
 **EPA AQUATOX Technical Note 1**

**A Calibrated Parameter Set for
Simulation of Algae in Shallow Rivers**

AQUATOX Technical Note 1

A Calibrated Parameter Set for Simulation of Algae in Shallow Rivers

Richard A. Park¹, James N. Carleton², Jonathan S. Clough³, and Marjorie C. Wellman²

¹Eco Modeling, Diamondhead MS 39525

²U.S. Environmental Protection Agency, Washington, DC 20460

³Warren Pinnacle Consulting, Inc., Warren VT 05674

January, 2009

INTRODUCTION

The AQUATOX aquatic ecosystem model contains constructs that represent responses of biological entities to numerous environmental factors, and simulations can include many taxa. Because large numbers of parameters must be chosen before simulations can take place, calibration of the model can be a daunting task, especially for novice users. The existence of a parameter set that can be used “off the shelf” potentially represents a great time and effort saver. This note describes development of one such parameter set, for photosynthetic algae in small to medium-sized shallow rivers in temperate North America.

SUMMARY OF APPROACH

AQUATOX was calibrated against data from three shallow rivers in Minnesota: the Crow Wing, Rum, and Blue Earth Rivers (Figure 1). These rivers are, respectively, nutrient-poor clear-water, moderately nutrient-enriched clear-water, and nutrient-enriched turbid. Simulations were run with a shared parameter set using AQUATOX Release 3, to obtain acceptable fits to observed data across all three sites. Goodness-of-fit to observed data was evaluated visually, and with relative bias and F tests. The resulting parameter set was verified by simulating a site on the Cahaba River, Alabama. Further verification was obtained by applying the original parameter set, without change, to nutrient-poor and nutrient-enriched, clear-water and turbid sites on the Lower Boise River, Idaho.

BACKGROUND

AQUATOX has been designed as a general ecological risk assessment model capable of representing the combined environmental fate and effects of conventional pollutants (*i.e.* nutrients, sediments) and toxic chemicals in aquatic ecosystems (Park *et al.* 2008). The model explicitly simulates competition, predation, and other kinds of interactions among user-definable groups in several trophic levels, including attached and planktonic algae, submerged aquatic vegetation, invertebrates of various guilds, and multiple size or age classes of several species of fish. Equations that represent these processes involve the biological components themselves (state variables), environmental drivers (*e.g.* flow, temperature), and chemical and biological factors that affect the state variables.

A challenge for users in setting up new simulations is assigning suitable values for parameters that govern state variables. Representative values may be difficult to find in the literature, and users may have difficulty knowing which parameters to modify during calibration, as well as by how much to vary them and in what order. To help address this concern AQUATOX comes bundled with libraries of parameter sets for many species, and these libraries are constantly being expanded and refined. In order to simulate a particular water body, however, modification of various parameters may still be necessary. Parameters may represent properties that are affected by ambient conditions or vary with local ecotypes. As an example, maximum photosynthetic rate (Pmax) would seem to be a basic property of an algal taxon, but at any given time the photosynthetic rate is affected by temperature, nutrients, light, etc. A well-chosen value for Pmax would be expected to be applicable to most sites where a specific algal group is present. This is the goal of a “global” parameter, and its existence would imply that new simulations could be set up without the need for significant re-calibration.

METHODS

To develop the initial calibration we worked with data provided by the Minnesota Pollution Control Agency (MPCA), which had found “significant and predictable” linear relationships between nutrients, algae, and biochemical oxygen demand in five medium to large rivers, in samples collected during 1999 and 2000 (Heiskary and Markus 2001, Heiskary and Markus 2003). Trophic conditions in these rivers span a nutrient gradient, from a relatively unenriched, predominantly forested watershed in the “Northern Lakes and Forests” ecoregion (Omernik 1987), to a relatively high-nutrient, predominantly row crop agricultural watershed in the “Western Corn Belt Plains” ecoregion. We first calibrated AQUATOX against data from each of these rivers simultaneously, *i.e.* using a single parameter set. We then tested the robustness of this parameter set by applying it to the Cahaba River in Alabama and the Lower Boise River in Idaho. Table 1 presents observed mean annual nutrient concentrations, temperatures and discharge in each of these rivers at the locations of interest.

Table 1. Mean annual conditions at the calibration and verification sites.

Site	Total N (mg/L)	Total P (mg/L)	TSS (mg/L)	Temp (deg. C)	Discharge (m³/d)
MN					
Crow Wing River	0.76	0.033	2.37	9.3	1.52E+06
Rum River	1.18	0.115	13.99	12.0	1.02E+06
Blue Earth River	6.80	0.204	82.48	10.6	1.49E+06
Lower Boise River, ID					
Eckert	0.128	0.060	5.15	10.5	3.90E+06
Middleton	1.763	0.325	13.89	11.7	1.07E+06
Parma	2.643	0.395	47.81	11.9	3.80E+06
Cahaba River, AL	1.131	0.198	15.77	18.0	6.63E+05

INITIAL CALIBRATION

We chose to focus our modeling efforts on specific sampled reaches within three of the five rivers monitored by MPCA. All three rivers are shallow (mean depth 1 m or less) and support diverse periphyton communities, which appear to vary in composition among rivers according to their position along enrichment and turbidity gradients (Heiskary and Markus 2001, Heiskary and Markus 2003). Based on MPCA data the Crow Wing River, which drains a heavily forested watershed, has relatively low concentrations of nutrients, and low water-column turbidity. The Rum River, draining a watershed with numerous dairy farms, has moderate nutrient concentrations and low turbidity. The Blue Earth River, whose watershed is composed largely of corn and soybean acreage with extensive tile drainage, has high nutrient concentrations and periodically high turbidity. The phytoplankton composition varies from river to river in a predictable fashion, apparently correlated with nutrient conditions. For example, in sampling conducted in 2000, cyanobacteria constituted only a tiny fraction of the sestonic algal biomass in the Crow Wing River but an important fraction in the Rum River, and were the dominant type in the Blue Earth River.

MPCA sampling data for nutrients, BOD₅, and total suspended solids (TSS) were available from two to five separate locations in each river on six to eight separate occasions between June and September of each of the years 1999 and 2000. These data were used to provide influent concentrations that drove the reach simulations. Biotic state variables were chosen to represent nutrient-poor, clear-water conditions characteristic of forested regions as well as nutrient-enriched, sporadically turbid conditions characteristic of agricultural regions. Because the objective was to obtain a set of state variables that would span broad conditions, the number of state variables was larger than might be necessary if a single river with static conditions were being simulated. By seeding the simulations with a range of taxa likely to thrive under a variety of conditions, the algal community responses to widely differing and changing conditions could be simulated using a single parameter set.

Simulated periphyton and phytoplankton communities consisted of broad taxonomic groups of green algae and cyanobacteria (“blue-greens”), as well as “low-nutrient” and “high-nutrient” adapted diatoms (Table 2). The simulated periphyton assemblage also specifically included the diatom *Nitzschia* and the filamentous green *Cladophora*, and the phytoplankton assemblage included the diatom *Navicula*, and *Cryptomonas*, for a mixture of organisms intended to represent potential algal responses throughout the range of simulated environmental conditions. Periphyton and phytoplankton groups were linked to each other in the model through sloughing and sinking, such that detached green algae become part of the sestonic green algal biomass, for example. Invertebrates were represented by broad guilds, with representative genera for shredders, suspension feeders, and grazers among the zoobenthos and zooplankton, as well as clams and snails. Fish species represented small and large forage, bottom, and game fish that are characteristic of different environmental conditions. All of the fauna were parameterized using the default parameter sets provided with AQUATOX version 3.

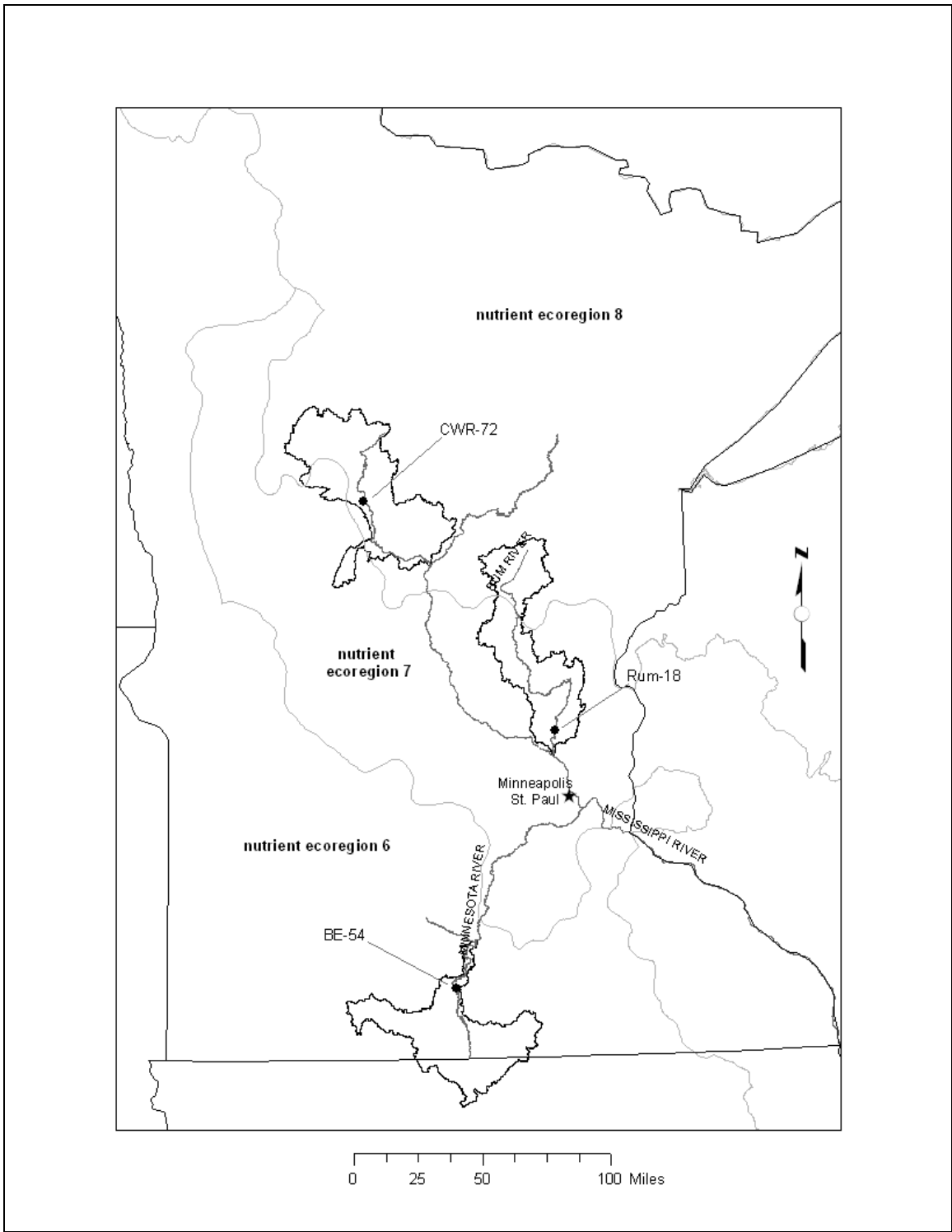


Figure 1. Locations of simulated Minnesota river reaches, with watersheds (HUC8), and aggregate level 3 nutrient ecoregions indicated.

Table 2. Select algal parameters employed in AQUATOX simulations.

Periphyton	Topt	Tmax	Tresp	LightSat	Pmax	Lightex	P half-sat	N half-sat	C half-sat	ExpMoCo	Fcrit	%sl
Low-nutrient diatoms	20	39	2	64	0.65	0.03	0.006	0.07	0.054	0.01	0.001 (0.003)	75 (90)
High-nutrient diatoms	20	35	1.8	22.5	2.3	0.03	0.055	0.2	0.054	0.01	0.004	60
Greens	25	42	2	70 (110)*	1.7 (2)	0.03	0.1	0.8	0.054	0.01	0.004 (0.003)	20 (60)
<i>Cladophora</i>	30	42	2	135	0.7 (1.4)	0.05	0.04	0.1	0.054	0.05	0.004	90
Blue-Greens	30	50	2	45	1.4	0.03	0.1	0.8	0.024	0.01	0.004	90
<i>Nitzschia</i>	25	39	2	82.5	0.5 (1.75)	0.03	0.095	0.4	0.054	0.05	0.001 (0.003)	50 (90)
Phytoplankton												
Low-nutrient diatoms	15	39	2	64	0.7	0.14	0.006	0.0154	0.054	0.05	NA	NA
High-nutrient diatoms	20	35	2	18	1.87	0.14	0.055	0.117	0.054	0.05	NA	NA
Greens	26	42	2	50 (110)	1.5 (1.65)	0.24	0.1	0.8	0.054	0.04	NA	NA
Blue-Greens	27	50	2	60	2.2	0.09	0.03	0.4	0.024	0.12	NA	NA
<i>Cryptomonas</i>	8	30	2	80 (110)	3	0.144	0.076	0.03	0.054	0.04	NA	NA

Key:

Topt = optimal temperature (deg C)

Tmax = maximum temperature (deg C)

Tresp = temperature response slope

LightSat = saturating light (Ly/day)

Pmax = maximum photosynthetic rate (1/day)

Lightex = light extinction coefficient 1/m-g/m3

P half-sat = phosphorus half-saturation constant (mg/L), Michaelis-Menten kinetics

N half-sat = nitrogen half-saturation constant (mg/L), Michaelis-Menten kinetics

C half-sat = inorganic carbon half-saturation constant (mg/L), Michaelis-Menten kinetics

ExpMoCo = exponential mortality coefficient (g/g-day)

Fcrit = critical force for periphyton scour (Newtons)

%sl = percent periphyton lost in slough event (%)

* Parameters in boldface were modified during calibration. Parameters enclosed in parentheses are the corresponding defaults. All other numbers are also model defaults.

Flow Data and Simulations

Biological responses in stream ecosystems can be highly sensitive to flow conditions. In the ideal case a modeler has access to reach-specific flow data, but if not flows may be estimated using other methods. For this exercise, USGS flow-gauging stations were conveniently located at the Rum-18 (Rum River, mile 18) and CWR-72 (Crow Wing River, mile 72) sampling sites (gauges 05286000 and 05244000 respectively). Recorded mean daily discharges at these locations supplied flow values for simulating these two sites. Unfortunately a gauging station was not present at BE-54 (Blue Earth River, mile 54); the nearest station on the Blue Earth River was 42 miles downstream, at gauge 05320000 near Rapidan Dam. Therefore, to provide flow estimates for the BE-54 AQUATOX simulation, a previously-derived Hydrologic Simulation Program-Fortran (HSPF) simulation of the river and its watershed at this location was employed (Donigian *et al.* 2005).

Nutrient and Suspended Solids Estimation

Nutrients support the bases of aquatic food chains, and nutrient state variables are required for AQUATOX to run. The available TP, total Kjeldahl nitrogen (TKN), nitrate (NO_3^-), and BOD_5 data collected by MPCA supplied the concentrations of these variables that were used to drive all three river simulations. Because AQUATOX is designed to process daily values of all inputs, it automatically applied linear interpolation between sampled dates to estimate concentrations of these constituents for the intervening days. AQUATOX applies this method for all input data where daily values are not provided by the user.

Total Suspended Solids (TSS) is a measure of suspended matter in the water, which can have significant effects on light transmission and consequently photosynthesis. Possession of daily site specific monitoring data would have been ideal, but was not the case. However, the available TSS observations were found to be correlated with flow in both the Blue Earth and Rum Rivers, such that daily estimates of TSS could be generated for use in the model. Because there was no gauge at BE-54, the relationship for BE-54 was based on a linear regression of TSS against ln-transformed flow at downstream gauge 05320000. The resulting time series provided a close match to most of the observed data (Figure 2). For the Rum River, a linear regression of TSS against flow was used, which provided reasonably good approximations of the observed data at this site as well (Figure 3). In contrast to the Rum and Blue Earth Rivers, the Crow Wing River exhibited no correlation between TSS and flow (this may have been because the river drains glacial outwash sands, only about 15% of the watershed for the reach is composed of agricultural land, and an estimated 57% is forest). In order to drive all three simulations with analogous forcing functions, an HSPF model of daily TSS in the Crow Wing reach (Donigian *et al.* 2005) was employed. It was felt that a well-calibrated HSPF simulation would provide a better representation of temporal trends in TSS than linear interpolation between the sampled points would have, despite discrepancies between some of the simulated and measured concentrations (Figure 4).

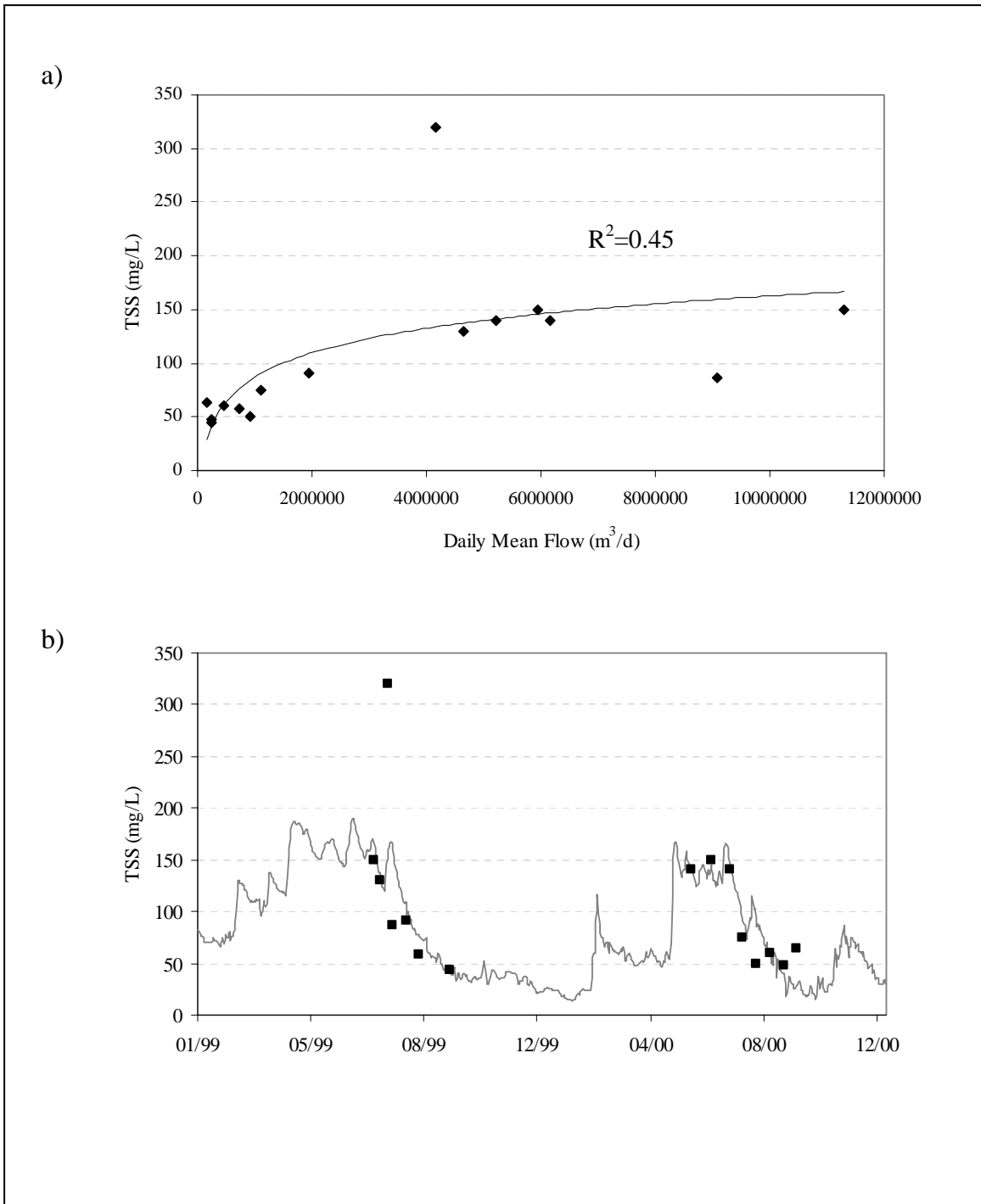


Figure 2. TSS at Blue Earth River 54: a) regression against ln-transformed daily flow at gauge 05320000; b) resulting simulated daily time series (line), and observed values (symbols).

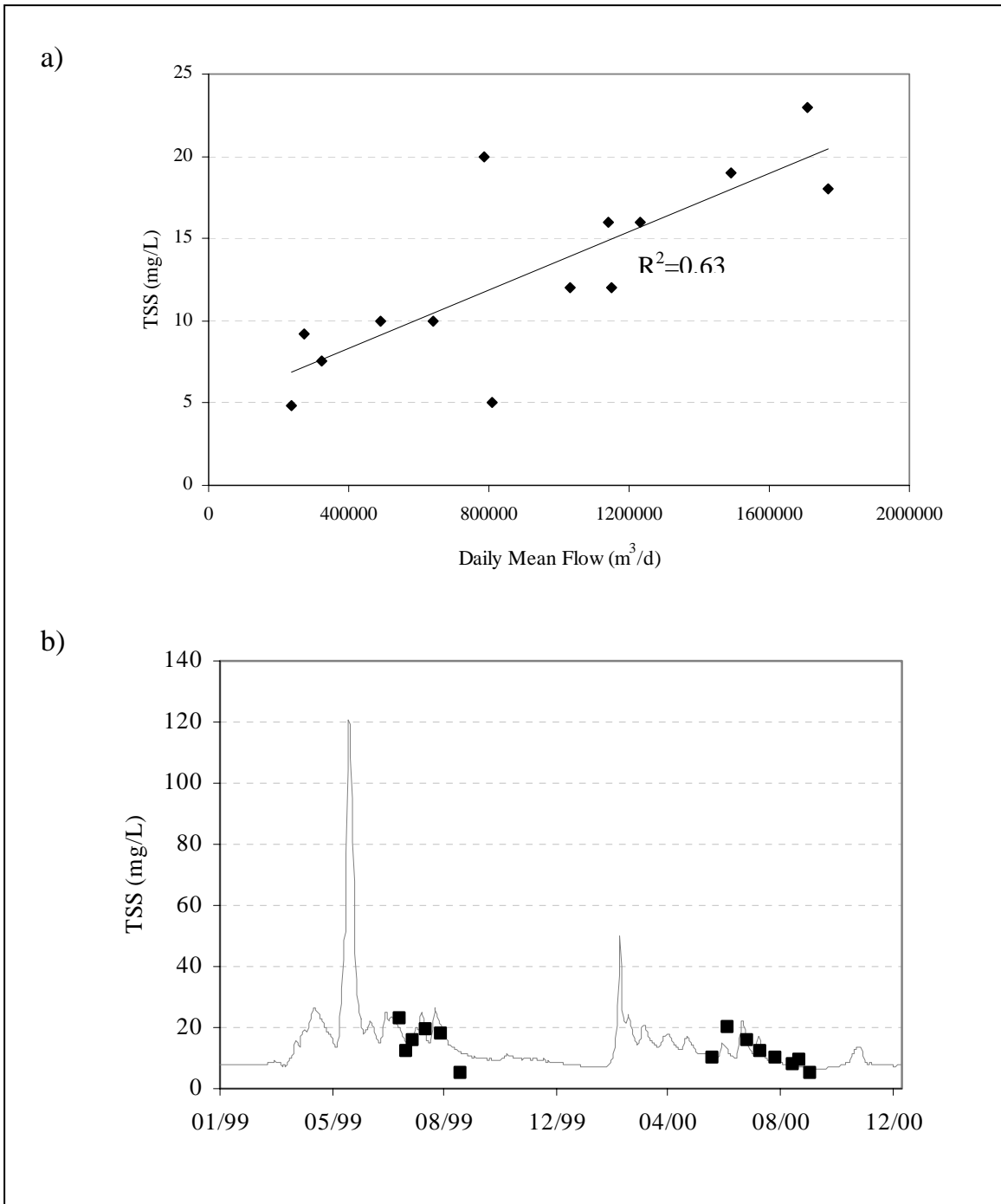


Figure 3. TSS at Rum River 18: a) linear regression against daily flow at gauge 05286000; b) resulting simulated daily time series (line), and observed values (symbols).

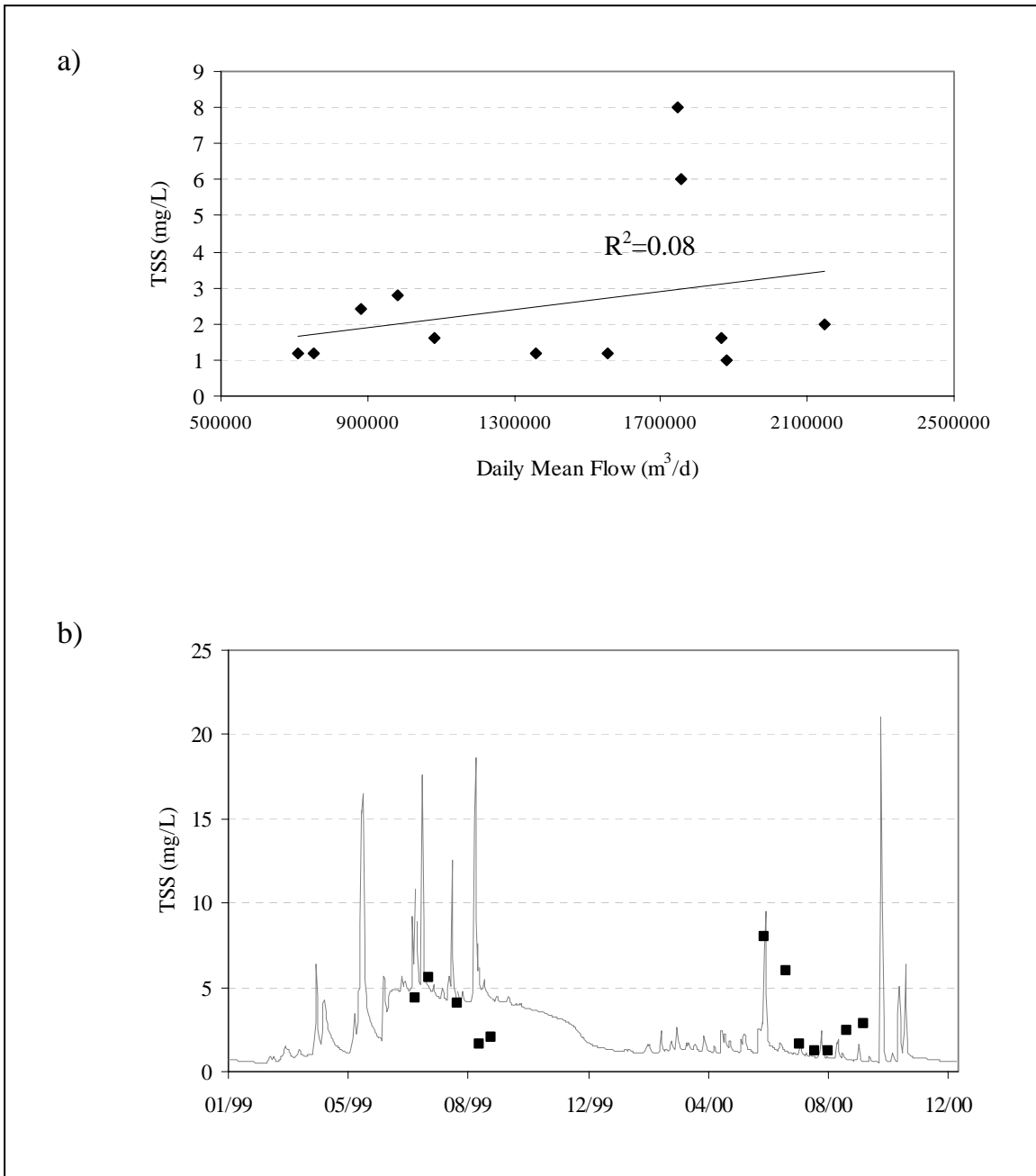


Figure 4. TSS at Crow Wing River 72: a) plot of TSS against daily flow at gauge 05244000; b) HSPF-simulated daily time series (line) and observed values (symbols).

Calibration Process

Calibration of AQUATOX for the Minnesota Rivers used observed sestonic and periphytic chlorophyll *a* as the primary target against which model output was optimized (via parameter modifications indicated in Table 2). Because there were only five to eight sestonic and one benthic chlorophyll *a* observations at each location in each of the two target years, calibration adequacy was evaluated subjectively, based on generally expected behavior (*e.g.* blooms occurring during summer) and approximate concordance with observed values (in terms of both magnitude and timing), as determined through graphical comparisons of model output and data (Figure 5).

Evaluation of Calibration

We also employed quantitative measures to evaluate the adequacy of the calibration and model performance. Relative bias is a robust measure of how well central tendencies of predicted and observed results correspond; a value of zero indicates that the means are the same (Bartell *et al.* 1992):

$$rB = (Pred_Bar - Obs_Bar)/Sobs$$

or:

$$\begin{aligned} rB &= \text{relative bias (standard deviation units);} \\ Pred_Bar &= \text{mean predicted value;} \\ Obs_Bar &= \text{mean observed value; and} \\ Sobs &= \text{standard deviation of observations.} \end{aligned}$$

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

$$F = Var_Pred/Var_Obs$$

where:

$$\begin{aligned} Var_Pred &= \text{variance of predictions;} \\ Var_Obs &= \text{variance of observations.} \end{aligned}$$

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. Small F values may indicate highly variable or uncertain observed data. Assuming normal distributions, the probability that the observed and predicted distributions are the same can be evaluated (Figure 6). Putting the two tests together, if a comparison has $rB = 0$ and $F = 1$, then the predicted and observed results are identical.

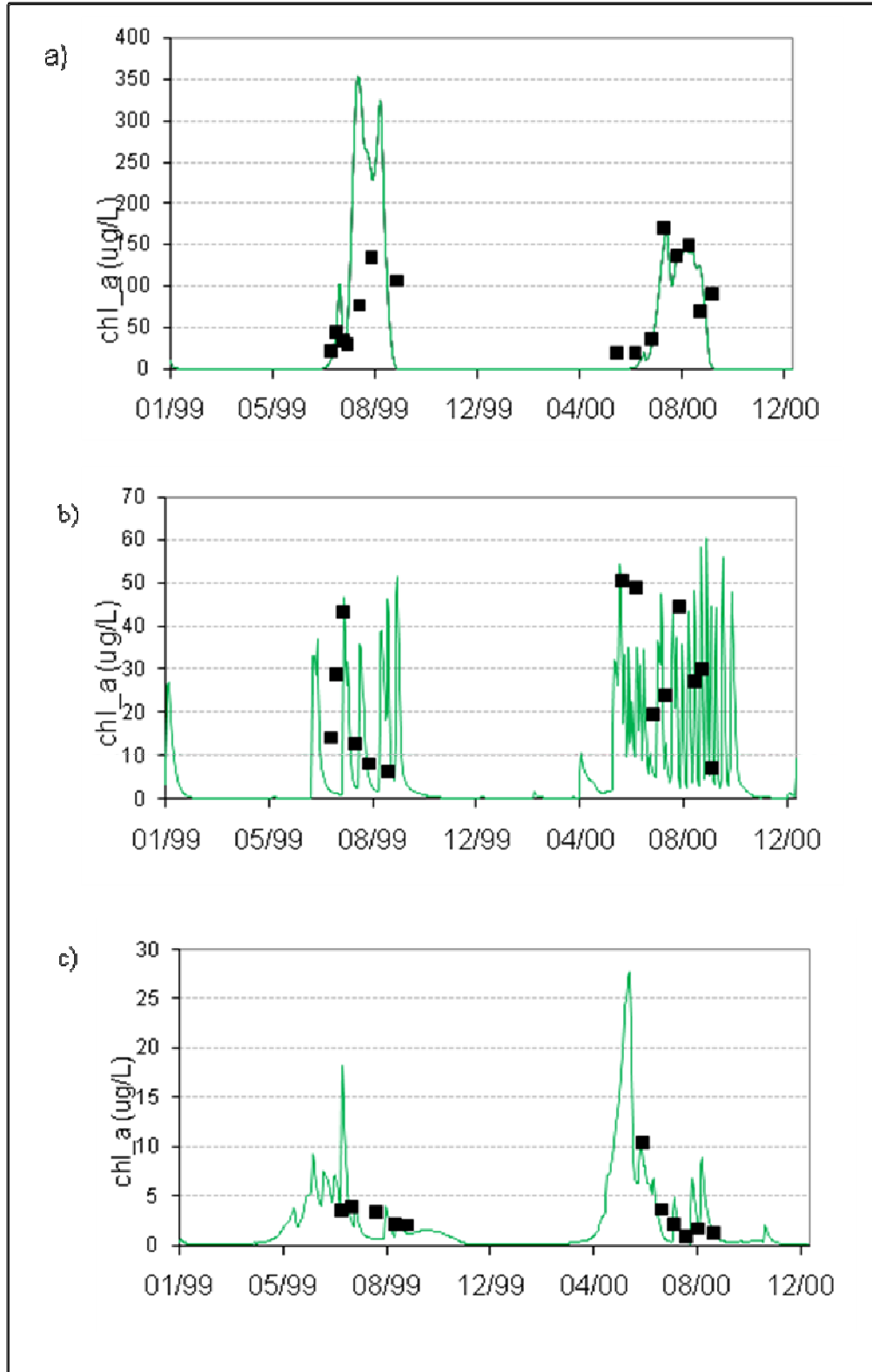


Figure 5. Observed (symbols) and calibrated AQUATOX simulations (lines) of sestonic chlorophyll *a* in three Minnesota rivers: a) Blue Earth at mile 54, b) Rum at mile 18, c) Crow Wing at mile 72. Note the order-of-magnitude range in scale among the figures.

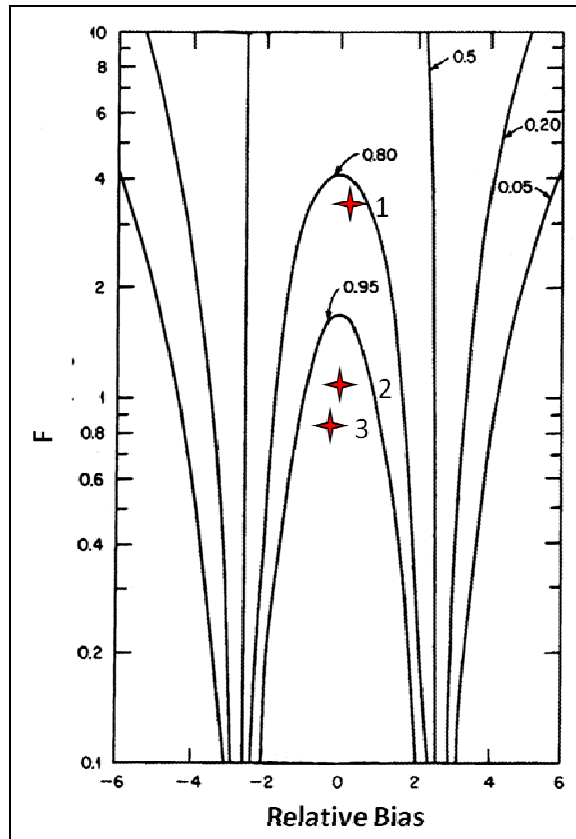


Figure 6. Overlap between model and data distributions based on relative bias and ratio of variances, F ; 1 = Blue Earth River, 2 = Crow Wing River, 3 = Rum River. Isopleths indicate the probability that the predicted and observed distributions are the same, assuming normality.

Application of these statistics to the three Minnesota simulations for the periods covered by the observed data indicates that in two simulations there is good overlap between the predicted and observed distributions, and in one simulation (BE-54) the model predicts greater variance (Figure 6). The central tendencies are similar between predicted and observed distributions for all three sites, as shown by the relative bias. Despite the fluctuations in predicted chlorophyll a , the predicted and observed variances are similar for the CWR-72 and Rum-18 simulations. Predicted periphyton sloughing events played a major role in determining the timing of chlorophyll a peaks in both simulations. The variance in predicted values is high in the BE-54 simulation, in which summer peak concentrations in 1999 appear to be overestimated by a factor of about two. The reason for this overestimation is not known, but may reflect uncertainties inherent in the HSPF-simulated flow and TSS values, the sparseness of water chemistry sampling data, and/or other limitations. Using the procedure described above, the probability that the BE-54 predictions and observations have the same distribution was found to be greater than 0.8. For the purpose of this analysis we therefore judged the calibration to be adequate.

Sensitivity Analysis

A *post-hoc* nominal-range sensitivity analysis of the BE-54 simulation identified the most sensitive cyanobacterial parameters (Figure 7). Two of these parameters, ‘Saturating Light’ and ‘Maximum Photosynthetic Rate’, were modified as part of the calibration process. The phytoplankton and periphyton parameters were linked in the analysis—that is, a 10% change in a parameter for the phytoplankton was also a 10% change in the same parameter for periphyton. When interpreting Figure 7, the vertical line at the middle of the ‘tornado’ diagram represents the deterministic model result. Red lines represent model results when the given parameter is reduced by 10%, while blue lines represent a positive 10% change in the parameter. The sensitivity statistic represents the average absolute percent change in model results divided by the percent change used to test model parameters. For example, if a 10% change in the parameter resulted in a 10% change in model results (in either the positive or negative direction), the sensitivity would be calculated as 100%. Similar to the findings of other investigators (Sourisseau *et al.*, 2008; Rashleigh *et al.*, 2009), the results of our analysis indicate that water column chlorophyll *a* is most sensitive to the cyanobacterial parameters ‘Optimal Temperature’ and ‘Maximum Photosynthetic Rate’.

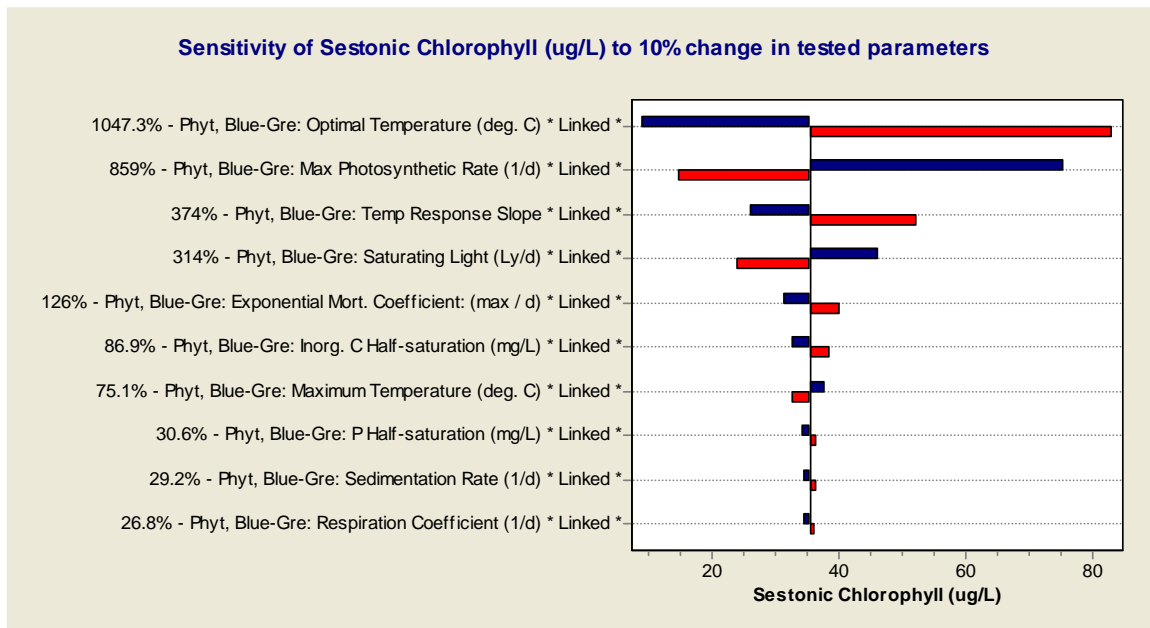


Figure 7. Tornado diagram showing relative sensitivity of sestonic chlorophyll *a* predictions to cyanobacteria parameters in simulations of the Blue Earth River. Red lines represent model results with a negative change in a parameter, and dark blue lines indicate model results with an increase in the parameter. The sensitivity statistic represents the average absolute percent change in model results divided by the percent change used to test model parameters.

PARAMETER SET VERIFICATION

The Cahaba River, AL

As a limited verification, the calibrated model was applied to a site on the Cahaba River south of Birmingham, Alabama, with modifications made to two parameters. The Crow Wing and Rum Rivers have cobbles and boulders and are more sensitive to high current velocities than the bedrock outcrops in the Cahaba River: not only is the bedrock hydrodynamically stable, it also provides abundant crevices and lee sides that serve as protected refuges for periphyton. For these reasons greater water velocity should be required in order to initiate periphyton scour in the Cahaba River than in the Crow Wing and Rum Rivers. With this rationale in mind, the critical force parameter for scour of periphyton (F_{crit}) was increased by about two-fold in the Cahaba River simulation to match model predictions against data. In locations with climates as different as Minnesota and Alabama one would expect different local ecotypes in resident algal species, with differing adaptations to temperature. With this rationale in mind, the optimum temperature values (T_{opt}) for green algae and cyanobacteria were also increased, by 5EC to 31EC and 32EC respectively. The resulting fit to observed data (Figure 8) was better than that obtained in the prior site-specific calibration (Park *et al.* 2002).

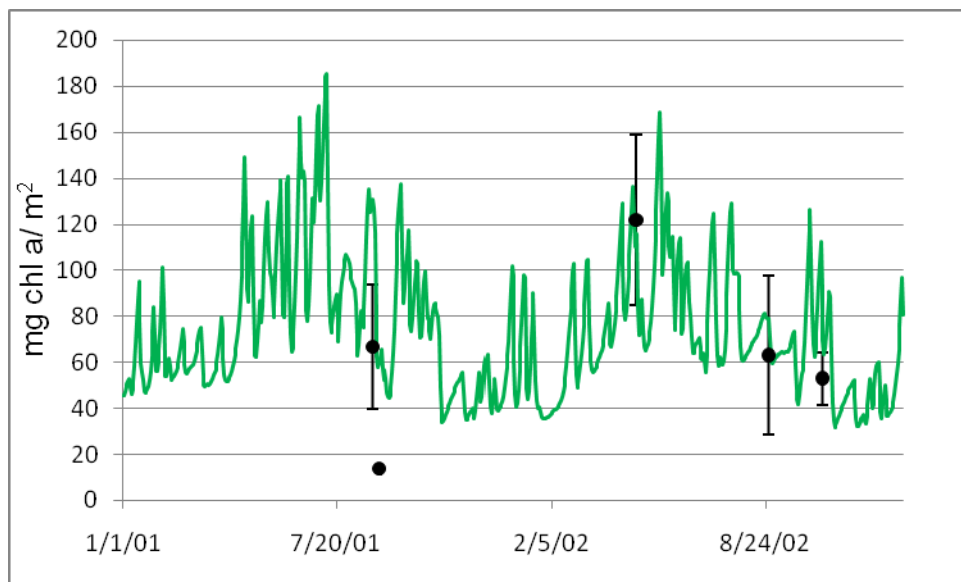


Figure 8. Observed (symbols with 1 standard deviation) and predicted (line) benthic chlorophyll *a* in the Cahaba River, Alabama.

The Lower Boise River, ID

As a further parameter set verification, the calibrated algal model was also applied to three dissimilar sites (Table 1) on the Lower Boise River, Idaho, without modification from the Minnesota calibration. The three sites cover a broad range of nutrient and turbidity conditions over a distance of 90 km (Figure 9). Eckert is a low-nutrient, clear-water site upstream of Boise; Middleton receives wastewater treatment effluent and is a

nutrient-enriched, clear-water site; and Parma is a nutrient-enriched, turbid site impacted by irrigation return flow from agricultural areas. Although the model overestimates periphyton at the Eckert site, the fit of this initial application (Figure 10) provides a promising starting point for further river-specific calibration.

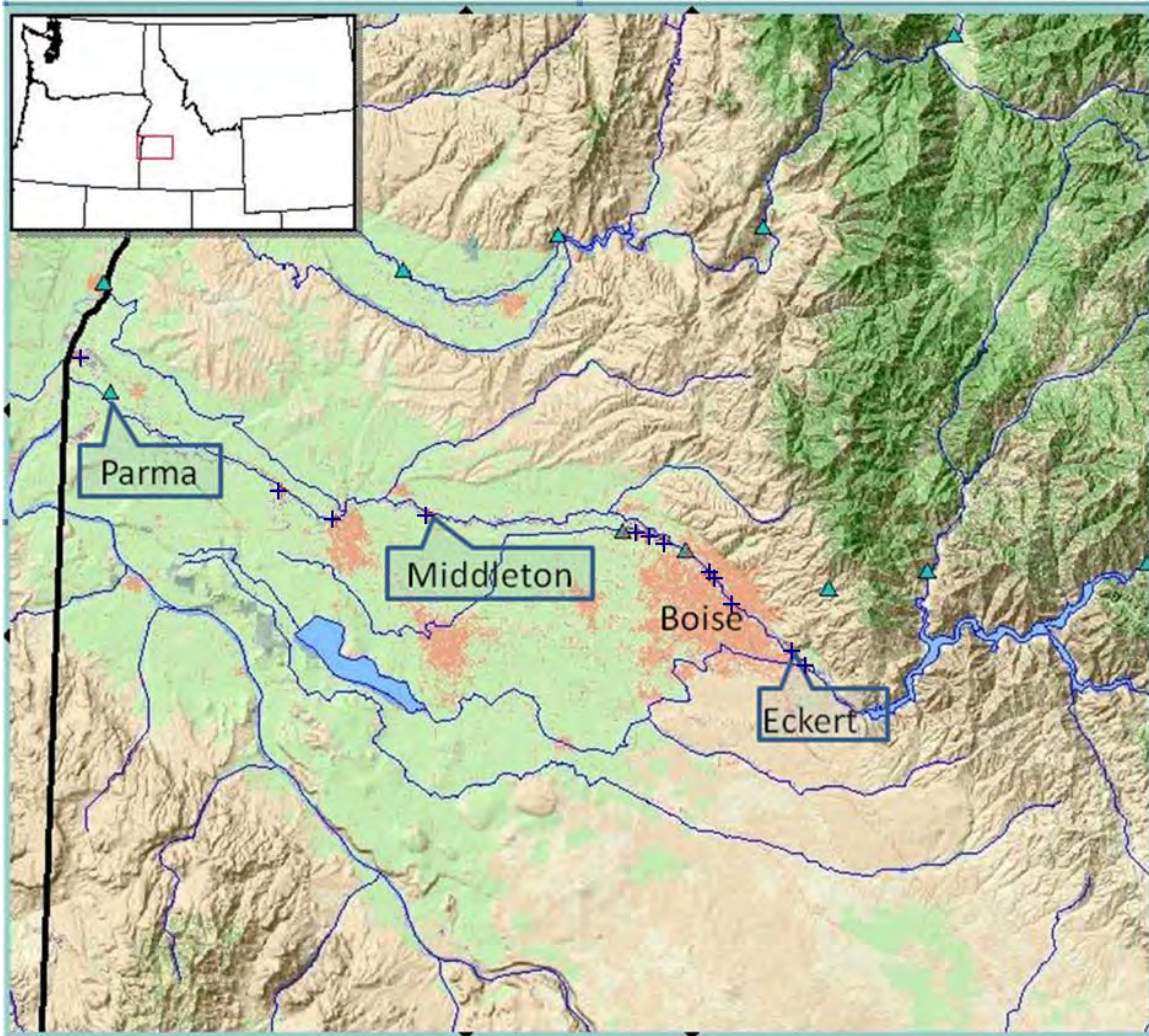


Figure 9. USGS gauging stations (triangles) and biological sampling stations (+) on the Lower Boise River, Idaho, with the three simulated sites indicated.

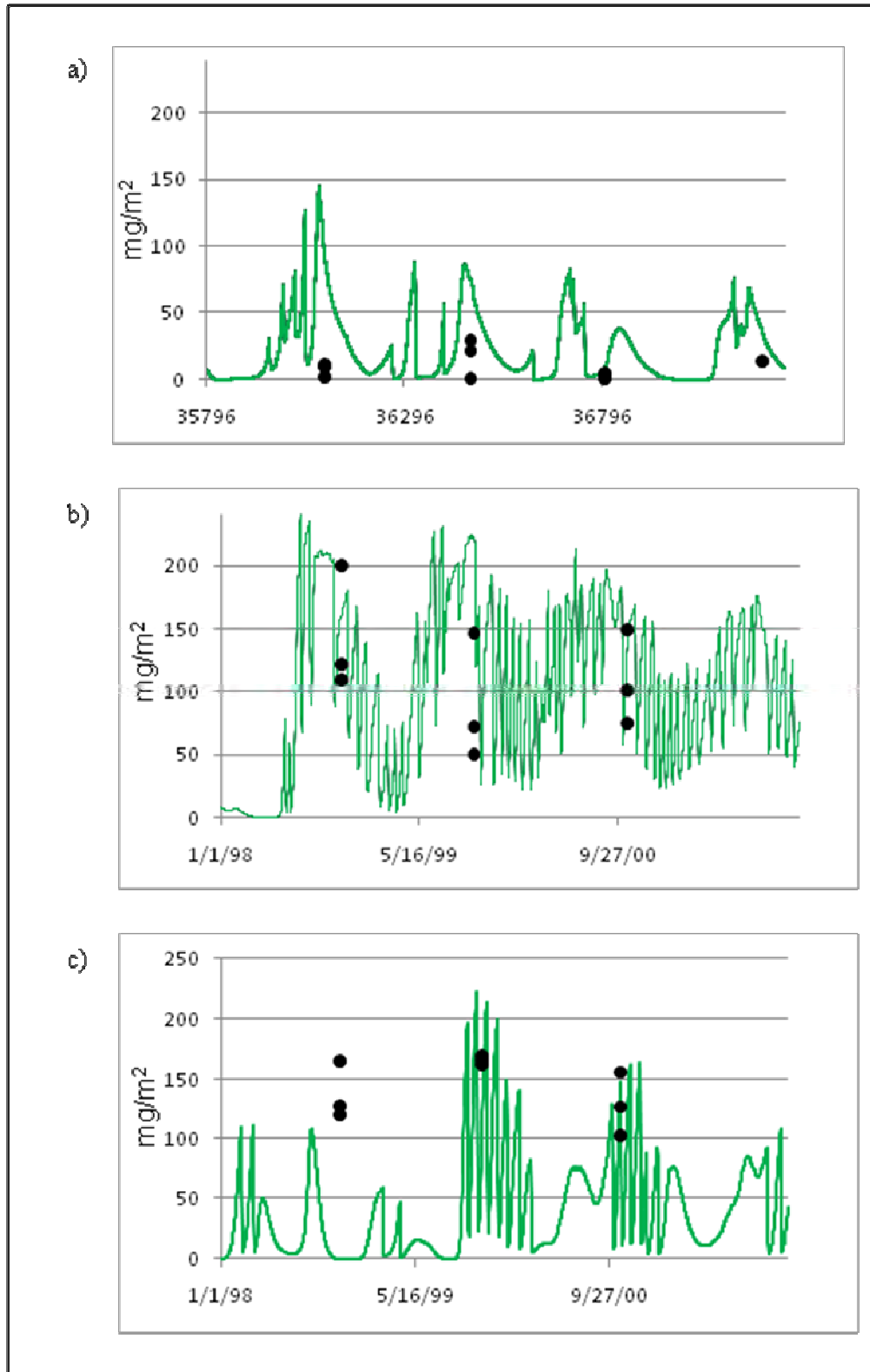


Figure 10. Predicted (line) and observed (symbols) benthic chlorophyll *a* (a) at Eckert Road, (b) near Middleton, (c) near Parma, Lower Boise River, Idaho.

CONCLUSIONS

Based upon evaluation of the simulations described in this note, the algal parameter set originally developed for Minnesota rivers (Table 2) appears to be fairly robust across wide nutrient and turbidity gradients in similarly-sized rivers, even in different regions of the country. These values may represent a global parameter set for algae in medium-sized rivers, and are suggested as a starting point for calibration of AQUATOX when simulating such systems. Future model comparisons against data from additional rivers may provide opportunities for further verification or refinement of these values. Sensitivity analysis produced two parameters relating to photosynthesis and temperature optima, to which special attention should be paid when further calibration is necessary.

ACKNOWLEDGMENTS

We are grateful to Tony Donigian and Jason Love for providing simulated influent loadings for the Minnesota rivers, and we are indebted to Steve Heiskary for providing us with MPCA's monitoring data, and for the logistical assistance he graciously provided during our site visits. We are grateful to Don Blancher, Susan Sklenar, and Lynn Wood for data and assistance on the Cahaba River; and to Tom Dupuis, Ben Nydegger, Kate Harris and Robbin Finch for data and assistance on the Boise River. We also thank Brenda Rashleigh for her review and useful suggestions. This work was conducted in part with Federal funds from the U.S. Environmental Protection Agency, Office of Science and Technology under contracts to AQUA TERRA Consultants and CH2M Hill.

Disclaimer

This document describes the development of a set of calibration parameters for the AQUATOX model, for the purpose of simulating algal growth in rivers. Anticipated users of this document include persons who are interested in using the model for this purpose, including but not limited to researchers and regulators. The model described in this document is not required, and the document does not change any legal requirements or impose legally binding requirements on EPA, states, tribes or the regulated community. This document has been approved for publication by the Office of Science and Technology, Office of Water, U.S. Environmental Protection Agency. Mention of trade names, commercial products or organizations does not imply endorsement or recommendation for use.

REFERENCES

- Bartell, S. M., R. H. Gardner, and R. V. O'Neill, 1992. *Ecological Risk Estimation*. Lewis Publishers, Boca Raton, Florida.
- Donigian, A. S., J. T. Love, J. S. Clough, R. A. Park, J. N. Carleton, P. A. Cocca, and J. C. Imhoff, 2005. Nutrient Criteria Development with a Linked Modeling System: Watershed and Ecological Model Application and Linkage. *in* 2005 TMDL Conference. Water Environment Federation, Philadelphia PA.
- Heiskary, S., and H. Markus, 2001. Establishing relationships among nutrient concentrations, phytoplankton abundance, and biochemical oxygen demand in Minnesota, USA, rivers. *Journal of Lake and Reservoir Management* 17:251-262.
- Heiskary, S., and H. Markus, 2003. Establishing Relationships Among In-Stream Nutrient Concentrations, Phytoplankton Abundance and Composition, Fish IBI and Biochemical Oxygen Demand in Minnesota USA Rivers. Minnesota Pollution Control Agency, St. Paul, MN.
- Omernik, J., 1987. Ecoregions of the conterminous United States. *Annals of the Association of American Geographers* 77:118-125.
- Park, R. A., E. C. Blancher, S. A. Sklenar, and J. L. Wood, 2002. Modeling the Effects of Multiple Stressors on a Use-Impaired River. *in* Society of Environmental Toxicology and Chemistry, Salt Lake City.
- Park, R. A., J. S. Clough, and M. C. Wellman, 2008. AQUATOX: Modeling environmental fate and ecological effects in aquatic ecosystems. *Ecological Modelling* 213:1-15.
- Rashleigh, B., M.C. Barber, and D.M. Walters, 2009. Foodweb modeling for PCBs in the Twelvemile Creek Arm of Lake Hartwell, South Carolina, USA. *Ecological Modelling* 220: 254-264.
- Sourisseau, S., A. Basseres, F. Perie, and T. Caquet, 2008. Calibration, validation and sensitivity analysis of an ecosystem model applied to artificial streams. *Water Research* 42:1167-1181.