VALIDATION OF AQUATOX VERSION 1.66, WITH DATA FROM LAKE ONONDAGA, NEW YORK

Introduction

"Lake Onondaga is arguably the most polluted lake in the United States" according to Effler (1996) in the preface to his comprehensive book, which serves as the primary reference for the following information and data on the lake. The shore of this lake in central New York State was industrialized before 1800, and over the last hundred years at least thirty different chemicals were produced from nearby salt and limestone deposits. Unfortunately, the lake was a convenient dumping ground for waste products. Production of soda ash resulted in waste beds as much as 21 m deep and 8.1 km^2 in area along 30% of the lake shore; the wastes include NaCl and $CaCl_2$ that easily leach into the lake. The salinity of the lake was around 3‰ (parts per thousand) prior to closure of the soda ash plant in 1986; by 1990 the salinity had decreased to 1.3‰. Nevertheless, this salinity creates unusual density gradients and intense stratification of the lake. A chlor-alkali plant produced NaOH and Cl by electrolysis, using Hg as the cathode. From 1946 to 1970 as much as 75,000 kg of Hg were discharged into the lake. Aside from an advisory against eating fish from the lake, the high mercury levels may have adversely affected the functioning of the lake ecosystem.

The lake has been a receptacle for most of the domestic waste and urban runoff from Syracuse and the surrounding area. Prior to 1960 untreated and poorly treated sewage was discharged directly to the lake. In 1960 the Metropolitan Sewer District (METRO) primary treatment plant was completed; in 1979 it was upgraded to secondary treatment; and in 1981 tertiary treatment (removal of phosphorus) was instituted. By design, there is little reduction in ammonia in the sewage effluent. At present nearly 20% of the annual inflow to the lake is from METRO. Most troubling are the combined sewer overflows (CSOs) that carry storm water and raw sewage into tributary creeks about 50 times a year. In 1991 there were 45 CSOs discharging into Onondaga Creek, 19 into Harbor Brook, and 2 into Ley Creek. The purpose of this study is to evaluate the validity of the AQUATOX model in representing eutrophication of a stratified urban lake receiving large amounts of point- and nonpoint-source nutrients and organic matter.

Onondaga is a glacial lake that is 7.6 km long and has a maximum width of 2 km; the watershed is 652 km^2. The surface area of the lake is 12E6 m^2, and the mean depth is 10.9 m, with a volume of 131E6 m^3; the maximum depth is 19.5 m. For a lake of this size it is appropriate to apply a one-dimensional model such as AQUATOX, which represents stratification into epilimnion and hypolimnion but assumes that the lake is well mixed horizontally.

Input Data

As a test of the application of AQUATOX, three levels of analysis were implemented using data that are generally available. With Effler's (1996) 832-page book as a resource, even more detailed analyses could have been performed, but they would have been beyond the scope of the present project. Therefore, some simplifications were taken in computing loadings and site characteristics. As shown in Table 1, mean annual values for nutrient and organic matter mass loadings and concentrations were used: first with mean monthly inflow data (first-level analysis) and then with daily inflow data (second- and third-level analyses).

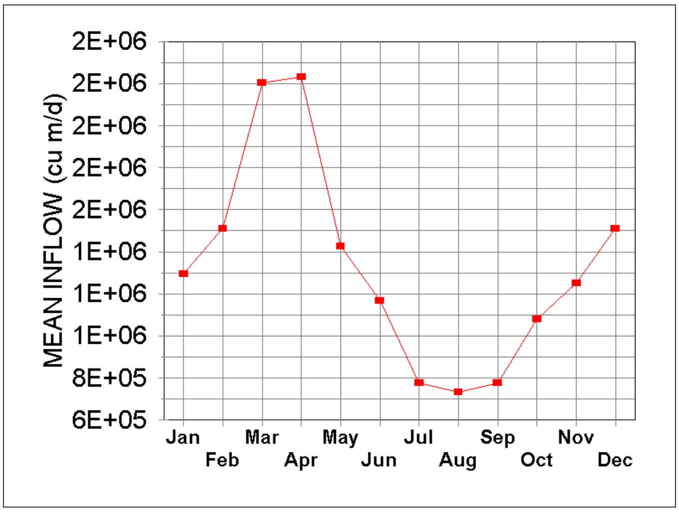
Table 1. Input Data

Variable	Source	Format
Inflow	Effler 1996, p. 103 www.waterdata.usgs.gov	[1] monthly values based on 28-yr means [2] daily values for 4 gauged streams; extrapolated to ungauged streams
Phosphorus, NPS METRO	Effler 1996, calc. from p. 162 Efffler 1996, calc. from p. 159 Effler 1996, p. 162	[1] mean loads, April-September, 1990 [2] mean annual conc., 7 tributaries, 1989-1990; mult. by respective inflow [1,2] mean loads, April-September, 1990
NO_x & NH_3, NPS METRO	Effler 1996, calc. from p. 138 Effler 1996, calc. from p. 128 Effler 1996, calc. from p. 138	[1] mean annual loads for 1989 [2] mean annual concentrations for 1989 for 4 tributaries [1,2] mean annual loads for 1989
Org. matter, NPS METRO	Effler 1996, calc. from p. 138 Effler 1996, calc. from p. 128 Effler 1996, calc. from p. 138	[1] back-calculated from organic-N [2] back-calculated from organic-N [1,2] mean annual loads for 1989
Epilimnion temperature	Effler 1996, p. 207	annual mean and range interpolated from figure for 1989
Hypolimnion temperature	Effler 1996, p. 247	annual mean and range interpolated from figure for 1981
Wind	Effler 1996, p. 248	mean value est. from figure for 30 years
Solar radiation	unpub. data, Lake George, N.Y.	observed annual mean and range
Initial conditions	Effler 1996	obs. data and professional judgment

[1] 1st-level analyses with monthly inflow data; [2] 2nd- and 3rd-level analyses with daily inflow data

AQUATOX can accept loadings data in a variety of formats. For the first-level analyses, constant mass loadings expressed as g/d were used for nutrients and organic matter. Mean monthly inflow values (**Figure 1**), based on a 28-yr dataset, primarily affected the retention time or flow-through rates for the lake. The intent was to use the model as if only general information was available.

Figure 1. Lake Onondaga mean daily inflow for each month, based on 28-yr record.



For the second- and third-level analyses, discharge data from the four gauged streams in the watershed (Onondaga Creek, Ninemile Creek, Ley Creek, and Harbor Brook, listed in order of importance) were downloaded from the U.S. Geological Survey Web site (see Table 1). Discharge from four ungauged streams was estimated, assuming that they had an aggregate flow rate that was 94% of the discharge of Ley Creek and Harbor Brook based on data in Effler (1996, p. 102). The loadings were then computed using average concentrations for the respective streams, assuming a constant relationship between concentration and discharge. Different average phosphate values were used for 1989 and 1990 for Onondaga and Ninemile Creeks, which varied considerably between the two years due to combined sewer overflows. Also, the concentration of ammonia in Ninemile Creek, which flows through the soda ash waste beds, exhibits an inverse relationship to flow rate according to Effler (1996, p. 131); therefore, his Equation 3.12 was used to compute the ammonia concentrations:

$$[T\ NH_3] \quad 0.20 \quad \frac{0.73}{Flow}$$

where:

$[T\text{-}NH_3]$	=	concentration of total ammonia (mgN/L),
Flow	=	flow rate (m^3/s).

Given the readily available hydrologic data, both 1989 and 1990 were simulated with daily loadings. Examination of the loading plots confirms that the streams draining into Lake Onondaga are indeed “flashy” or subject to fast runoff with distinct peaks (**Figure 2**), and the nutrient and organic matter loadings vary accordingly (**Figures 3-6**).

Figure 2. Lake Onondaga inflow.

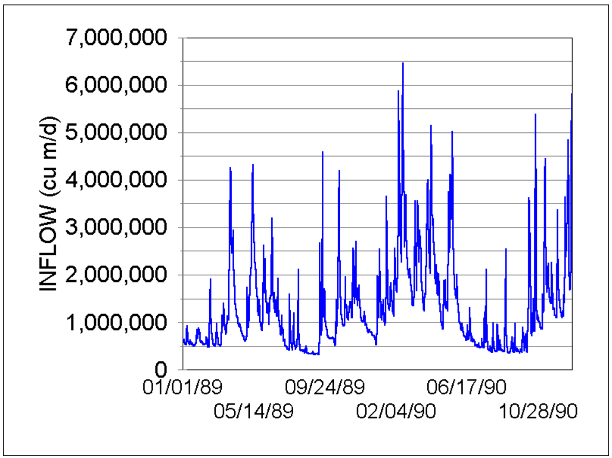


Figure 3. Lake Onondaga phosphate loadings.

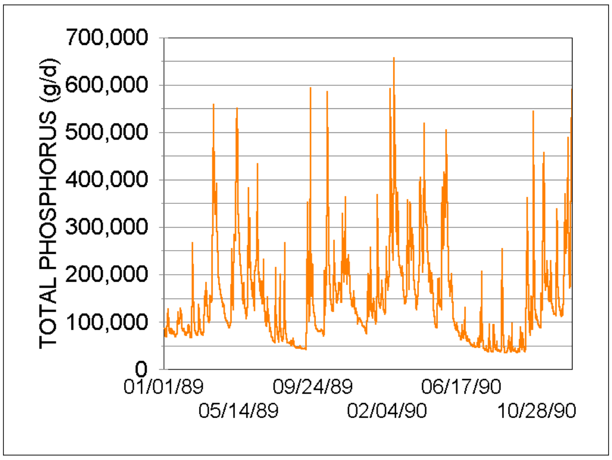


Figure 4. Lake Onondaga ammonia loadings.

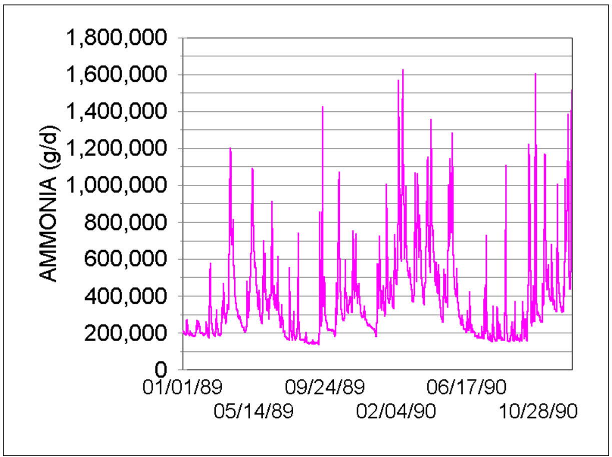
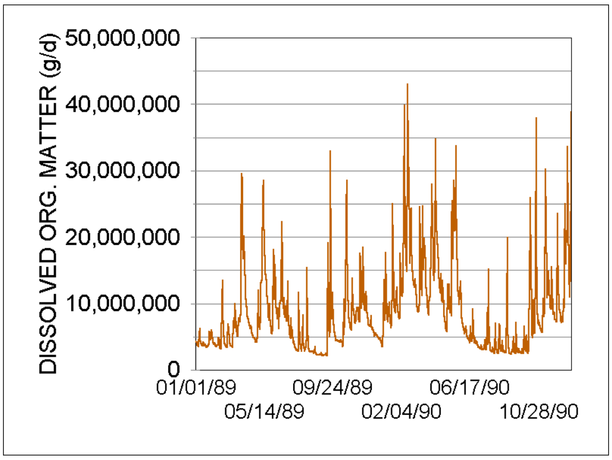


Figure 5. Lake Onondaga DOM loadings.



In the second-level analysis no attempt was made to fine-tune the model. In the third-level analysis the model input was specifically modified to represent better the known site-specific characteristics of this unusual lake. No changes were made in the computer program, but several work-arounds were used; these are available to any model user. Also, another algal group was parameterized—something any knowledgeable user could implement. Altogether, one additional day was spent incorporating the greater detail into the simulations; more time could have been spent to obtain an even better calibration.

It appears that the salinity gradient in the lake is restricting the mixing depth. The model computes the depth of the well mixed layer (epilimnion) using a robust regression equation with the fetch (distance across which the wind can blow) as the independent variable. This equation is based on a dataset for 167 lakes. By back-calculating from the regression equation, a fetch (*Length*) of 0.779 km was found to give the observed well mixed depth (*MaxZMix*) of 7.75 m:

$$\begin{array}{rl} \mathit{MaxZMix} & \mathit{Length}^{0.336} \cdot 0.569 \\ \log(\mathit{Length}) & \dfrac{\log(7.75)}{0.336} \quad 0.245 \\ \mathit{Length} & 779 \ \mathrm{m} \end{array}$$

The spring bloom was reported to be due to cryptomonads, a flagellated algal group. Using values from Collins and Wlosinski (1983), a cryptomonad compartment was parameterized. Version 1.66 of AQUATOX can simulate three algal groups, generally diatoms, green algae and blue-green algae. Diatoms and green algae are more important than blue-greens in Lake Onondaga, so cryptomonads were substituted for blue-greens. This is appropriate because the model assumes that blue-greens occupy the top meter of water unless the wind exceeds 3 m/s, when Langmuir stripes form, and cryptomonads also tend to move toward the surface.

The first- and second-level implementations had cladocerans (*Daphnia*) and predatory zooplankton as the two zooplankton compartments. However, rotifers are important grazers on cryptomonads, and predatory zooplankton probably are unimportant in the lake, so rotifers were substituted for predatory zooplankton in the third-level analysis. Furthermore, the food preferences for rotifers were changed to force them to “eat” cryptomonads in the model. In addition, the zoobenthos, (*Tubifex tubifex*) feeding rates and catfish initial conditions were calibrated in order to model sediment oxygen demand.

First-Level Results

Initially, the lake was simulated using monthly averages for inflow and annual averages for nutrient and organic-matter loadings, similar to a screening-level application. The maximum chlorophyll *a* predictions were of the same magnitude as those observed in Lake Onondaga, and the observed summer biomass values were bounded by the predictions. However, the algal bloom in early May was missed entirely and several summer fluctuations were missed (**Figure 6**). The spring bloom was due to cryptomonads, which were not modeled. Evidently the fluctuations in summer biomass were due to a succession of algal blooms and crashes involving greens, flagellated greens, and diatoms; whereas the model predicted diatoms to be the dominant phytoplankton. Site-specific calibration (third-level analysis of this study) would be necessary to represent this detailed succession. Plots of cumulative distributions emphasize the differences between the predicted (**Figure 7**) and observed (**Figure 8**) chlorophyll values. The lack of low predicted values compared to the uniform distribution of observed values between 5 and 80 μg/L is obvious.

Figure 6. Predicted and observed chlorophyll in Lake Onondaga, New York, in 1990.

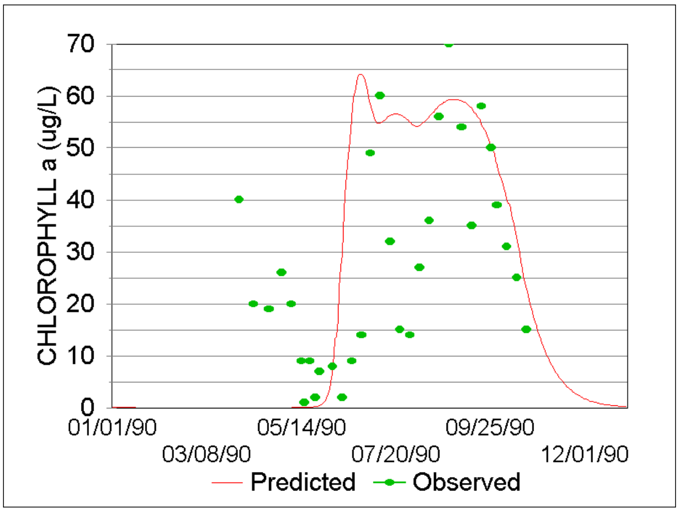


Figure 7. Cumulative distribution of predicted chlorophyll in Lake Onondaga in 1990.

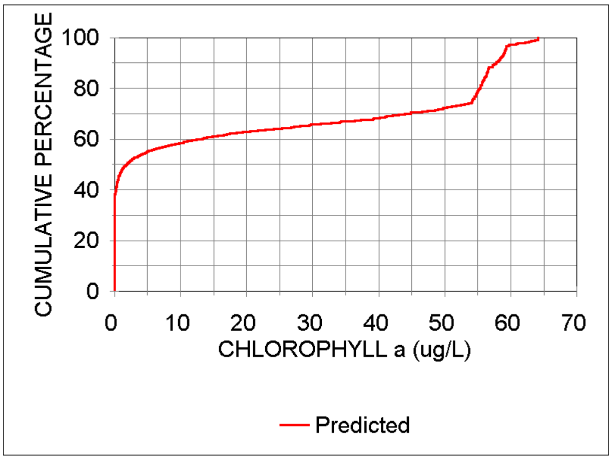
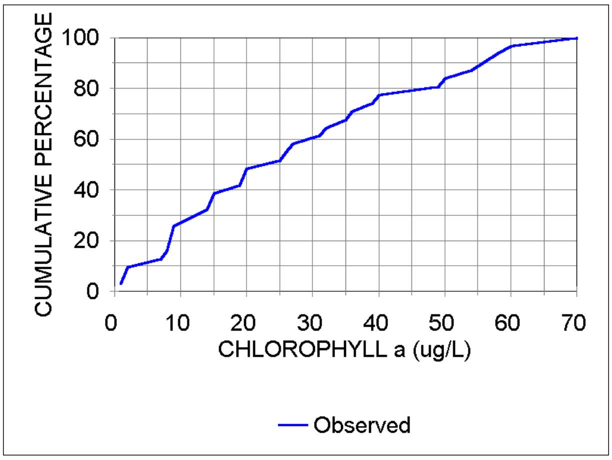
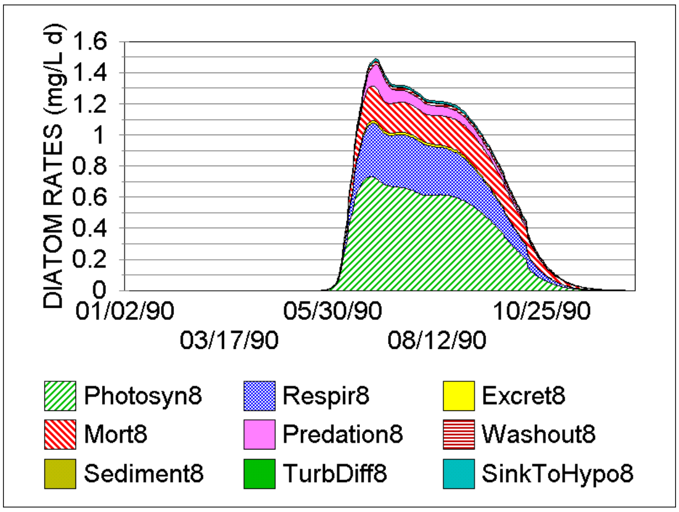


Figure 8. Cumulative distribution of observed chlorophyll from Lake Onondaga in 1990.



Examination of the epilimnetic diatom rates (**Figure 9**, an area graph that displays individual rates for each day) reveals that growth — represented by photosynthesis (Photosyn8) balanced against respiration (Respir8) and, to a minor degree, excretion (Excret8) — occurs over the entire summer and early fall. Nonpredatory mortality (Mort8) is important, and predation (Predation8) is less important. Washout (Washout8), loss to bottom sediments (Sediment8), mixing with the hypolimnion (TurbDiff8), and sinking to the hypolimnion (SinkToHypo8) are unimportant.

Figure 9. Predicted rates for diatoms in Lake Onondaga in 1990.



Dissolved oxygen is another environmental variable that is important from a regulatory perspective, with 5 mg/L being the standard applicable to Lake Onondaga. The predicted epilimnion values (**Figure 10**) indicate a late winter dissolved oxygen sag under the ice that cannot be confirmed due to a lack of observed data. However, observed low values during the summer were not represented by the first-level model application. Interestingly, these low values are not represented by the site-specific Lake Onondaga model either (Effler 1996, p. 712). The lack of agreement may be due to several factors. The crashes of the successive algal blooms observed in the lake undoubtedly created labile detritus that exerted oxygen demand; furthermore, reduced chemical species, especially methane and Fe^{++}, transported from the anoxic hypolimnion are not modeled in AQUATOX. The pronounced sag in October is due to the admixture of a large volume of anoxic hypolimnetic waters during overturn. The hypolimnion predictions indicate anoxic conditions in the middle of summer, and the episode is remarkably close to the observed conditions (**Figure 11**).

Figure 10. Dissolved oxygen in the Lake Onondaga epilimnion in 1990.

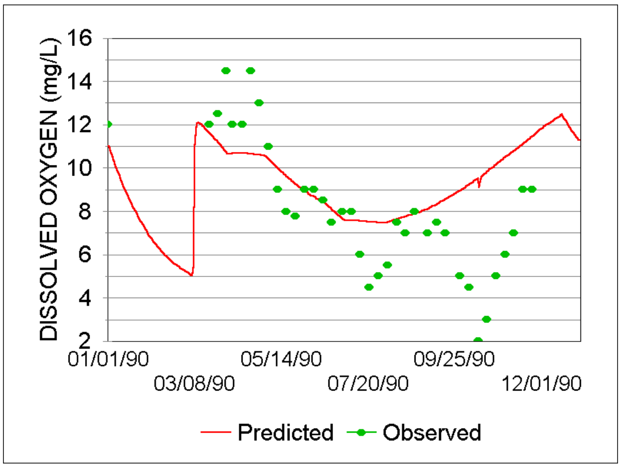
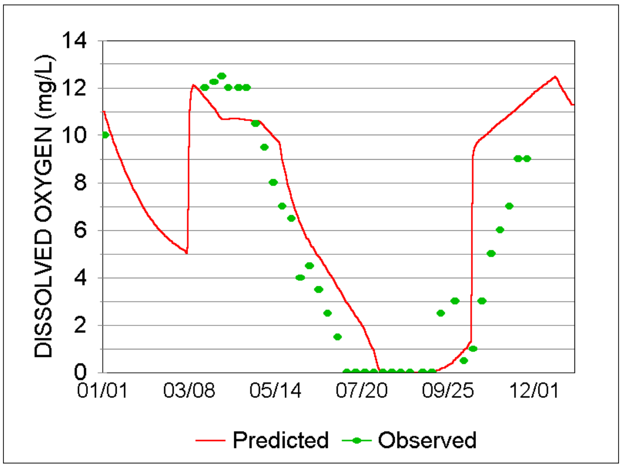


Figure 11. Dissolved oxygen in the Lake Onondaga hypolimnion in 1990.



Second-Level Results

The prediction of chlorophyll concentrations is no better with the daily data (**Figure 12**) than with monthly loadings. The maximum values of the 1990 summer bloom are predicted reasonably well, but neither of the spring blooms is predicted. The algal rates (not shown) do not differ significantly from those predicted with the monthly loadings. The summer epilimnetic oxygen sags again are poorly represented (**Figure 13**). The 1989 hypolimnetic anoxia occurs too late in the summer, although its magnitude is accurately predicted. The 1990 period of anoxia is well represented (**Figure 14**).

Figure 12. Chlorophyll in Lake Onondaga based on daily loadings.

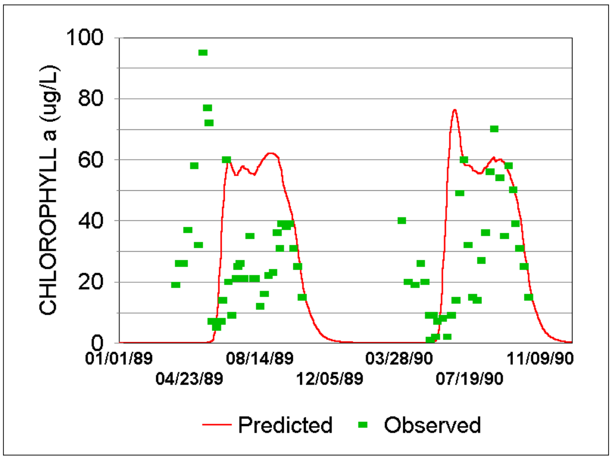


Figure 13. Dissolved oxygen in Lake Onondaga epilimnion, based on daily loadings.

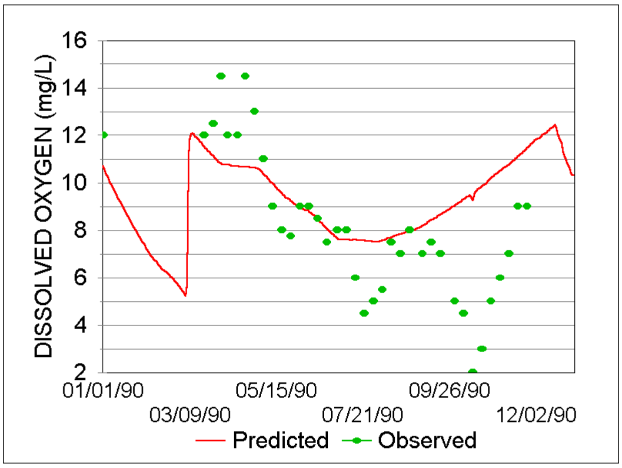
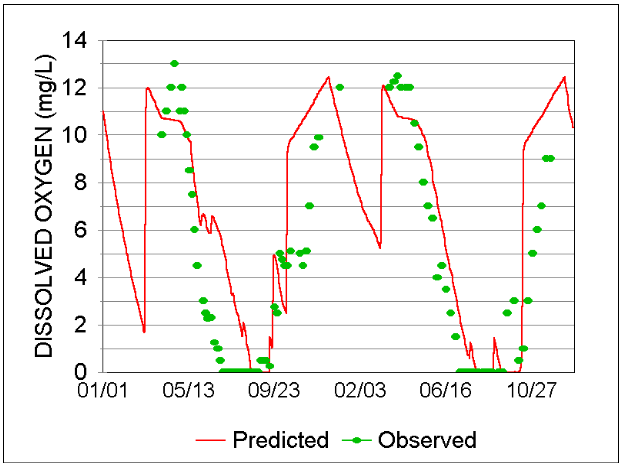


Figure 14. Dissolved oxygen in Lake Onondaga hypolimnion, based on daily loadings.



Examination of multiple model runs suggests that the model is sensitive to the feeding rate of the zoobenthos (modeled as *Tubifex tubifex*). As formulated, feeding gradually converts refractory detrital sediment to labile detritus, which creates additional oxygen demand. Slower feeding delays the onset of hypolimnetic anoxia. If the 1989 period is considered as "spin-up" so the simulation can recover from the effects of poor initial conditions and only 1990 results are considered, then the model can be judged as an adequate representation.

The herbivorous zooplankton exhibit realistic seasonal fluctuations in biomass. *Daphnia* is the surrogate herbivorous zooplankter represented in the model run, and the observed mean biomass of 0.625 mg/L for cladocerans during the growing season is about four times higher than predicted. The fish are dominated by catfish in the simulation, compared to dominance by planktivorous fish in the lake, although the initial condition for catfish of 5 mg/L is forcing that result in the two-year simulation. The gradual decrease in the fish stocks over the two-year period also could be a function of inappropriate initial conditions, or it may indicate that zoobenthos production is not simulated properly—another consequence of the sensitivity to zoobenthic feeding rates. Unfortunately, zoobenthic biomass and production data are unavailable.

Figure 15. Predicted herbivorous zooplankton (*Daphnia*) biomass in Lake Onondaga.

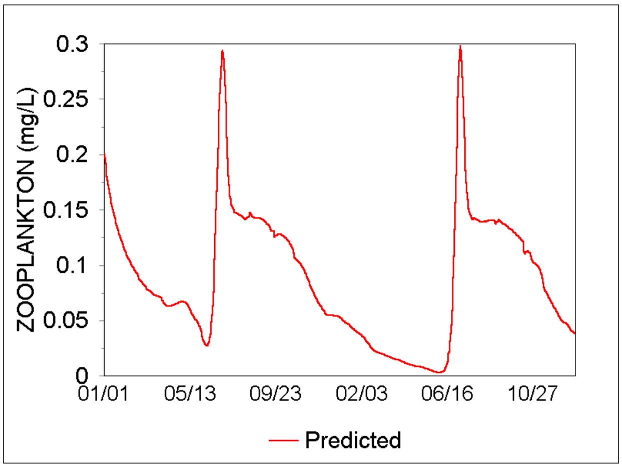
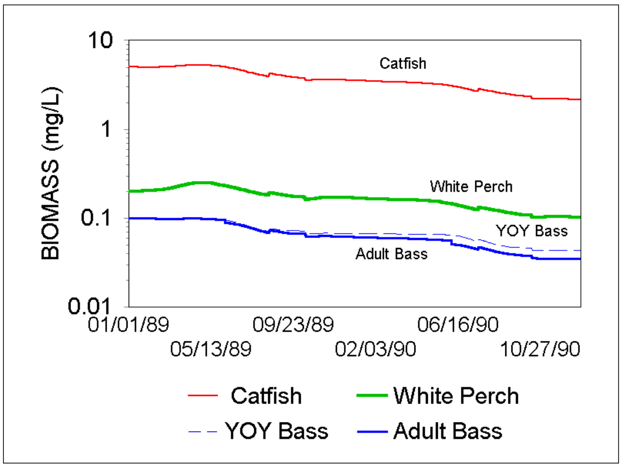


Figure 16. Predicted fish biomass in Lake Onondaga.



Third-Level Results

Detailed site information was used to obtain a satisfactory calibration to 1989 data for Lake Onondaga. This is demonstrated by both the dissolved oxygen and chlorophyll *a* trends. The epilimnetic dissolved oxygen (**Figure 17**) exhibits a sag during the fall overturn, and the summer values are realistically lower than in the first- (**Figure 10**) and second-level (**Figure 13**) analyses. These reflect the simulation of a larger volume of anoxic hypolimnion admixed during overturn and the oxygen demand created by successive crashes of algal blooms. The high observed oxygen values are not predicted well; however, it is generally more important to predict the low values than the high values. The hypolimnetic anoxia is represented even better than in the first- (**Figure 11**) and second-level (**Figure 14**) analyses. The calibration of *Tubifex tubifex* and adjustment of catfish initial conditions were necessary to model adequately the dynamics of sediment oxygen demand.

Figure 17. Dissolved oxygen in Lake Onondaga epilimnion based on calibrated model.

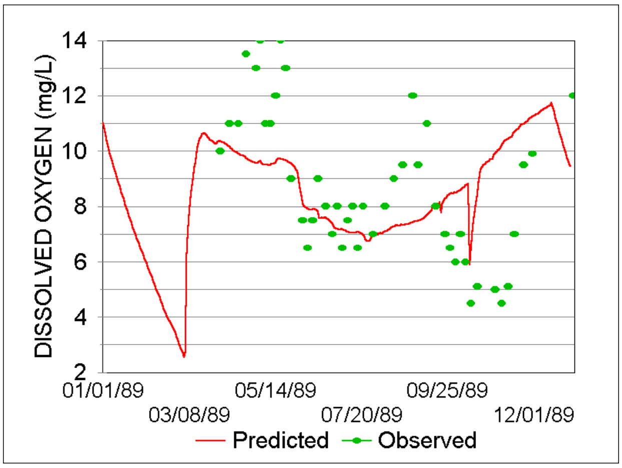
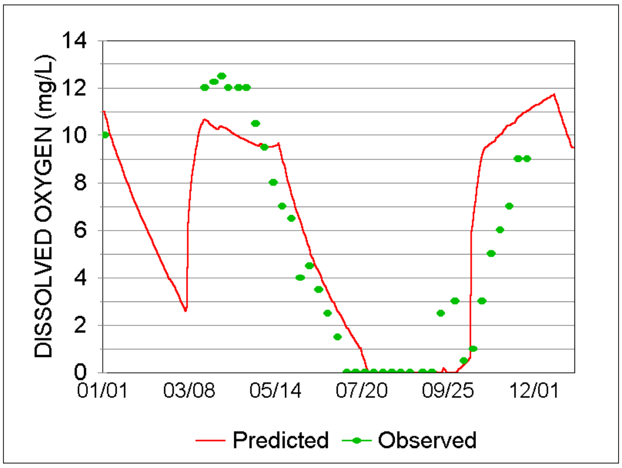
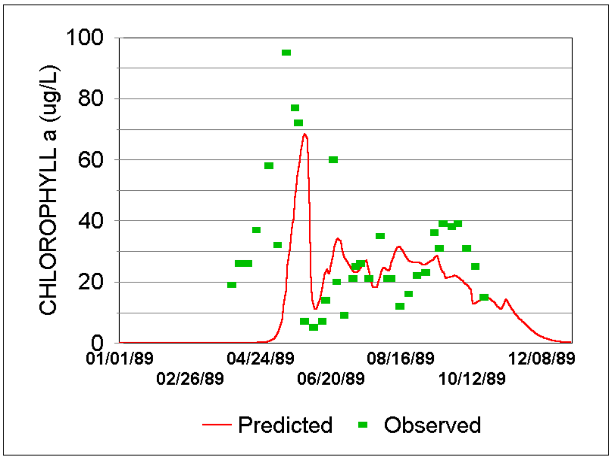


Figure 18. Dissolved oxygen in Lake Onondaga hypolimnion based on calibrated model.



The predicted chlorophyll *a* trends of the improved application are reasonably representative of the trends observed during 1989; they are much better than those simulated in the first- (**Figure 6**) and second-level (**Figure 12**) analyses. The factors contributing to the improvement are the forcing of a shallow epilimnion, inclusion of cryptomonads and rotifers that account for the spring algal bloom and subsequent crash, and more dynamic nutrient cycling due to improved loadings data and dynamic sediment release. All these changes could have been made by a knowledgeable user; they did not involve changing the AQUATOX code.

Figure 19. Chlorophyll in Lake Onondaga based on calibrated model.



The calibrations were preformed using 1989 data and keeping 1990 data separate from the process. As a further check on the model validity, both 1989 and 1990 were simulated. As might be expected, the test revealed some transient behavior, especially with respect to zoobenthos and fish populations. However, the validity of the epilimnetic and hypolimnetic dissolved oxygen simulations held (**Figure 20** and **Figure 21**). Also, the simulations of chlorophyll represented significantly different algal responses in the two years (**Figure 22**), and the simulated 1990 algal blooms—although larger than observed—were within historic ranges observed in the lake.

Figure 20. Dissolved oxygen in Lake Onondaga epilimnion in 1989 and 1990; simulation based on calibration for 1989.

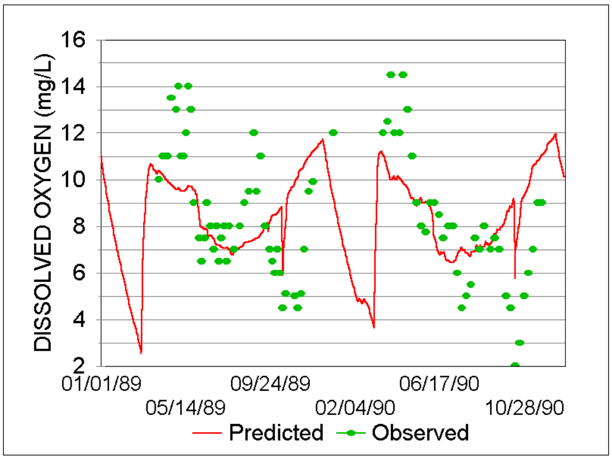


Figure 21. Dissolved oxygen in Lake Onondaga hypolimnion in 1989 and 1990; simulation based on calibration for 1989.

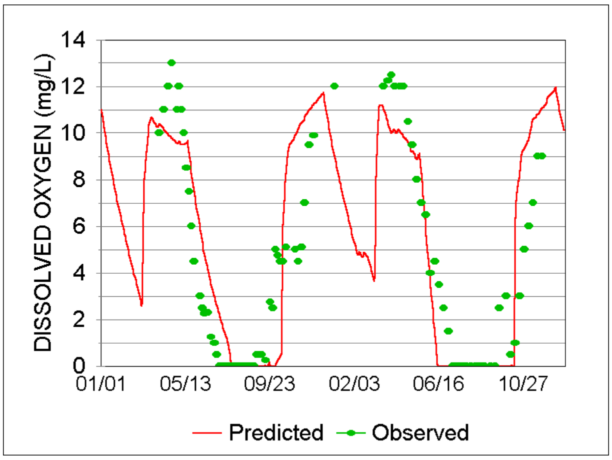
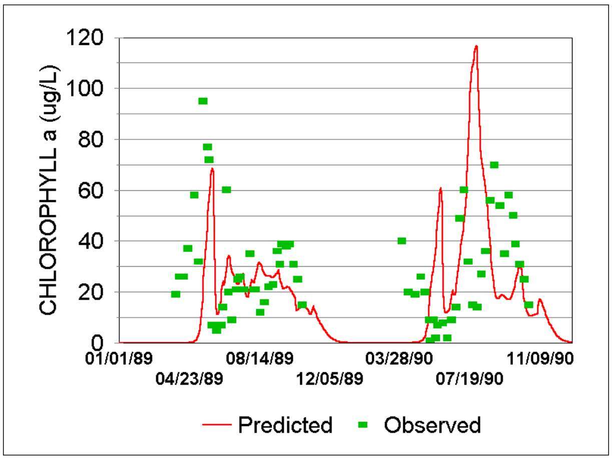


Figure 22. Chlorophyll in Lake Onondaga in 1989 and 1990; based on 1989 calibration.



In order to test the null hypothesis that the predicted and observed distributions are the same, cumulative distributions were obtained (**Figures 23-25**). These were compared using the Kolmogorov-Smirnov test. The distributions for epilimnetic oxygen were significantly different, but those for hypolimnetic oxygen and chlorophyll were not shown to be significantly different at the 0.05 level (**Tables 2-5**).

Figure 23. Cumulative distributions of predicted and dissolved oxygen in Lake Onondaga epilimnion in 1989 and 1990.

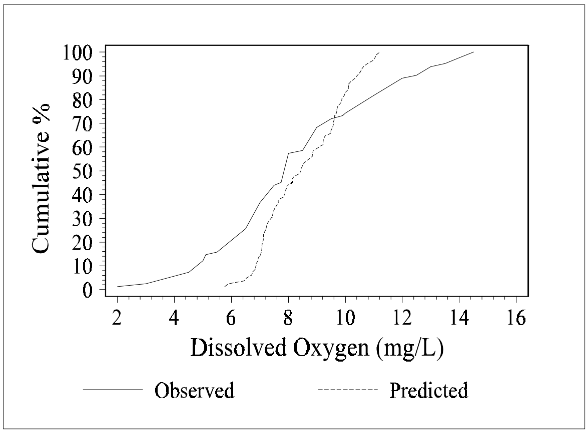


Figure 24. Cumulative distributions of predicted and dissolved oxygen in Lake Onondaga hypolimnion in 1989 and 1990.

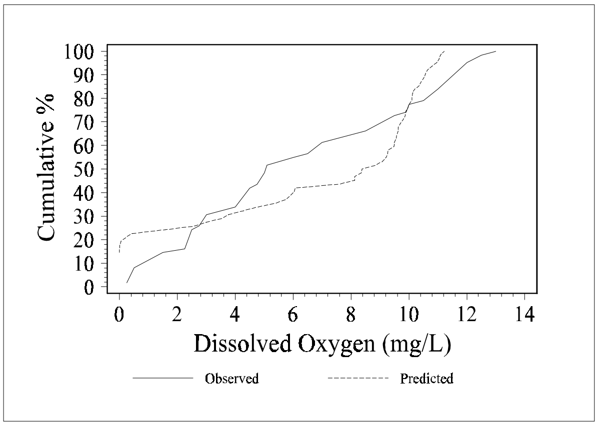


Figure 25. Cumulative distributions of predicted and observed chlorophyll in Lake Onondaga epilimnion in 1989 and 1990.

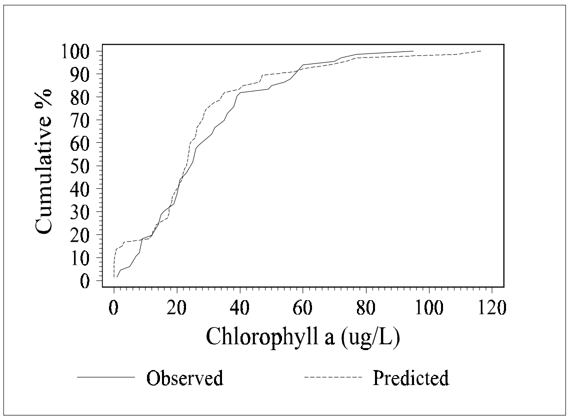


Table 2. Summary Statistics for Dissolved Oxygen in Lake Onondaga Epilimnion

Time Period	Group	Oxygen (mg/L)					
		No. of Obs.	Mean	Median	Std. Dev.	Std. Err.	p-value from KS Test
1989-1990	Observed	82	8.46	8.00	2.82	0.31	0.025*
	Predicted	82	8.53	8.45	1.41	0.16	

* Significantly different at α=0.05.

Table 3. Summary Statistics for Dissolved Oxygen in Lake Onondaga Hypolimnion

Time Period	Group	Oxygen (mg/L)					
		No. of Obs.	Mean	Median	Std. Dev.	Std. Err.	p-value from KS Test
1989-1990	Observed	62	6.27	5.10	3.98	0.51	0.131[a]
	Predicted	62	6.52	8.61	4.19	0.53	

[a] Not significantly different at α=0.05.

Table 4 Summary Statistics for Chlorophyll in Lake Onondaga Epilimnion

Time Period	Group	Chlorophyll (mg/L)					
		No. of Obs.	Mean	Median	Std. Dev.	Std. Err.	p-value from KS Test
1989-1990	Observed	66	28.98	25.00	19.87	2.45	0.319[a]
	Predicted	66	26.65	23.12	23.07	2.84	

[a] Not significantly different at α=0.05. Statistics courtesy of Jie Tao and William Warren-Hicks, The Cadmus Group.

AQUATOX routinely performs paired simulations of perturbed and controlled conditions to facilitate quantitative risk assessment and environmental decision making. As an example, the default control run for 1989 for Lake Onondaga provided a simulation without the loadings of nutrients and organic matter from the metropolitan sewage treatment plant. The results were interesting: the predicted epilimnetic dissolved oxygen increased measurably (**Figure 26**); although the hypolimnetic oxygen still dropped below the 5 mg/L standard, anoxia was not forecast (**Figure 27**); and the algal blooms were predicted to be slightly less severe during the summer (**Figure 28**), with a noticeable shift to more desirable diatoms in a fall bloom. Keep in mind that these were one-year simulations and were still affected by internal nutrient loadings from sediments.

Figure 26. Predicted epilimnetic dissolved oxygen in Lake Onondaga with and without METRO sewage effluent.

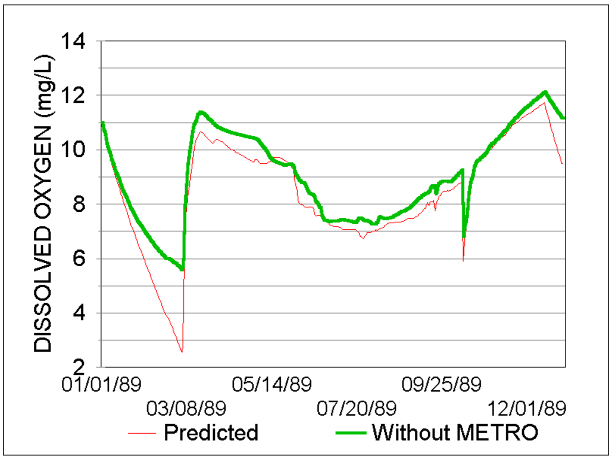


Figure 27. Predicted hypolimnetic dissolved oxygen in Lake Onondaga with and without METRO sewage effluent.

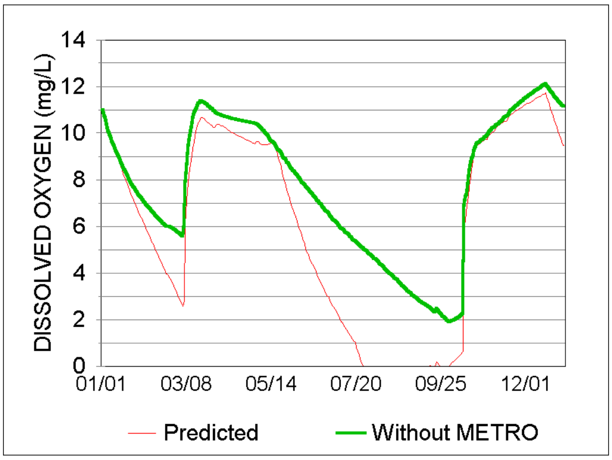
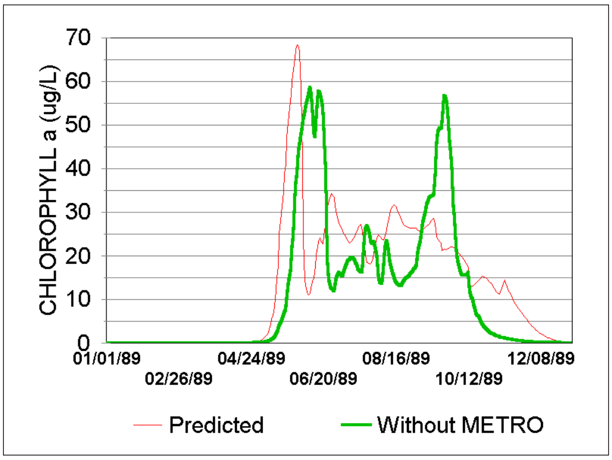


Figure 28. Predicted chlorophyll in Lake Onondaga with and without METRO sewage effluent.



The model seemed to be sensitive to zoobenthic feeding, so sensitivity analysis was performed. The maximum consumption rate for *Tubifex tubifex* was calibrated at 0.25 g/g·d for the third-level analysis, reflecting the interference of low oxygen levels with feeding behavior. For the sensitivity analysis, that value was taken as the mean for a normal distribution with a standard deviation of 0.1 and was used in a Latin hypercube sampling with ten iterations. The parameter values spanned a range from no feeding, and therefore limited sediment-water interaction, to doubled feeding rates with accelerated sediment-water interaction. The results demonstrate the influence that simulated feeding has on utilization and mobilization of detrital sediments and subsequently on the predicted hypolimnetic anoxia (**Figure 29**). Given the pool of nutrients tied up in the bottom sediments, the potential for release, and the annual overturn that mixes hypolimnetic and epilimnetic water, it is not surprising that increased recycling affects all the ecosystem; this includes epilimnetic nutrients (**Figure 30**), cryptomonad blooms (**Figure 31**), and epilimnetic dissolved oxygen (**Figure 32**).

Figure 29. Sensitivity of hypolimnetic dissolved oxygen to zoobenthic feeding in AQUATOX.

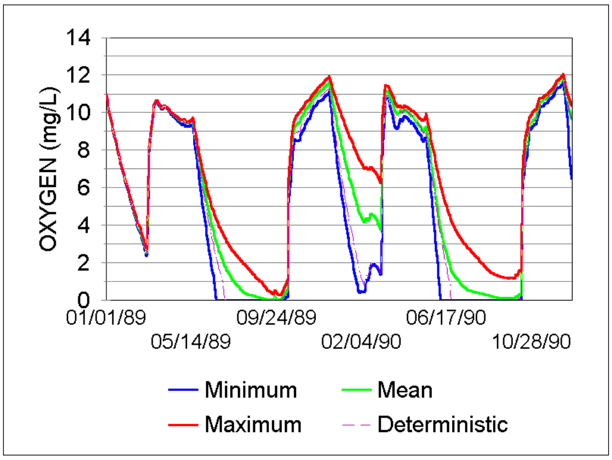


Figure 30. Sensitivity of epilimnetic phosphate to zoobenthic feeding in AQUATOX.

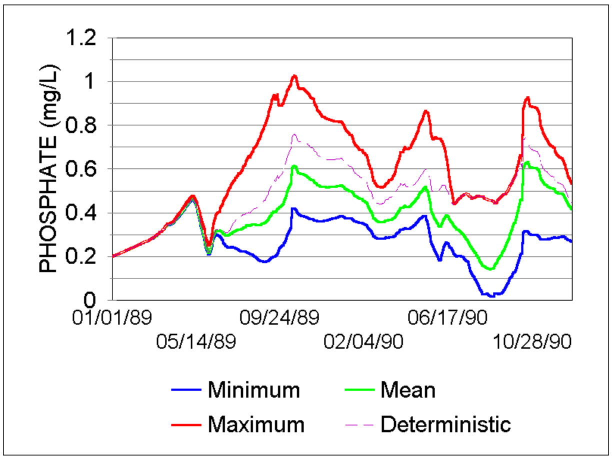


Figure 31. Sensitivity of cryptomonad blooms to zoobenthic feeding in AQUATOX.

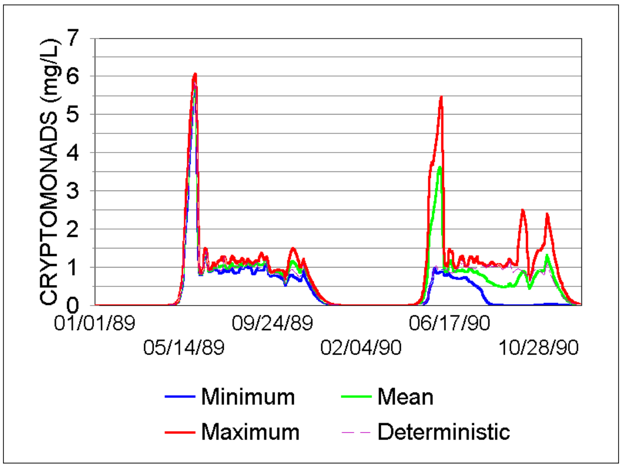
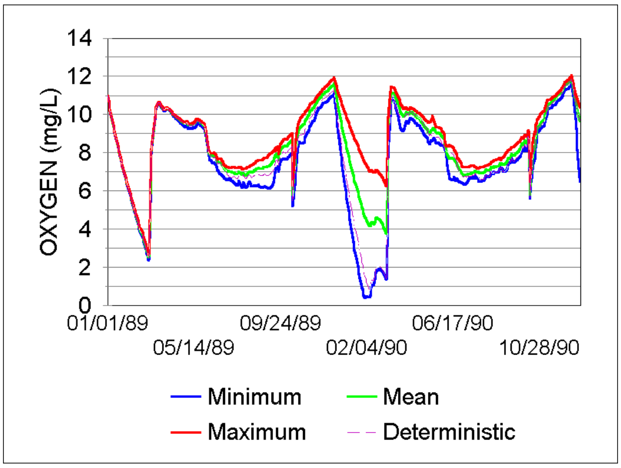


Figure 32. Sensitivity of epilimnetic oxygen to zoobenthic feeding in AQUATOX.



Conclusions

AQUATOX is seen to be a powerful tool for assessing eutrophication problems. It can be applied as a screening-level model with readily available data; it can import time series data for more detailed analyses; and it can be calibrated to represent site-specific conditions. These approaches are illustrated by increasingly detailed applications to Lake Onondaga, New York, a heavily polluted lake affected by both municipal sewage effluent and urban runoff. Paired control and perturbed simulations provide insights and estimates of impacts suitable for quantitative risk assessment and environmental decision making. Uncertainty analysis with efficient Latin hypercube sampling can be used to assess sources of uncertainty, including sensitivity to key parameters.

References

Collins, Carol D., and Wlosinski, Joseph H. 1983. *Coefficients for Use in the U.S. Army Corps of Engineers Reservoir Model, CE-QUAL-R1.* Vicksburg, Miss.: Environmental Laboratory, U.S. Army Engineer Waterways Experiment Station, 120 pp.

Effler, Steven W. 1996. *Limnological and Engineering Analysis of a Polluted Urban Lake.* New York: Springer-Verlag, 832 pp.