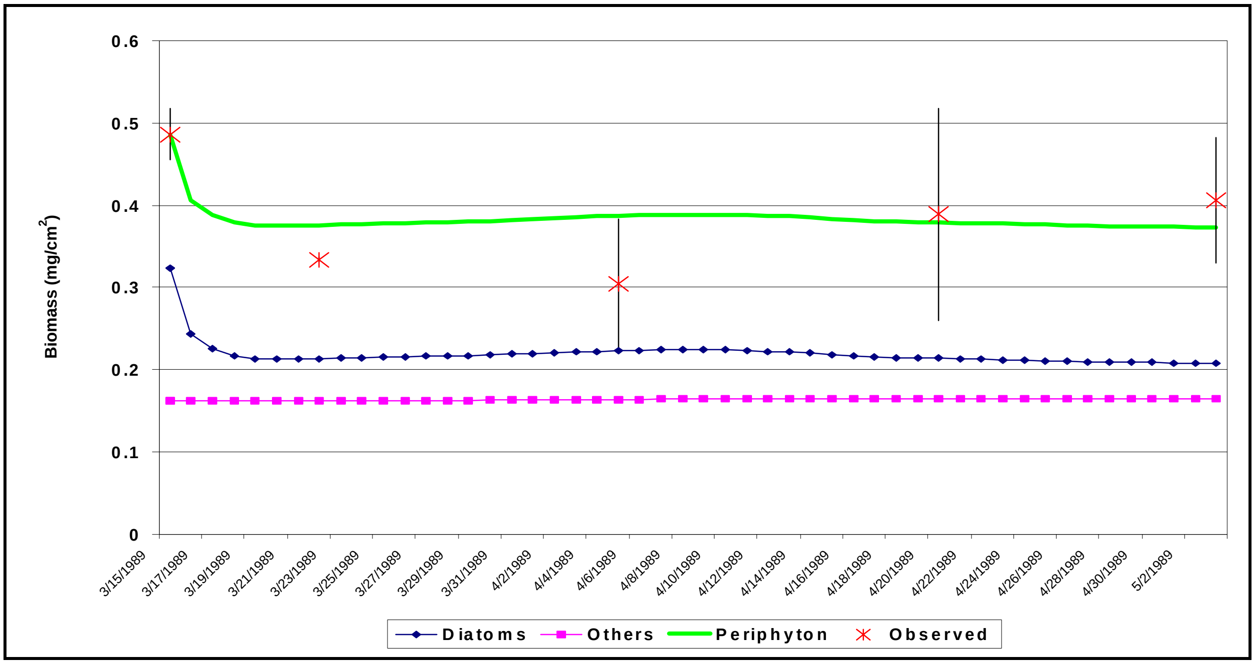

Figure 19. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of N in Spring, 1989

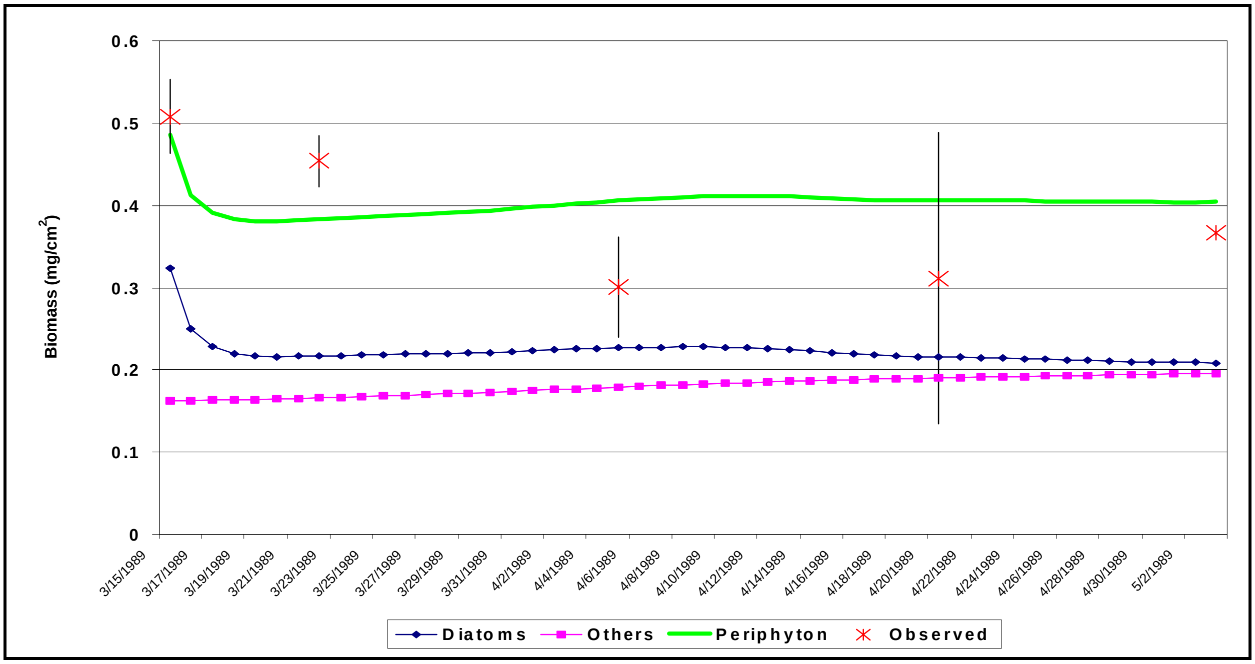

Figure 20. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of P in Spring, 1989.

The simulation of the control channel, with grazers removed, seems to fit the exponential buildup of biomass in the first several weeks in the Spring, 1989 experiment (**Figure 18**). However, the timing of the apparent sloughing is off and the maximum value cannot be confirmed by the data (**Figure 18**). Nevertheless, it is instructive to compare the results from this experiment with those of the companion experiment with addition of N and P; without the addition of nutrients periphyton growth is much slower and senescence and sloughing occurs at a lower biomass (**Figure 19**).

The exponential buildup of periphyton biomass in the Spring, 1990, experiment seems to fit the observed data well (**Figure 20**). Statistically, the simulation of the summer experiment is similar to the observed (**Table 5**); however, the data do not support the predicted simple exponential increase in biomass over the seven weeks (**Figure 21**); possibly light is more limiting for part of the experiment than represented by the model.

Similar to the simulations of the grazed nutrient enrichment experiments, the predicted biomasses in the control channels with grazers provide mean responses that are similar to the observations but do not represent the 0.1 to 0.2 g/m^2 temporal and within-sample fluctuations (**Figure 22 - Figure 24**).

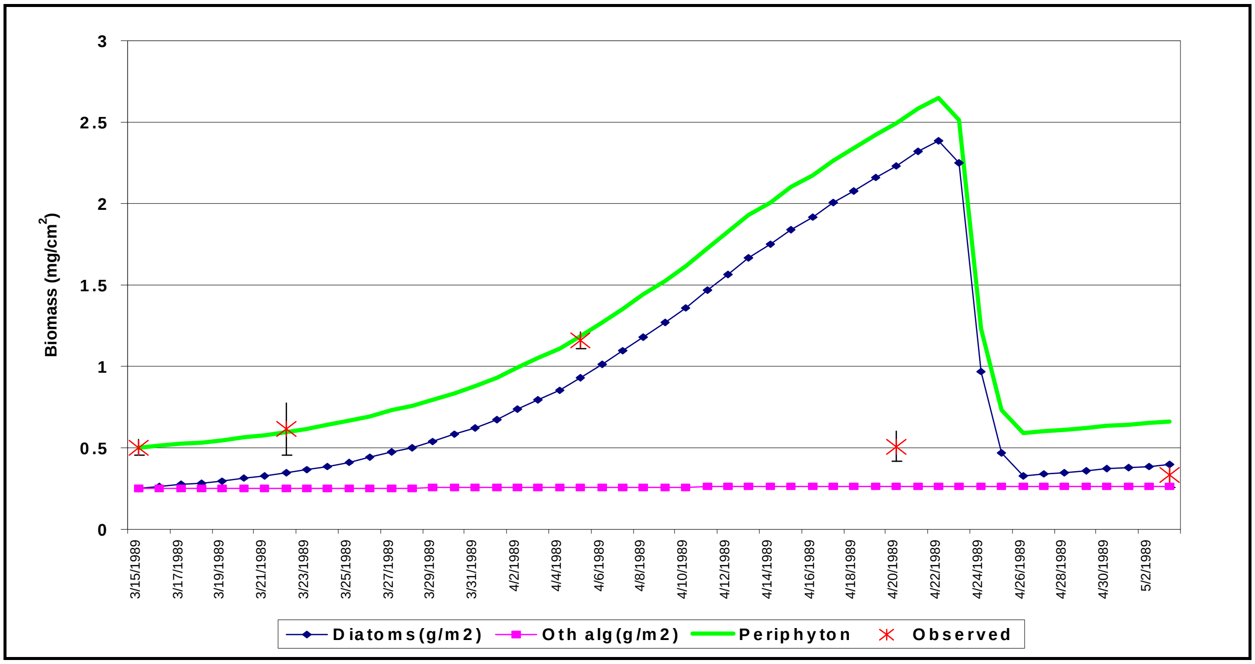

Figure 21. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993, pers. comm.) in control channel in Walker Branch, Tennessee, with removal of grazers in Spring, 1989.

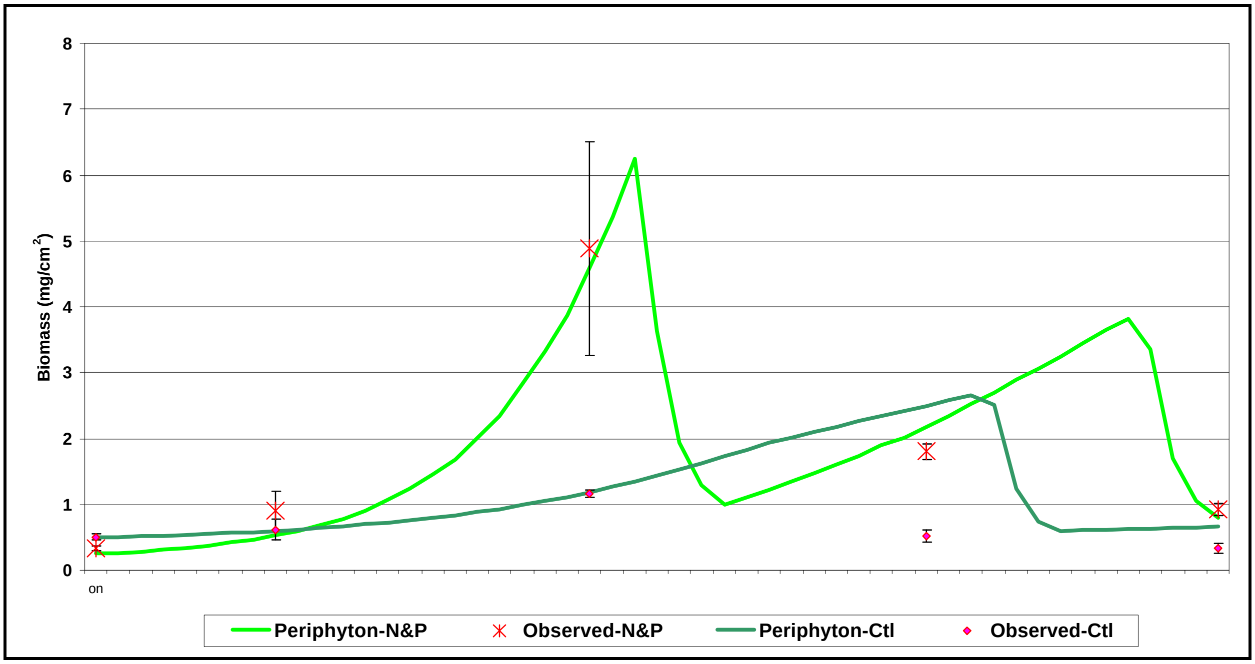

Figure 22. Control and nutrient-enriched predicted and observed periphyton biomass for Walker Branch, Tennessee, without grazers in Spring, 1989. This figure combines **Figure 9** and **Figure 18** for purposes of comparison.

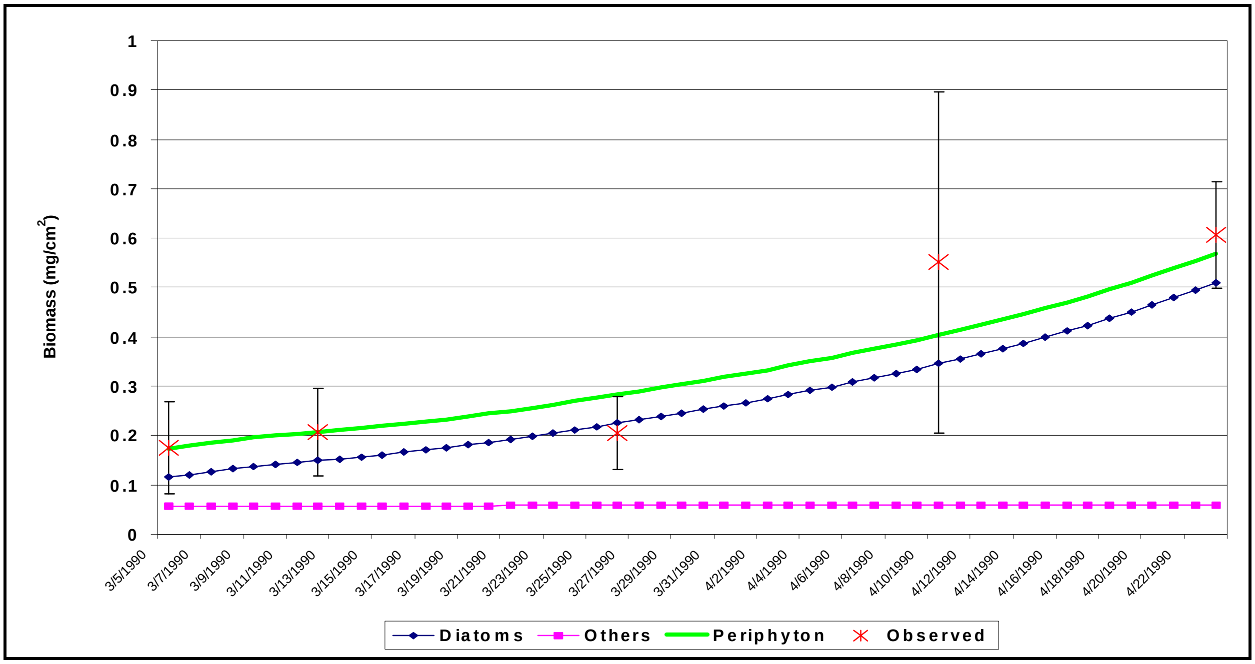

Figure 23. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in control channel in Walker Branch, Tennessee, with removal of 90% of grazers in Spring, 1990.

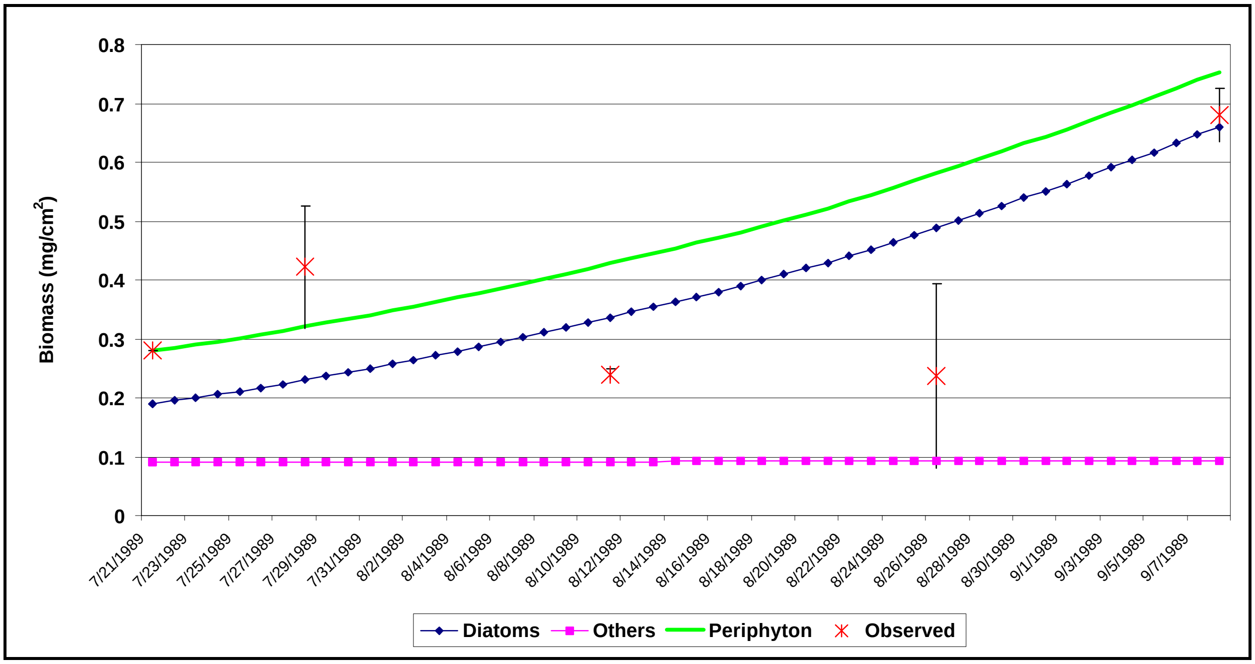

Figure 24. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in control channel in Walker Branch, Tennessee, with removal of grazers in Summer, 1989.

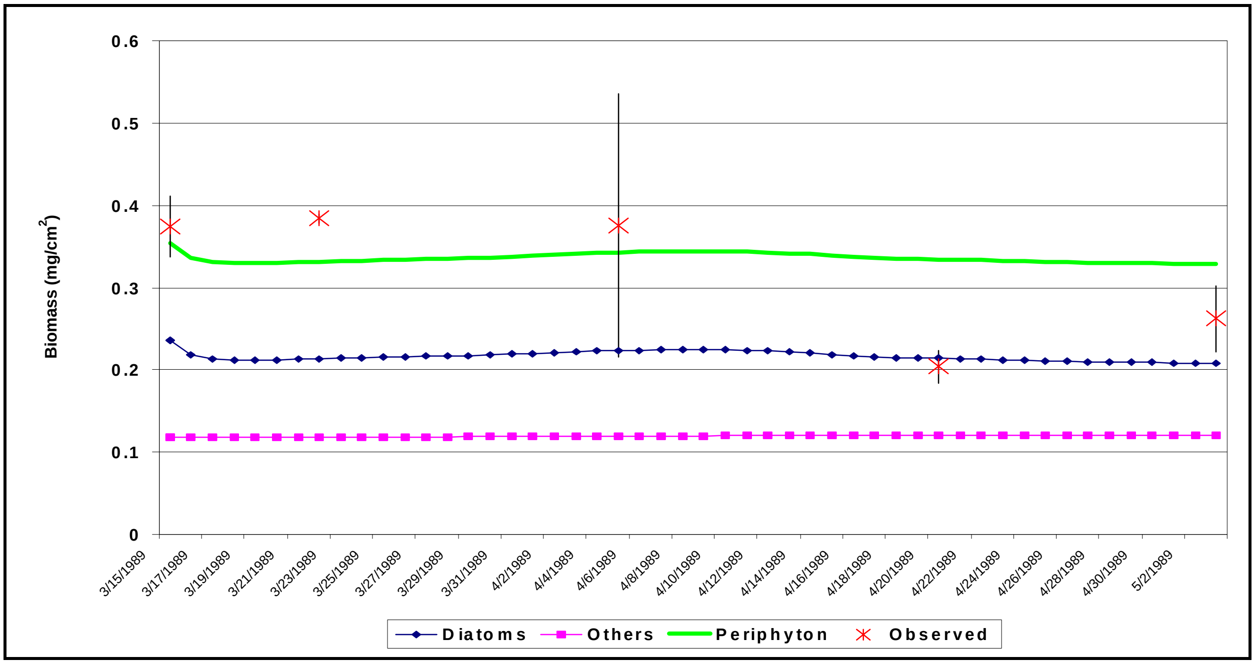

Figure 25. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in control channel in Spring, 1989.

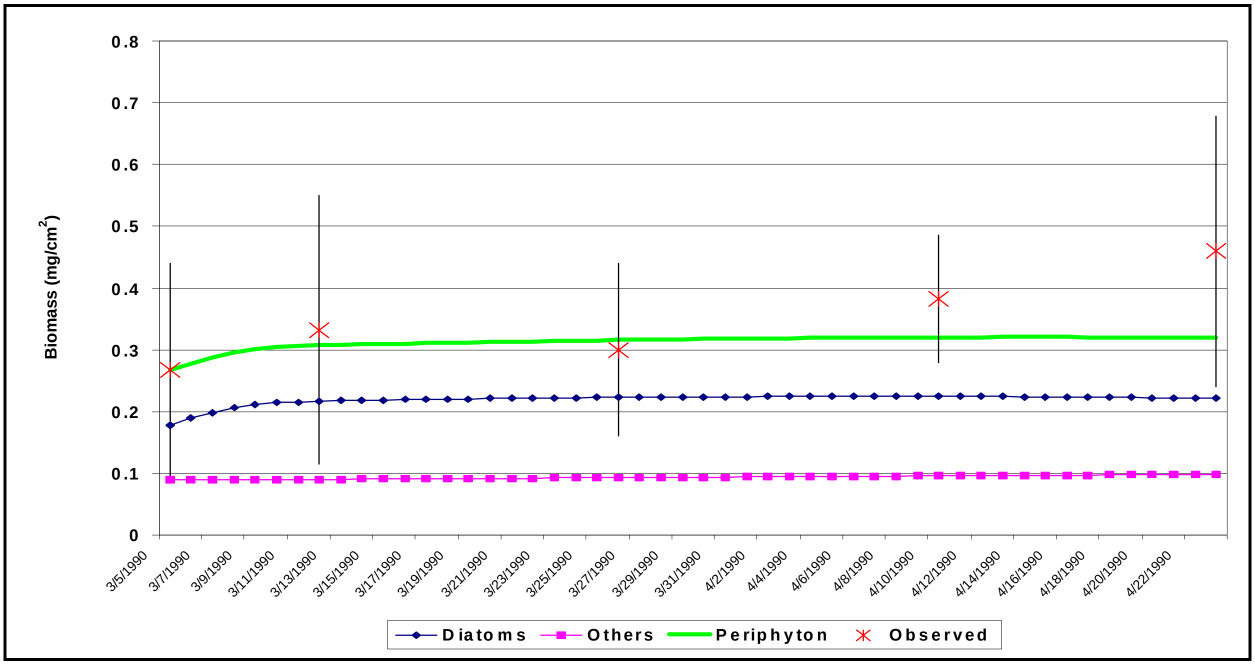

Figure 26. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in control channel in Walker Branch, Tennessee, in Spring, 1990.

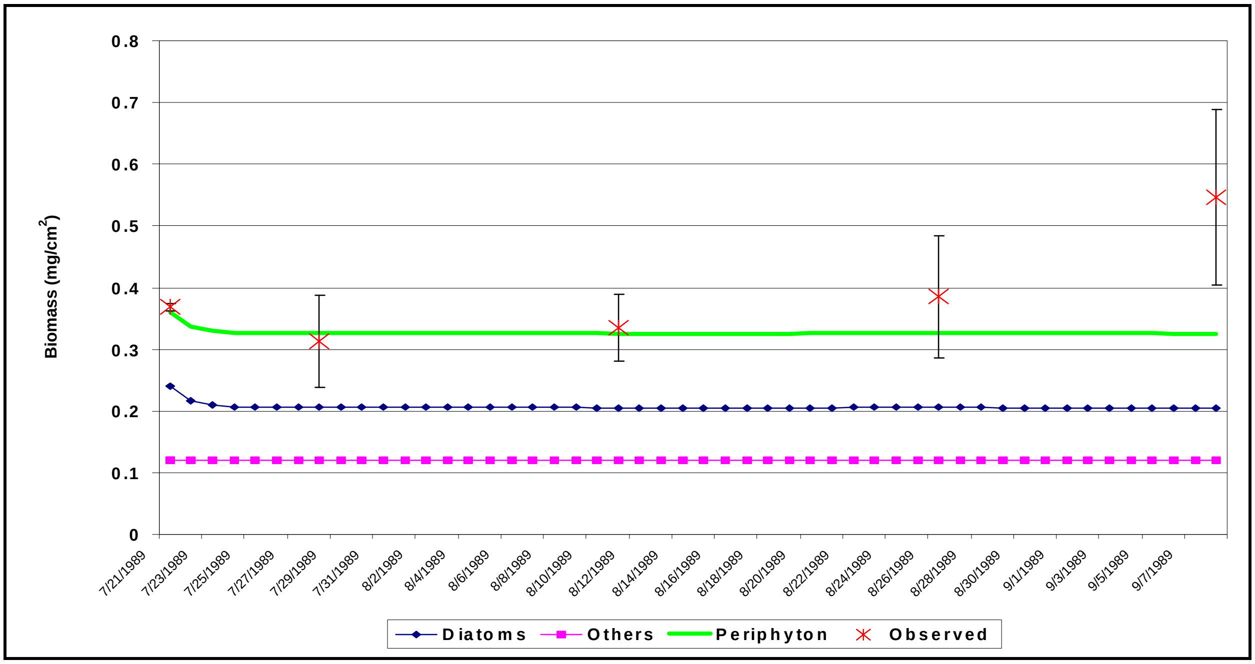

Figure 27. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in control channel in Walker Branch, Tennessee, in Summer, 1989.

Simulations of experiments with high light levels and no grazing in Summer, 1989, are difficult to evaluate because the predicted dynamic responses, with buildup of biomass followed by sloughing, cannot be confirmed by the data. In fact, statistically the predicted and observed distributions for the unenriched experiment are quite different (**Table 5**). The predicted patterns are intriguing in that they predict stimulation of algal growth and sloughing both without (**Figure 25**) and with (**Figure 26**) addition of nutrients and in the absence of grazers. The addition of nutrients decreases the predicted doubling time from 6.7 days to 5.7 days. This indicates that light and not nutrients are limiting in the summer. The nitrate and phosphate concentrations in the stream are twice those of the spring experiments, probably because the nutrients are not being assimilated as quickly by periphyton in the heavily shaded stream in the summer. Unfortunately, carbon fixation rates observed by Rosemond (1993, pers. comm.) at the beginning and end of the experiment do not confirm high productivity in the unenriched experiment. However, based on the increase in observed biomass from the initial value to that eight days later (**Figure 25**), a doubling time of as little as 3 days is possible. As shown in **Figure 27**, the model predicts a substantial algal response to high light, especially when compared to the comparable treatment with natural, low light.

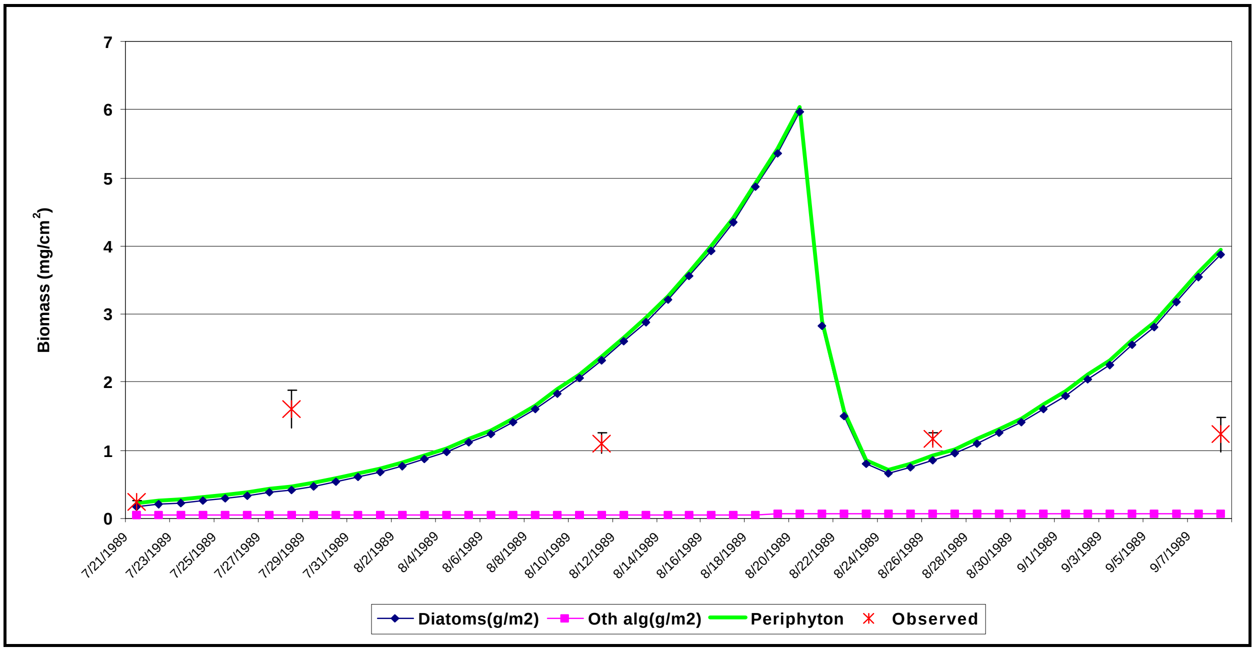

Figure 28. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, channel without addition of nutrients but with high light levels and removal of grazers in Summer, 1989.

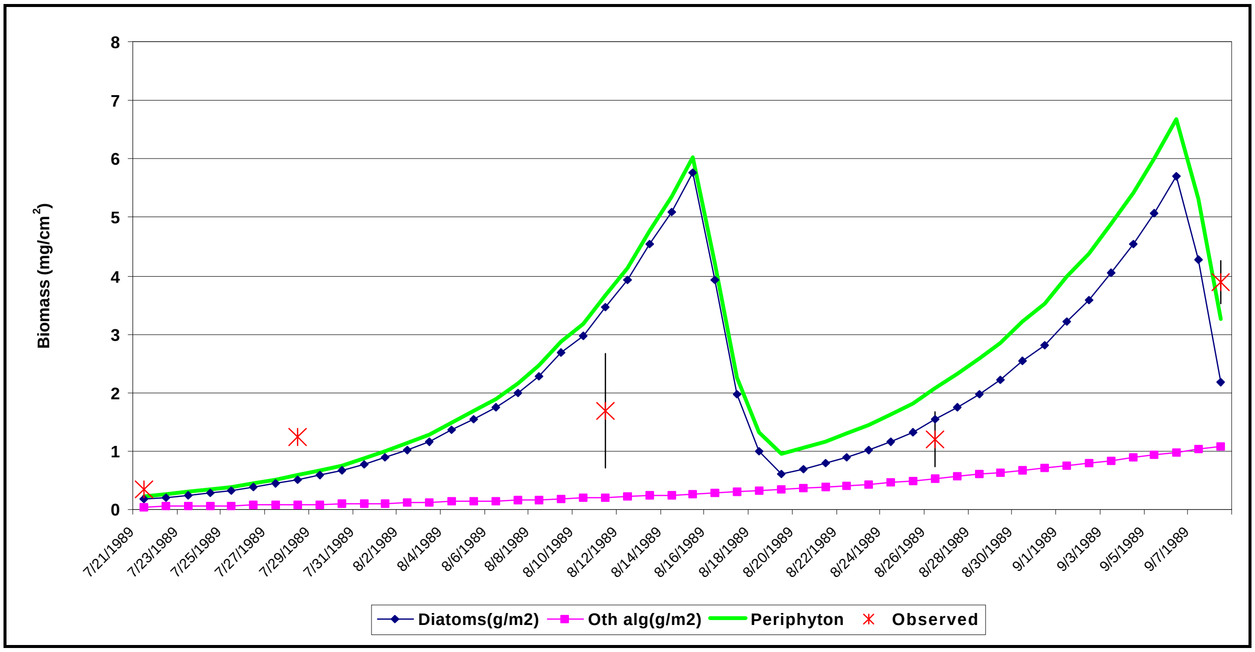

Figure 29. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of N and P, high light levels, and removal of grazers, Summer, 1989.

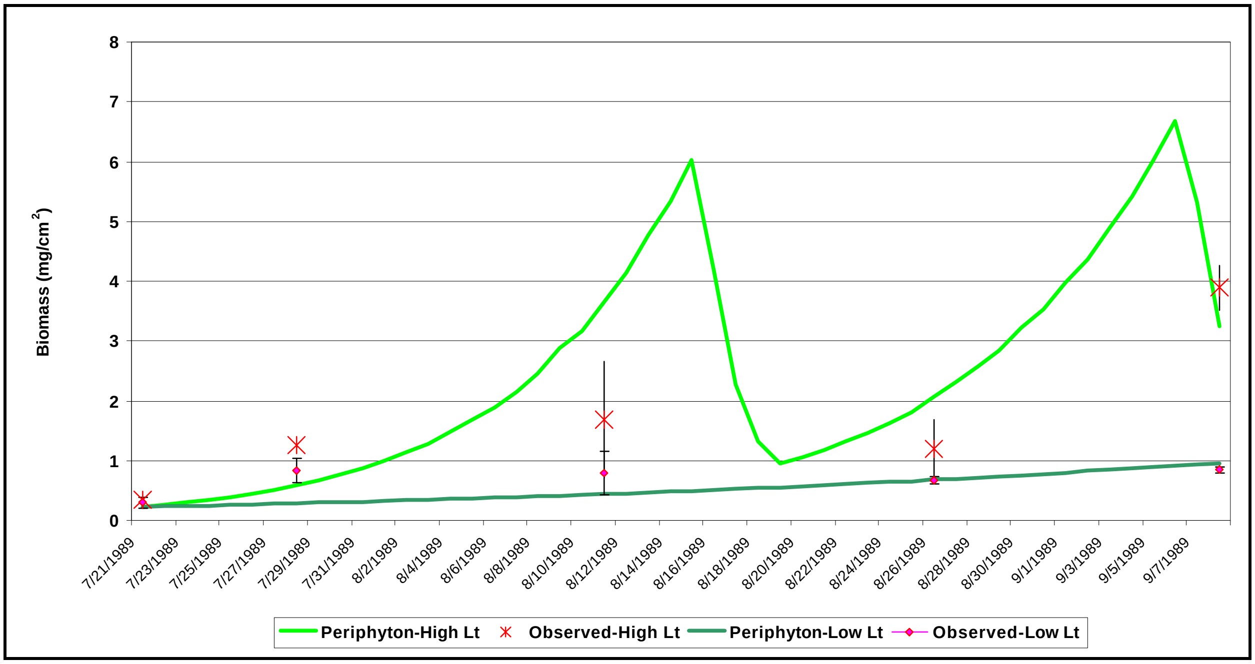

Figure 30. Low-light and high-light predicted and observed biomass of periphyton in Walker Branch, Tennessee, with addition of N and P and removal of grazers in Summer, 1989. This figure combines **Figure 13** and **Figure 26** for purposes of comparison.

With grazers present the results are quite different in the high-light experiments. Without the addition of nutrients the grazers are able to consume most of the algal production (**Figure 28**); the model gives an acceptable fit to all the observed data by passing within one standard deviation of all the points. However, the model predicts a slight increase in biomass of greens, in contrast to Rosemond's (1993) observation that greens decreased due to the competitive advantage of diatoms. With the addition of nutrients the grazers are unable to keep pace with algal production in both the simulation and in the experiment (as Rosemond, 1993, concluded), and the fit of the prediction to the observed data point on the last day is almost exact, although the model overestimates biomass in the intervening weeks (**Figure 29**).

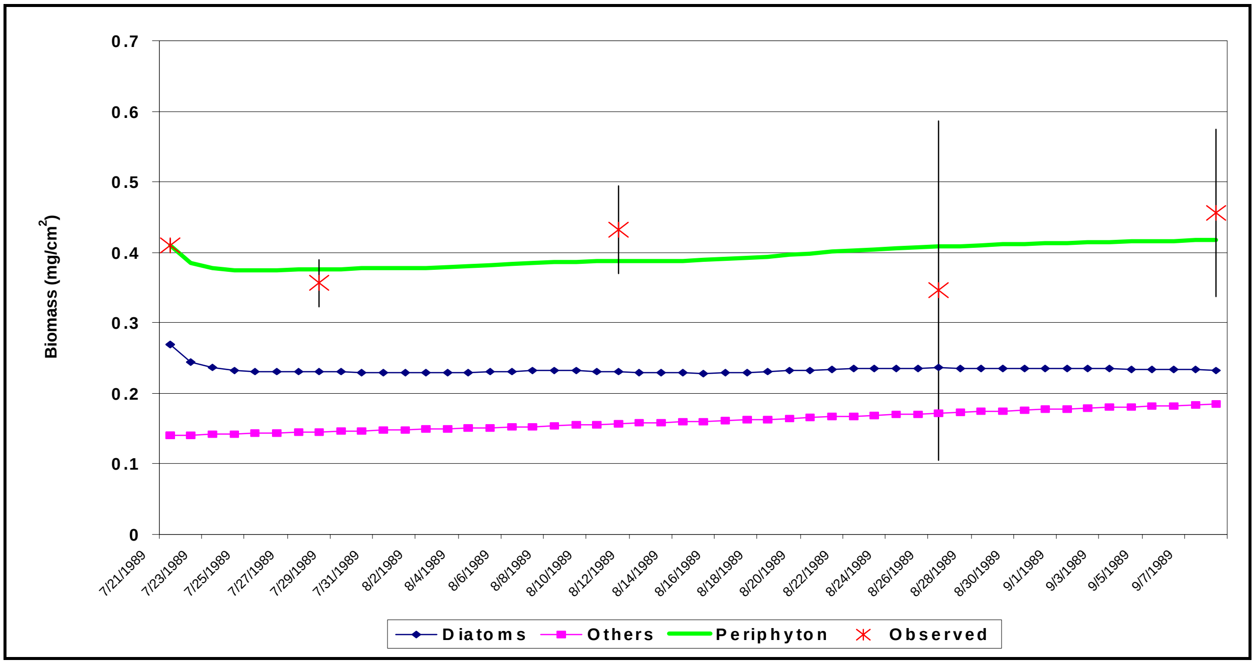

Figure 31. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, channel without addition of nutrients but with high light levels, Summer, 1989.

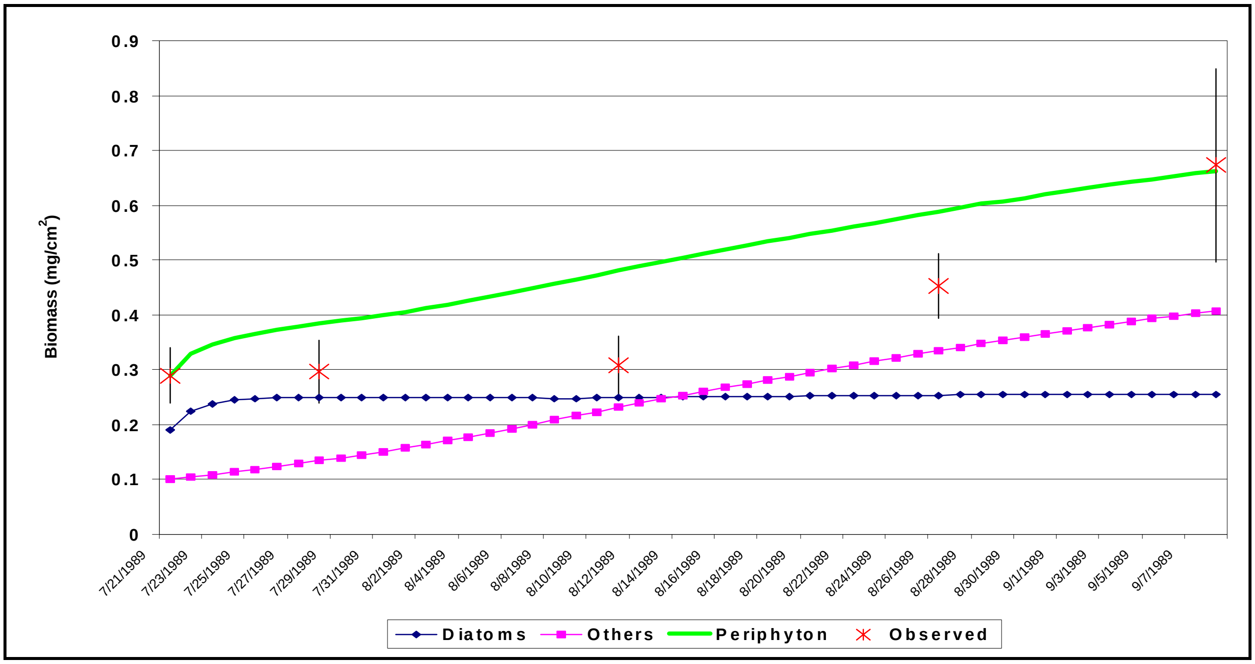

Figure 32. Comparison of predicted biomass of periphyton, constituent algae, and observed biomass of periphyton (Rosemond, 1993) in Walker Branch, Tennessee, with addition of N and P and high light levels, Summer, 1989.

Process-level Verification

Walker Branch is a simple spring-fed woodland stream ecosystem with periphyton, grazers (almost entirely one species of gastropod), detrital loadings from upstream, low nutrient levels, spring-moderated temperatures, and low light levels. Through careful factorial experiments conducted in stream-side channels and stream enclosures, nutrients, light, and grazing were manipulated in Spring and Summer (Rosemond, 1993). Twenty control and perturbed treatments form the basis for calibration of the periphyton submodel in AQUATOX. The ability of one set of parameters to represent all twenty treatments is evidence of the robustness of the model for representing woodland streams. The fact that the model demonstrates bottom-up and top-down controls on the periphyton with multiple limiting factors suggests that there is a sound scientific basis for the formulations.

Rosemond (1993) came to the conclusion that

> "the biomass, productivity, and taxonomy of the periphyton community in this study were strongly limited by nutrients and light and controlled by herbivory. The addition of nutrients and light and the removal of snails resulted in a shift in the algal community from one composed of chlorophytes and cyanophytes, and characterized by low biomass... to a community of filamentous diatoms, with high biomass.... Removal of herbivores, alone, resulted in taxonomic shifts towards diatoms, but with little increase in biomass or productivity. When nutrients were added alone, biomass and productivity were not strongly affected. However, it was the interaction between all three factors that produced the greatest effects on biomass and productivity, indicating simultaneous limitation by light, nutrients, and herbivory."

The simulations presented in the previous section provide a rigorous, mathematically coherent confirmation of most of Rosemond's (1993) conclusions.

Grazing by large, long-lived populations of gastropods was shown to suppress periphyton biomass under all circumstances except the combination of high nutrients and high light. Both N and P, singly and especially in combination, were shown to stimulate periphyton growth, resulting in either buildup of periphyton biomass (to higher levels than observed by Rosemond, 1993) or trophic transfer to gastropods. Periphyton growth can occur under the low light conditions provided by the dense forest canopy; however, elevated light levels, approaching those of an unshaded stream, were shown to stimulate growth, especially if coupled with enriched nutrient conditions.

As periphyton biomass, including associated detritus, accumulates with low or no grazing it is vulnerable to sloughing. AQUATOX is formulated to represent sloughing as a function of biomass and deteriorating environmental conditions including decreasing nutrients and decreasing light, the latter as a function of both incident solar radiation and self-shading. Generally the predicted buildup of biomass and sloughing were shown to be consistent with the observed data and the experience of the field investigator (Rosemond, pers. comm.). Sloughing is also a function of water velocity, which could not be investigated using the experimental data with near-constant velocities. However, in the validation exercise described in the next section, daily varying discharge was a factor in a simulation of periphyton sloughing from natural cobbles in the stream.

Validation

A validation for a woodland stream was performed using a two-year bimonthly data set from Walker Branch, Tennessee (Rosemond, 1993). Periphyton biomass and gastropod densities were measured on cobbles in the stream channel. Because it involved continuous, ambient stream conditions (**Table 6**), in contrast to the seven-week stream-side and channel enclosure studies used for calibration, a successful simulation can be considered a validation of the periphyton submodel for this system.

Table 6. Loadings and Initial Conditions Used in 2-year Simulations of Walker Br.

October 1, 1988 to November 1, 1990			
	Treatment	Constant Flow	Daily Flow
Initial gastropod biomass (g/m^2)*		8	8
Nutrients (mg/L)	NH_4-N	0.0001 to 0.0065	0.0001 to 0.0065
	NO_3-N	0.0009 to 0.0435	0.0009 to 0.0435
	PO_4-P	0.0008 to 0.0053	0.0008 to 0.0053
Light (Ly/d)$^+$		8.4 to 115	8.4 to 115
Velocity (cm/s)		13.0	7.0 to 23.0
Initial algal biomass (g/m^2)*	Diatoms	0.022	0.022
	Greens	0.023	0.023

$^+$ Light was reported by Rosemond (1993) as photosynthetic active radiation, which was multiplied by 2 to provide total radiation values used by AQUATOX *Ash-free dry weight

First, the model was run for the two-year period using a constant flow rate and a velocity of 13 cm/s. This corresponded closely to the conditions under which the model was calibrated except that the velocity was greater than in the experiments. The predictions fell below all the observed points, but passed within one standard deviation of all but one point (?). Mean predicted biomass was 0.280 g/m^2 compared to observed biomass of 0.413 g/m^2, with rB = -0.148 and F = 0.589, indicating that the means and variances are similar at the 95% confidence level. The gastropod biomass increased to 15 g/m^2, which probably is above the maximum biomass in the stream.

Then the model was run using observed daily flow rates. The results are somewhat different in this simulation that more accurately represents the dynamics of the natural stream system (?). The predictions pass within one standard deviation of all thirteen points, passing very close to some of the observations. The mean predicted periphyton biomass was 0.328 g/m^2, compared to the observed biomass of 0.413 g/m^2, with an rB of -0.942; and the F value is 1.13, confirming that the predicted and observed distributions are similar at the 95% confidence level.

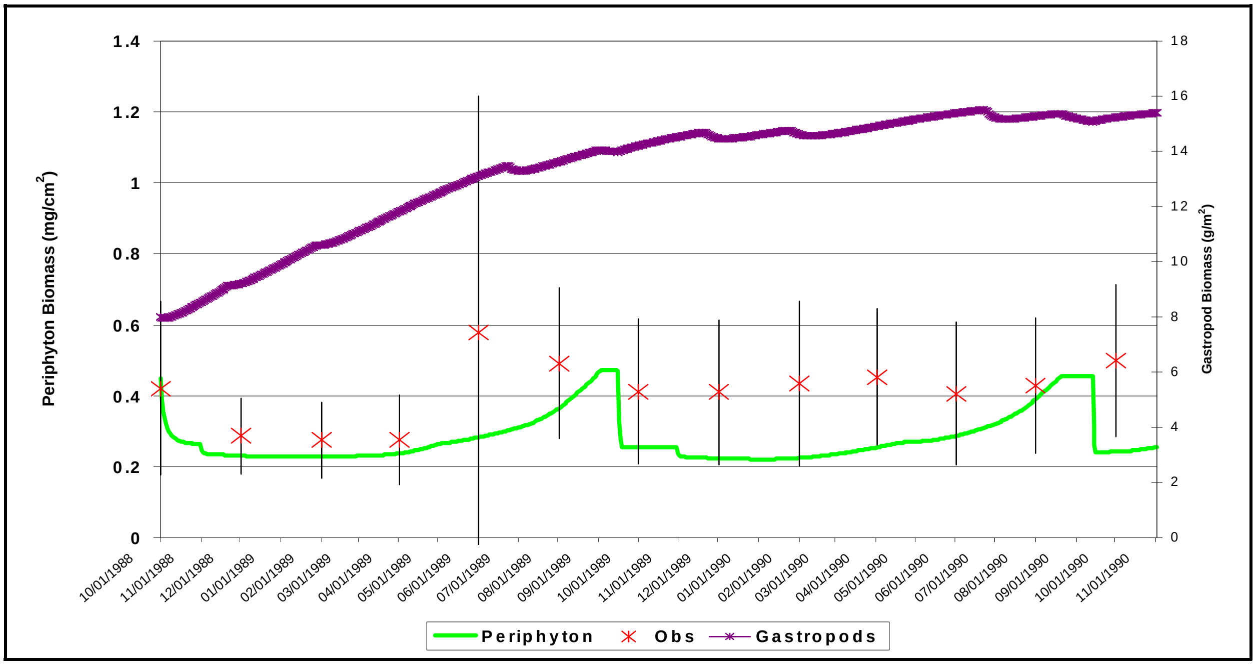

Figure 33 Comparison of predicted and observed (Rosemond, 1993) biomass of periphyton and predicted biomass of gastropods on cobbles in Walker Branch, Tennessee, with constant flow in 1989 and 1990.

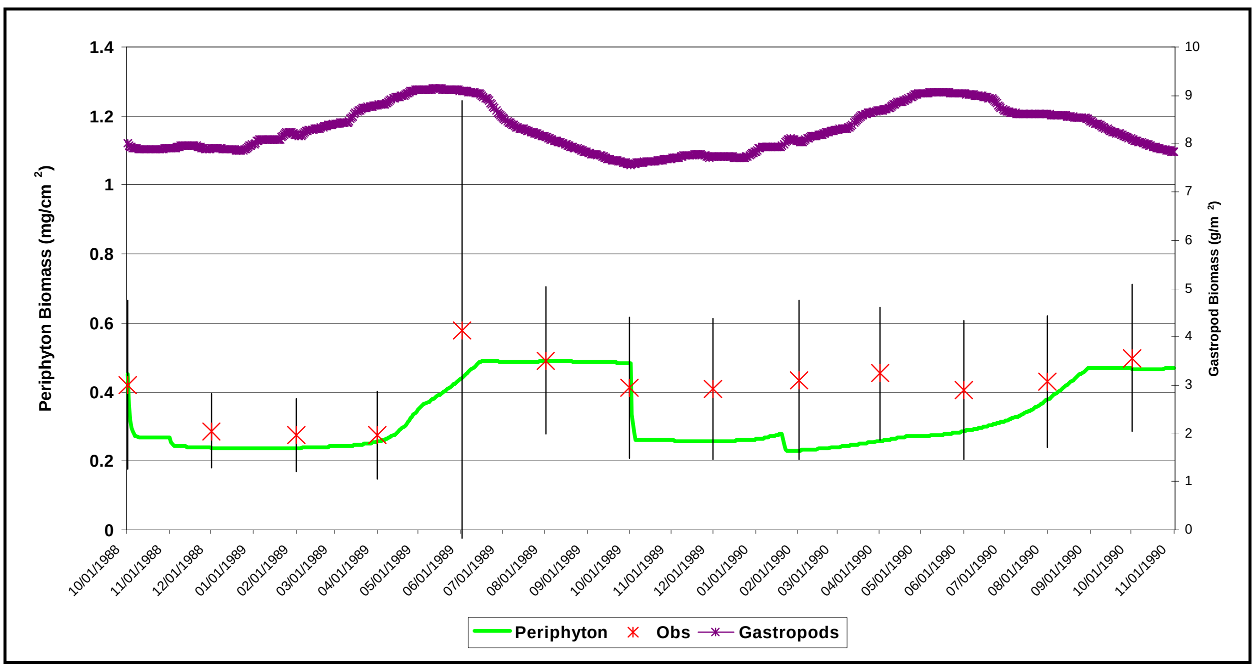

Figure 34. Comparison of predicted and observed (Rosemond, 1993) biomass of periphyton and predicted biomass of gastropods in Walker Branch, Tennessee, with daily varying flow rates in 1989 and 1990.

After a decrease in the biomass of greens at the beginning of the simulation, perhaps due to an inappropriate initial condition, the fluctuations in periphyton are due to diatoms (**Figure 32**). Long periods with only base flow allow predicted diatom biomass to accumulate until finally a small runoff event initiates massive sloughing. Gastropods exhibit a stable fluctuation in predicted biomass between 8 and 9 g/m^2, and grazing pressure on diatoms is intense when diatoms reach a biomass of 0.20 mg/cm^2, the minimum biomass for feeding by gastropods (**Figure 33**). Loss due to photorespiration also increases with biomass buildup due to self-shading.

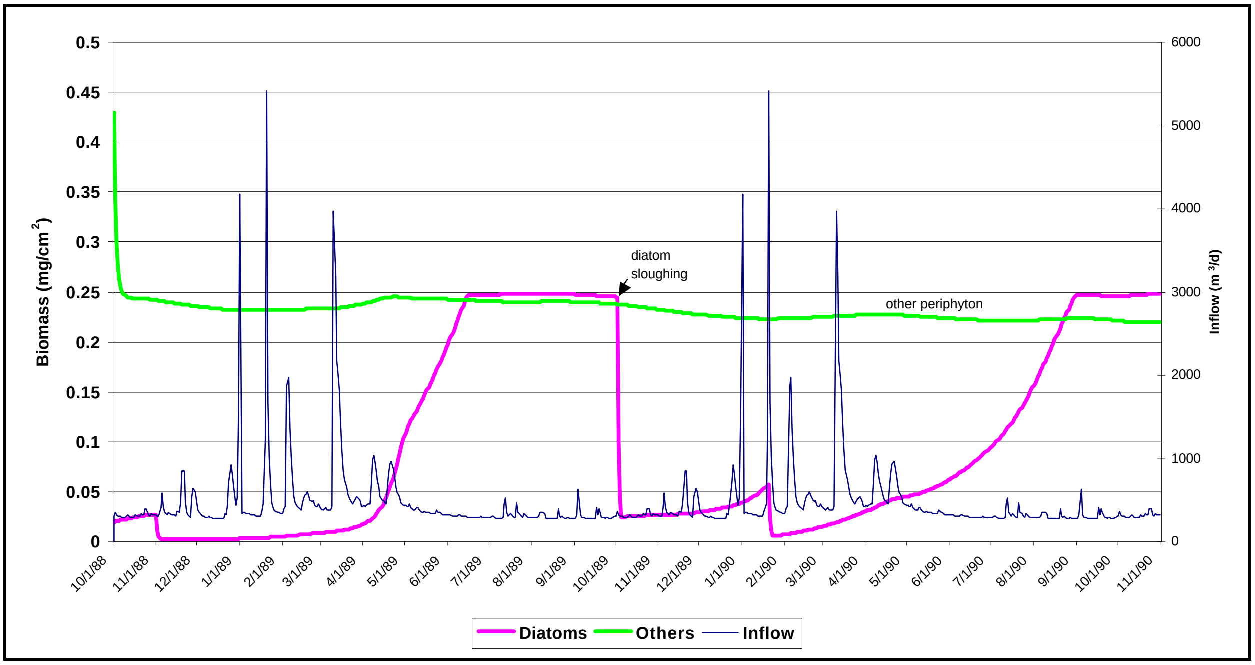

Figure 35. Predicted biomass of periphytic diatoms and other algae on cobbles in Walker Branch, Tennessee, with daily varying inflow in 1989 and 1990.

Conclusions

The periphyton submodel, with the newly formulated sloughing function, provides enhanced capability for simulating periphyton growth as a result of eutrophication or nutrient enrichment. The weight of evidence based on predicted and observed maximum and mean periphyton biomass, biomass variance, visual inspection, and process rate plots, strongly suggests that the model provides a good fit to the periphyton data in twenty treatments. The model also satisfactorily simulated gastropod biomass. Using a single parameter set, the model performed well in simulating nutrient-poor and nutrient-enriched, low- and high-light conditions, and grazing and lack of grazing in a woodland stream. An independent, two-year data set from Walker Branch was used to validate the model for continuous ambient woodland stream conditions, including low light, low nutrients, variable temperature, intense grazing, and daily varying stream flow. Visual inspection, statistics, and consideration of process plots all confirm that the model provides a realistic representation of the woodland stream ecosystem.

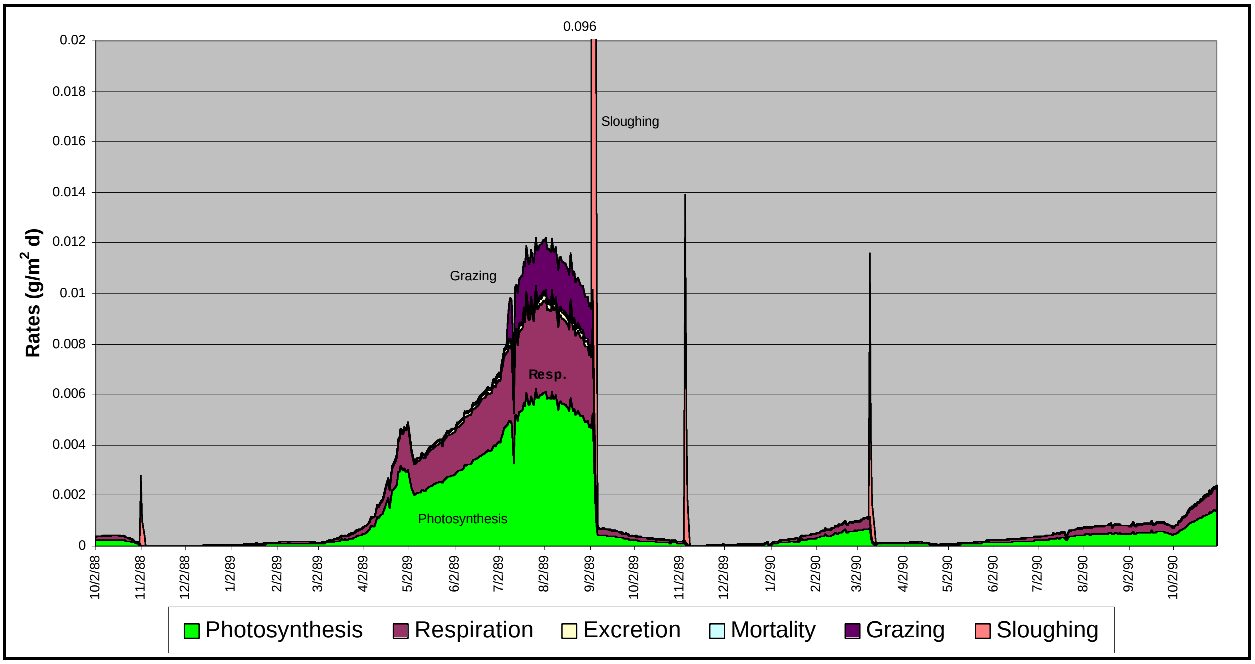

Figure 36. Predicted process rates affecting diatoms on cobbles in Walker Branch, Tennessee, with daily inflow in 1989 and 1990.

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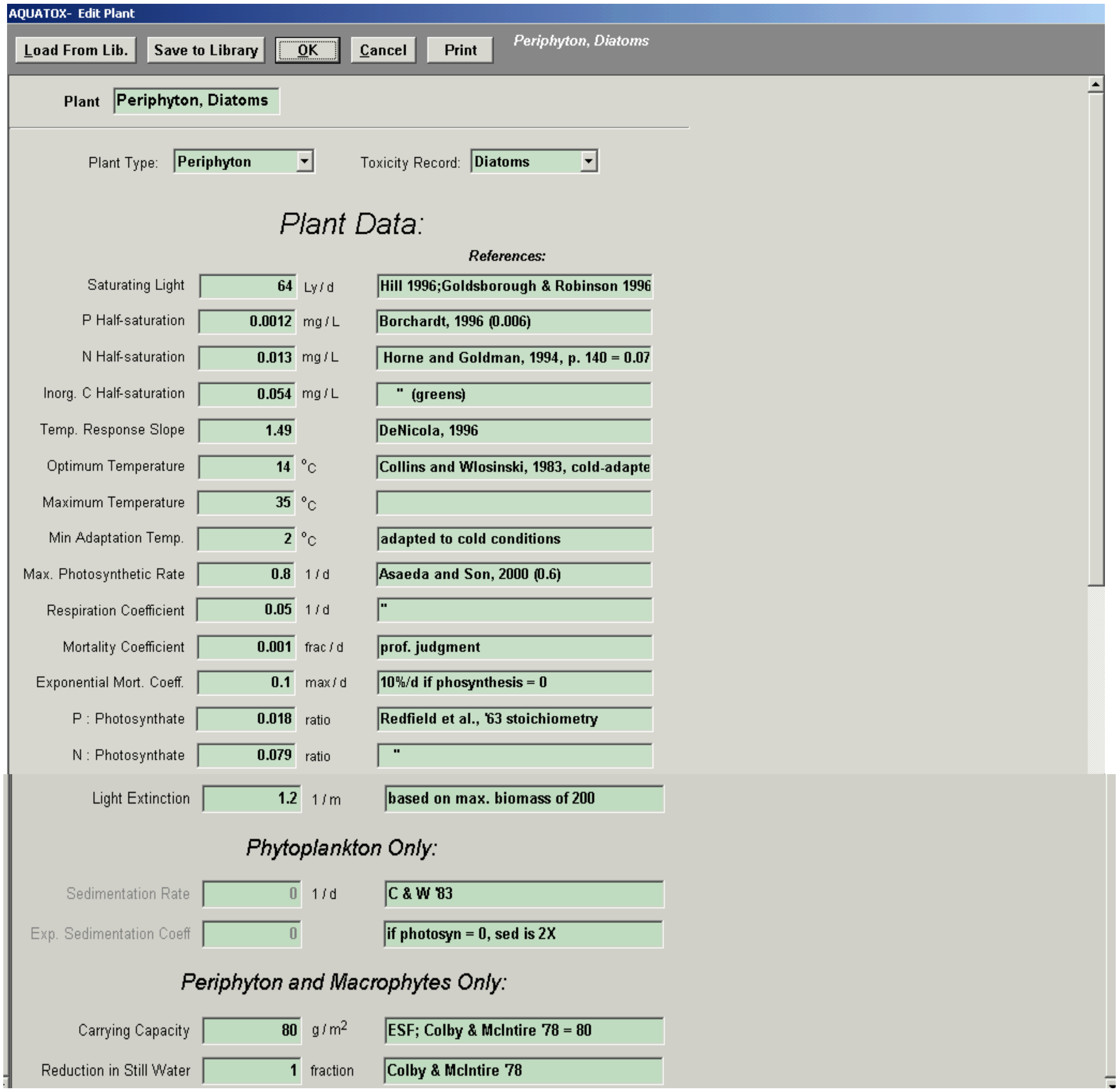
Appendix—Biotic Parameters

Periphyton, Diatoms



AQUATOX- Edit Plant

Load From Lib. | Save to Library | OK | Cancel | Print — *Periphyton, Diatoms*

Plant: Periphyton, Diatoms

Plant Type: Periphyton — Toxicity Record: Diatoms

Plant Data:

			References:
Saturating Light	64	Ly / d	Hill 1996;Goldsborough & Robinson 1996
P Half-saturation	0.0012	mg / L	Borchardt, 1996 (0.006)
N Half-saturation	0.013	mg / L	Horne and Goldman, 1994, p. 140 = 0.07
Inorg. C Half-saturation	0.054	mg / L	" (greens)
Temp. Response Slope	1.49		DeNicola, 1996
Optimum Temperature	14	°C	Collins and Wlosinski, 1983, cold-adapte
Maximum Temperature	35	°C	
Min Adaptation Temp.	2	°C	adapted to cold conditions
Max. Photosynthetic Rate	0.8	1 / d	Asaeda and Son, 2000 (0.6)
Respiration Coefficient	0.05	1 / d	"
Mortality Coefficient	0.001	frac / d	prof. judgment
Exponential Mort. Coeff.	0.1	max / d	10%/d if phosynthesis = 0
P : Photosynthate	0.018	ratio	Redfield et al., '63 stoichiometry
N : Photosynthate	0.079	ratio	"
Light Extinction	1.2	1 / m	based on max. biomass of 200

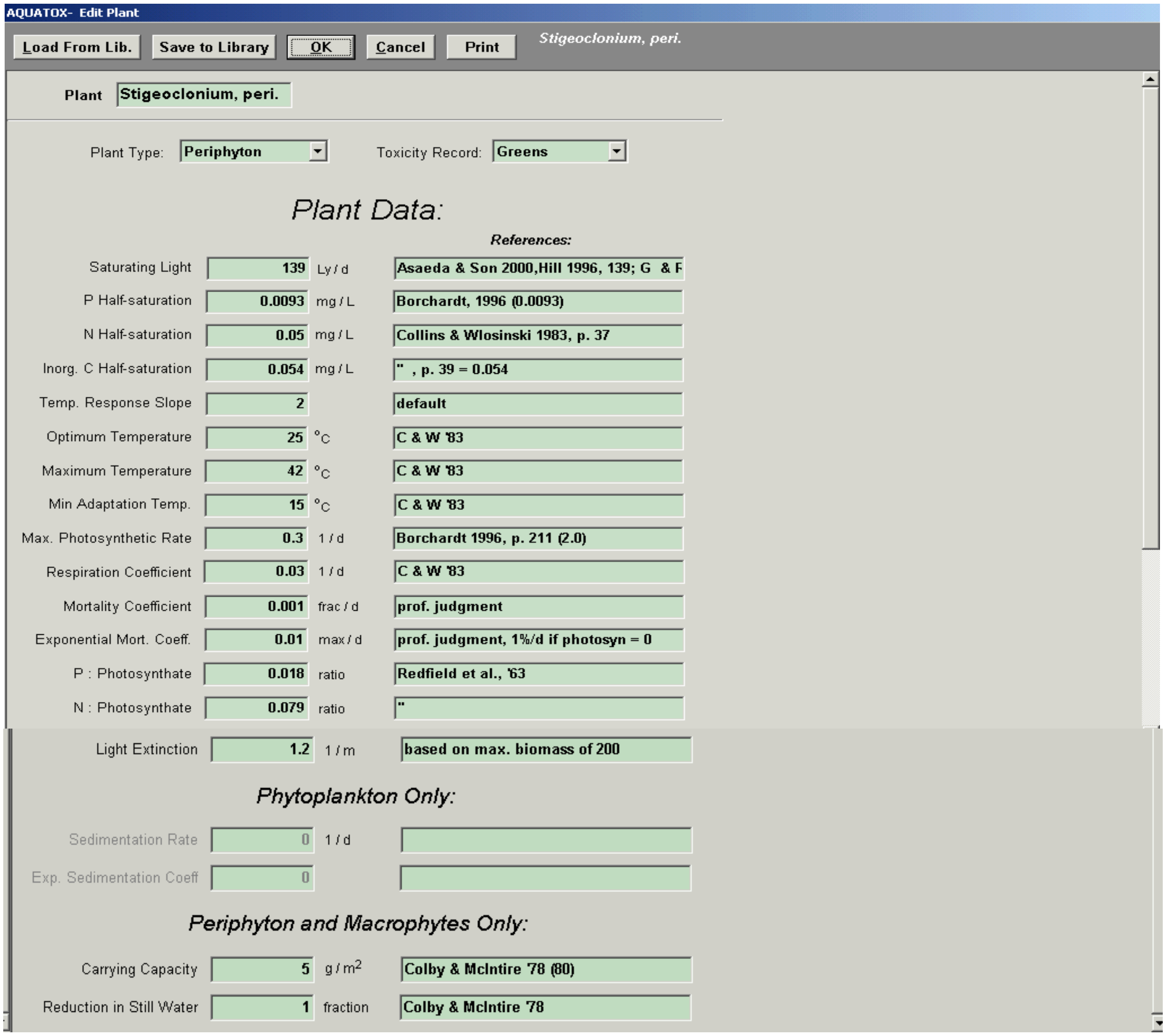
Phytoplankton Only:

Sedimentation Rate	0	1 / d	C & W '83
Exp. Sedimentation Coeff	0		if photosyn = 0, sed is 2X

Periphyton and Macrophytes Only:

Carrying Capacity	80	g / m^2	ESF; Colby & McIntire '78 = 80
Reduction in Still Water	1	fraction	Colby & McIntire '78

Periphyton, *Stigeoclonium tenue*


AQUATOX- Edit Plant

Load From Lib. | Save to Library | OK | Cancel | Print | Stigeoclonium, peri.

Plant: Stigeoclonium, peri.

Plant Type: Periphyton   Toxicity Record: Greens

Plant Data:

			References
Saturating Light	139	Ly / d	Asaeda & Son 2000,Hill 1996, 139; G & F
P Half-saturation	0.0093	mg / L	Borchardt, 1996 (0.0093)
N Half-saturation	0.05	mg / L	Collins & Wlosinski 1983, p. 37
Inorg. C Half-saturation	0.054	mg / L	" , p. 39 = 0.054
Temp. Response Slope	2		default
Optimum Temperature	25	°C	C & W '83
Maximum Temperature	42	°C	C & W '83
Min Adaptation Temp.	15	°C	C & W '83
Max. Photosynthetic Rate	0.3	1 / d	Borchardt 1996, p. 211 (2.0)
Respiration Coefficient	0.03	1 / d	C & W '83
Mortality Coefficient	0.001	frac / d	prof. judgment
Exponential Mort. Coeff.	0.01	max / d	prof. judgment, 1%/d if photosyn = 0
P : Photosynthate	0.018	ratio	Redfield et al., '63
N : Photosynthate	0.079	ratio	"
Light Extinction	1.2	1 / m	based on max. biomass of 200

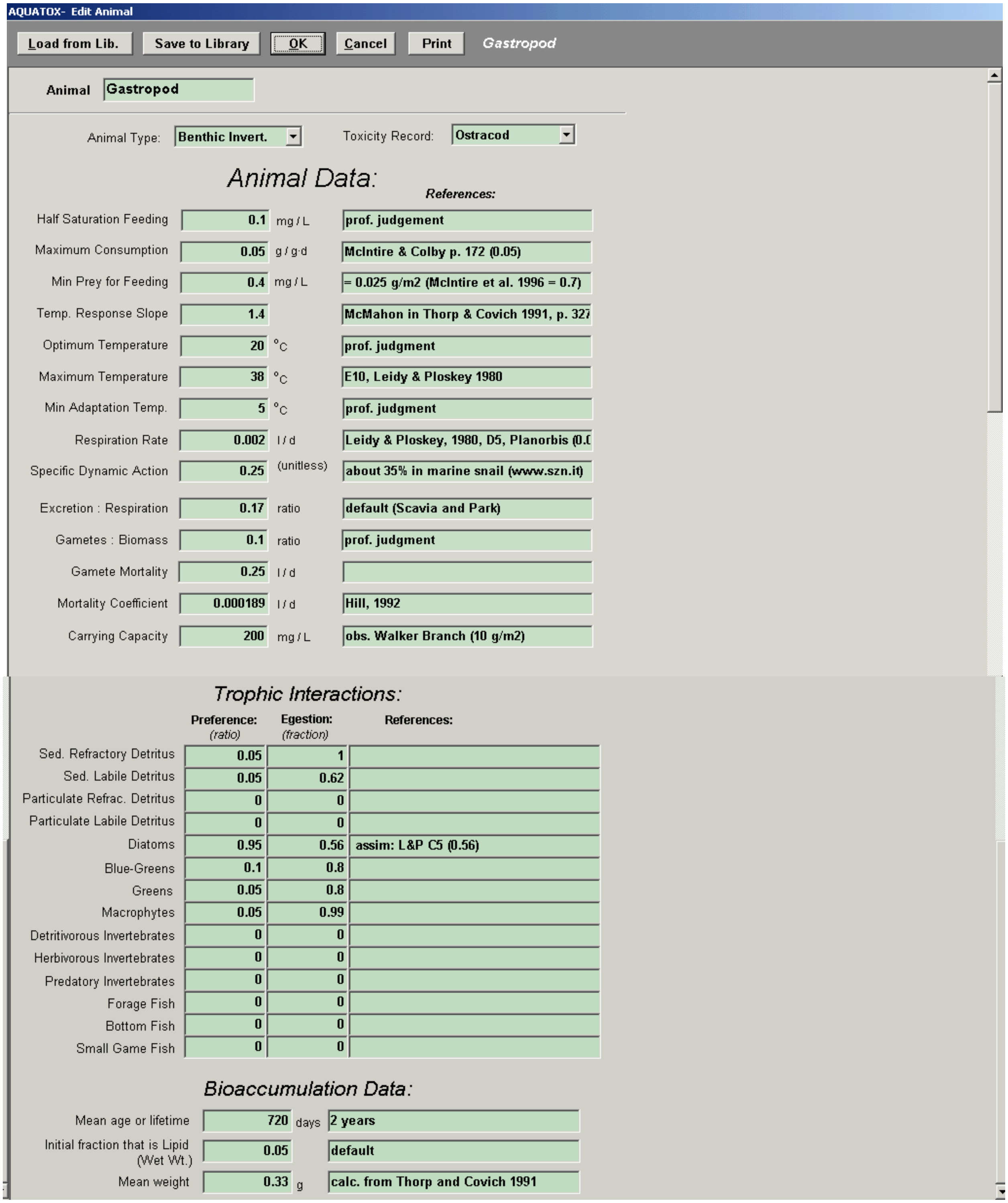
Phytoplankton Only:

Sedimentation Rate	0	1 / d	
Exp. Sedimentation Coeff	0		

Periphyton and Macrophytes Only:

Carrying Capacity	5	g / m2	Colby & McIntire '78 (80)
Reduction in Still Water	1	fraction	Colby & McIntire '78

Gastropod


AQUATOX- Edit Animal
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OK
Cancel
Print
Gastropod
Animal Gastropod
Animal Type: Benthic Invert.
Toxicity Record: Ostracod
Animal Data:
References:
Half Saturation Feeding 0.1 mg / L prof. judgement
Maximum Consumption 0.05 g / g·d McIntire & Colby p. 172 (0.05)
Min Prey for Feeding 0.4 mg / L = 0.025 g/m2 (McIntire et al. 1996 = 0.7)
Temp. Response Slope 1.4 McMahon in Thorp & Covich 1991, p. 327
Optimum Temperature 20 °C prof. judgment
Maximum Temperature 38 °C E10, Leidy & Ploskey 1980
Min Adaptation Temp. 5 °C prof. judgment
Respiration Rate 0.002 l / d Leidy & Ploskey, 1980, D5, Planorbis (0.0
Specific Dynamic Action 0.25 (unitless) about 35% in marine snail (www.szn.it)
Excretion : Respiration 0.17 ratio default (Scavia and Park)
Gametes : Biomass 0.1 ratio prof. judgment
Gamete Mortality 0.25 l / d
Mortality Coefficient 0.000189 l / d Hill, 1992
Carrying Capacity 200 mg / L obs. Walker Branch (10 g/m2)
Trophic Interactions:
Preference: (ratio) Egestion: (fraction) References:
Sed. Refractory Detritus 0.05 1
Sed. Labile Detritus 0.05 0.62
Particulate Refrac. Detritus 0 0
Particulate Labile Detritus 0 0
Diatoms 0.95 0.56 assim: L&P C5 (0.56)
Blue-Greens 0.1 0.8
Greens 0.05 0.8
Macrophytes 0.05 0.99
Detritivorous Invertebrates 0 0
Herbivorous Invertebrates 0 0
Predatory Invertebrates 0 0
Forage Fish 0 0
Bottom Fish 0 0
Small Game Fish 0 0
Bioaccumulation Data:
Mean age or lifetime 720 days 2 years
Initial fraction that is Lipid (Wet Wt.) 0.05 default
Mean weight 0.33 g calc. from Thorp and Covich 1991