Draft Submitted for Publication in the Proceedings of the
6th International Estuarine and Coastal Modeling Conference

Calibration Performance of a Two-Dimensional, Laterally-Averaged Eutrophication Model of a Partially Mixed Estuary

James D. Bowen[1], A.M. ASCE

Abstract

Eutrophication modeling of the estuarine portion of the Neuse River, North Carolina was conducted to predict the water quality improvement associated with a 30 percent nutrient loading reduction to the estuary. An existing two-dimensional, laterally-averaged model (CE-QUAL-W2) was applied to predict water quality conditions in the lower 80-km of the estuary. During model calibration it was found that the extent to which the model explained observed variability in water quality parameters varied widely. Correlation coefficients between model predictions and observations were 0.93 for salinity, 0.77 for nitrite+nitrate, and 0.69 for dissolved oxygen, but only 0.25 for chlorophyll-a. The relatively poor chlorophyll-a calibration performance was ascribed to the model's inaccuracy in predicting the timing and location of algal blooms. Good agreement was observed, however, between cumulative frequency distributions of chlorophyll-a observations and predictions. Predicted cumulative frequency distributions of chlorophyll-a concentrations matched observations to within a factor of two for frequencies between 0.01 and 0.99, although the maximum observed values were much higher than model predicted maximums. These peak chlorophyll values are of particular concern to the regulatory community as they result in water quality standard violations. A sensitivity analysis, performed to explore the model's capability to predict these highest concentrations, indicated that changes in algal growth parameters alone would not increase predicted maximum concentrations to observed values. It appears from model results that residence time is an important factor in limiting the maximum predicted chlorophyll-a concentrations.

Introduction

North Carolina's Neuse River Estuary has experienced the adverse effects of nutrient enrichment for decades. It is widely believed, however, that these problems

---

[1] Assistant Professor, Department of Engineering Technology, University of North Carolina at Charlotte, Charlotte NC 28223 (704) 547-3130

have worsened lately as a result of increases in human and livestock population and agricultural activity in the watershed. In an attempt to reverse the ecological and water quality trends, the State of North Carolina has drafted regulations aimed at reducing nitrogen loading to the estuary by 30 percent. The State has also funded water quality modeling and monitoring research to investigate the relationship between nutrient loading and estuarine water quality. As part of this effort, eutrophication modeling of the estuary is being performed. In this article we report on some aspects of the models's ability to simulate observed spatial and temporal distributions of key water quality parameters.

Previous studies of water quality in the Neuse River estuary have largely been observational. Long-term monitoring studies have shown that nutrient concentrations generally decrease downstream, although at different rates, such that the time-averaged N:P ratio decreases downstream (Christian et al., 1991; Paerl et al., 1995). Nitrate concentrations in the upper estuary are generally more than an order of magnitude higher than the lower estuary. Temporal variability in both nutrient concentrations, chlorophyll-a concentrations, and primary productivity are significant, with variations occurring both seasonally and associated with loading events from high river flows (Rudek et al., 1991; Boyer et al., 1993; Mallin et al. 1993; Paerl et al., 1995). The monitoring data suggests that limitation of phytoplankton productivity may result from low temperature, light, or nutrients at certain times and places within the estuary, and that accumulation of chlorophyll biomass is also affected greatly by changing water residence times.

The Neuse Estuary is considered to be a hyper-eutrophic estuary, and has experienced serious blue-green algae blooms in the oligohaline portion of the estuary since at least the 1970's (Hobbie and Smith, 1975; Paerl, 1987). Unfortunately, these problems seem to have spread and intensified in the last few years. In 1995, heavy summer rains followed by a prolonged period of density stratification lead to summer widespread algal blooms and anoxia (defined here as DO concentration < 2 mg/l), and massive fish kills (Paerl and Pinckney, 1996). An outbreak of the toxic algae *Pfiesteria piscicida* (Burkholder et al., 1995) also occurred, and was considered to be the cause of many of the fish deaths. A similar scenario occurred in 1996, after the passage of Hurricane Fran. Anoxia and fish kills occurred along the entire estuary. A smaller, although significant fish kill occurred in the middle estuary in late July, 1998 (Leuttich et al., in press).

Nutrient bioassays have suggested that a 30% reduction in nutrient loading might be sufficient to produce a noticeable decrease in algal productivity (Paerl, 1987). Based upon this work and additional expert assessment, the state adopted the 30% nutrient reduction level as the initial goal of its management strategy for the Neuse River. The state's management strategy also includes, however, an effort to develop and calibrate a eutrophication model of the Neuse Estuary, and revise the 30% reduction target, if warranted. The ultimate objective of this modeling study is to determine the water quality consequences of nutrient loading reduction. Of particular interest is the estuary's predicted response to a load reduction of 30%. Two previous transport model studies have been completed for the Neuse River Estuary. Lung (1988) used WASP to investigate the factors related to blue-algal blooms. Robbins and Bales (1995) used a two-dimensional, vertically-averaged circulation and transport This model predicted that lateral variations in longitudinal water velocities could be significant during certain forcing conditions within the estuary.

In this article we report on the calibration performance of a two-dimensional laterally-averaged model of the Neuse River Estuary. This model has been previously calibrated to data from 1991 that had extensive hydrodynamic information, but very limited water quality information (Bowen and Hieronymus, in press). Here we make use of the extensive hydrodynamic and water quality monitoring data on the Neuse Estuary now being collected (Luettich et al., in press). These data allow us to look carefully at the degree to which the model simulates observed spatial and temporal distributions of nutrients, dissolved oxygen, and chlorophyll-a. Through this analysis we are able to assess, to some extent, the utility of the model with regard to environmental management of the Neuse Estuary.

Description of the Study Site

North Carolina's Neuse River drains approximately 16,000 km^2, and empties into the southwestern corner of the Pamlico Sound. In the river's headwaters is the Raleigh-Durham metropolitan area, with nearly a million inhabitants. Approximately 1.5 million people live in the entire river basin. The lower basin is used intensively for agricultural and livestock production. The estuary occupies the lower 80 km of the river (Figure 1). It is broad and shallow, with average depths ranging from approximately 4 m near New Bern to 6 m at the mouth.

Surface water loadings to the estuary come from two rivers and nine creeks, as well from direct runoff and precipitation. Three of these water bodies (Neuse River, Trent River, Swift Creek) account for more than 90% of the total watershed area (Bales and Robbins, 1999). None of the remaining creeks has a watershed area more than 1.1% of the total. Direct runoff to the estuary accounts for 3.9% of the watershed area.

For the purposes of this study, the Neuse River Estuary between Streets Ferry and Oriental can be divided into three sections, as was done in studies of benthic nutrient and dissolved fluxes (NC DWQ, 1998). The upper estuary, from Streets Ferry to just upstream of Upper Broad Creek, is oligohaline. Velocities and salinities in this section are strongly affected by riverine flushing (Giese et al., 1985). The upper estuary is considered eutrophic and has experienced numerous blooms of blue-green algae (Hobbie and Smith, 1975; Paerl, 1987).

The middle estuary is much wider and generally shallower than the upper estuary. It runs southwesterly to Cherry Point, where the estuary makes a perpendicular bend to the northeast. Cherry Point is considered the downstream extent of the middle estuary.

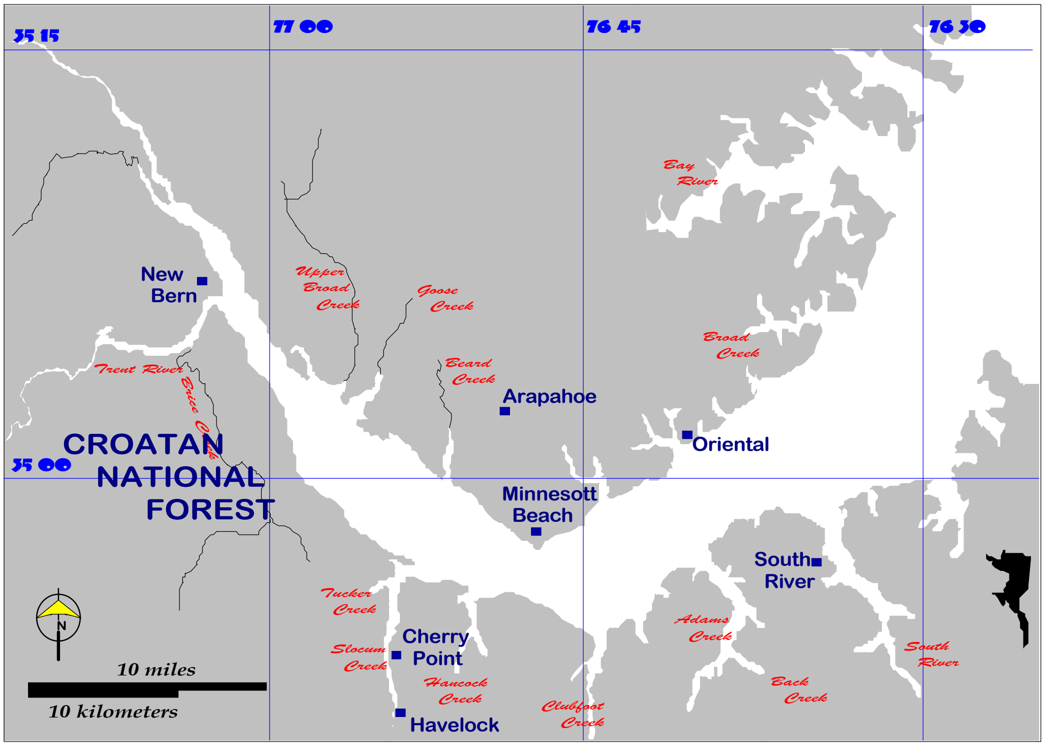

Figure 1. Neuse River Estuary, North Carolina

The lower estuary is generally wider and deeper than the other sections. The middle and lower estuary reaches are considered to be mesohaline and mesotrophic. Recently dinoflagellate blooms have plagued these sections of the estuary (Rudek et al., 1991; Mallin and Paerl, 1994).

Methods and Procedures

The Neuse River Estuary is a relatively long, narrow, partially-mixed estuary. Significant longitudinal and vertical variations in water quality conditions have been observed (e.g. Christian et al. 1991). For these reasons, the two-dimensional, laterally-averaged water quality model CE-QUAL-W2 (W2) was chosen for application to the Neuse River Estuary (Cole and Buchak 1995).

W2 is a coupled hydrodynamic/water quality model. Its water quality algorithms incorporate 23 constituents (W2 Version 3), 18 of which are used in this application. These 18 constituents are linked to one another to simulate: 1) phytoplankton uptake and release of nutrients and CO_2 through photosynthesis and respiration; 2) remineralization of carbon and nutrients through phytoplankton mortality, exudation, and water column respiration; 3) consumption and production, and transport of dissolved oxygen through respiration, reaeration, and photosynthesis; and 4) recycling of nutrients and consumption of DO through sediment diagenesis.

In this application of W2, certain modifications were made to the standard water quality routines. First of all, three separate algal groups were used: 1) dinoflagellates and diatoms, 2) chlorophytes and cryptophytes, and 3) blue-green algae. The sediment diagenesis model was also modified to include both labile and refractory organic matter state variable, as well as an aqueous sediment oxygen demand (i.e., sulfide) state variable.

A nineteen month period in 1997 and 1998 was simulated using the model (Table 2). Model boundary conditions were developed using data from the U.S. Geological Survey (river flows, Neuse River bathymetry), the North Carolina Division of Water Quality (water quality of Neuse and Trent Rivers, wastewater treatment plant loadings, the U.S. Weather Service (meteorologic forcings at Cherry Point Naval Air Station), and the UNC Institute of Marine Sciences (elevation, water quality). Model spatial resolution (Table 2) was established by comparing results of salinity simulations for various numbers of Neuse River model segments ranging from 35 to 140 (Bowen and Hieronymus, in press). Temporal resolution was set according the model's auto time-stepping routines.

The two years simulated, 1997 and 1998, were very different hydrologically.. All seven months in 1997 (May - December) had Neuse River flows below the monthly average. Two relatively high-flow events, which occurred in early June and early August, brought the flow only up to the average monthly values. In contrast, 1998 was an exceedingly wet year. Springtime flows were significantly above average. Runoff decreased markedly after April, and the remainder of 1998 was characterized by streamflows below monthly averages.

Table 1. Model Application Summary

Characteristic	Value
Modeled Region	Streets Ferry - Oriental, North Carolina
Model Time Period	June 1, 1997 - December 31, 1998
Horizontal Grid Resolution	62 segments, length approx. 1 km.
Vertical Grid Resolution	18 layers, 0.5 m thick
Temporal Resolution	approx. 6 min.
Temporal Resolution - upstream flow boundary conditions	daily flows and nutrient concentrations, hourly temperatures, weekly data for other water quality constituents
Temporal Resolution - downstream elevation boundary conditions	water levels every 15 min., water quality profiles bi-weekly
Meteorologic Forcing Data	hourly air and dewpoint temperatures, hourly cloud cover, and wind speed and direction, daily precipitation

Calibration of the model was performed first on the hydrodynamic aspects of the model and then on water quality. Parameters adjusted during hydrodynamic calibration included the maximum and minimum eddy viscosities and diffusivities, and horizontal momentum and mass dispersion coefficients. Water quality calibration focused on specification of the algal growth parameters that quantify nutrient, temperature, and light limited growth rates. Calibration of dissolved oxygen is ongoing at this time, and will not be discussed.

Results

The relatively dry conditions in the Summer of 1997 and the very wet conditions in early 1998 produced significant salinity variations in the normally mesohaline middle portion of the Neuse Estuary. Summer salinities in the bottom waters near Cherry Point went as high as 17 PSU (Figure 2). By March of 1998 salinities dropped to less than 4 PSU, and did not recover to the values of the previous summer until very late in the year. Top to bottom differences in salinity were quite variable. These patterns were also seen

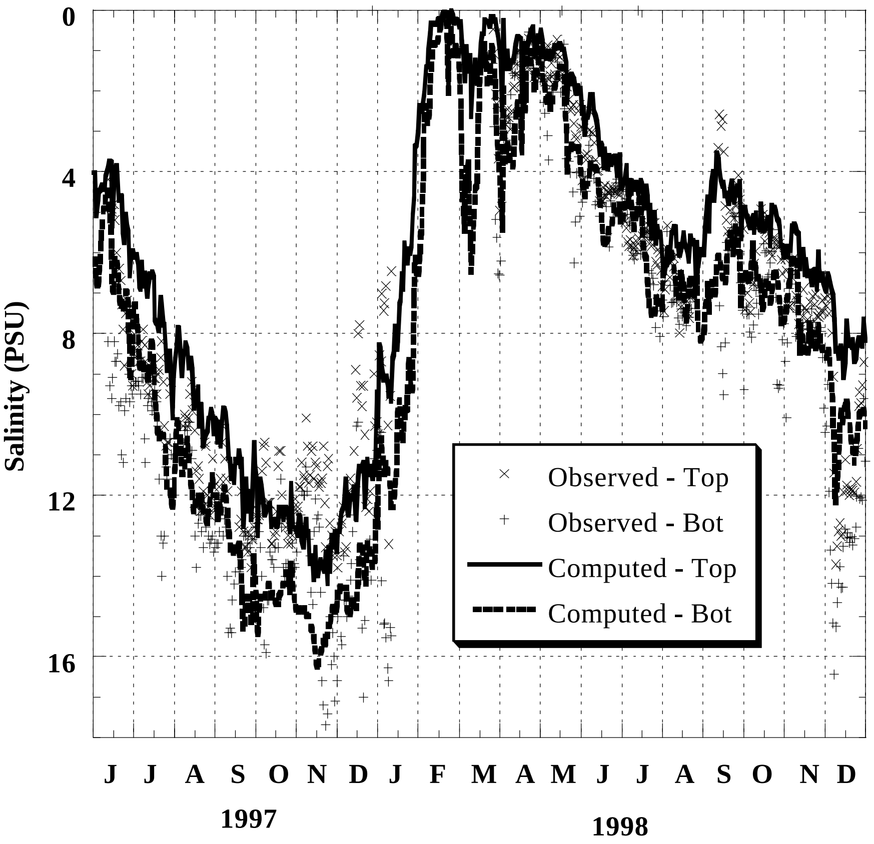

Figure 2. Observed (symbols) and Predicted (lines) Salinities in the Neuse River Estuary at Cherry Point, North Carolina.

in the model predictions (Figure 2), although the model generally seems less dynamic with regard to stratification as compared with the observed data. Observed chlorophyll-a concentrations in the surface waters of the Neuse Estuary were also quite variable spatially and temporally. Over the nineteen month time period simulated (June ‘97 - December ‘98), concentrations above the water quality standard value of 40 µg/l were observed in April, June, and August of 1998 in the middle and lower estuary (Figure 3). In 1997, the summertime peak chlorophyll concentrations were generally lower and were

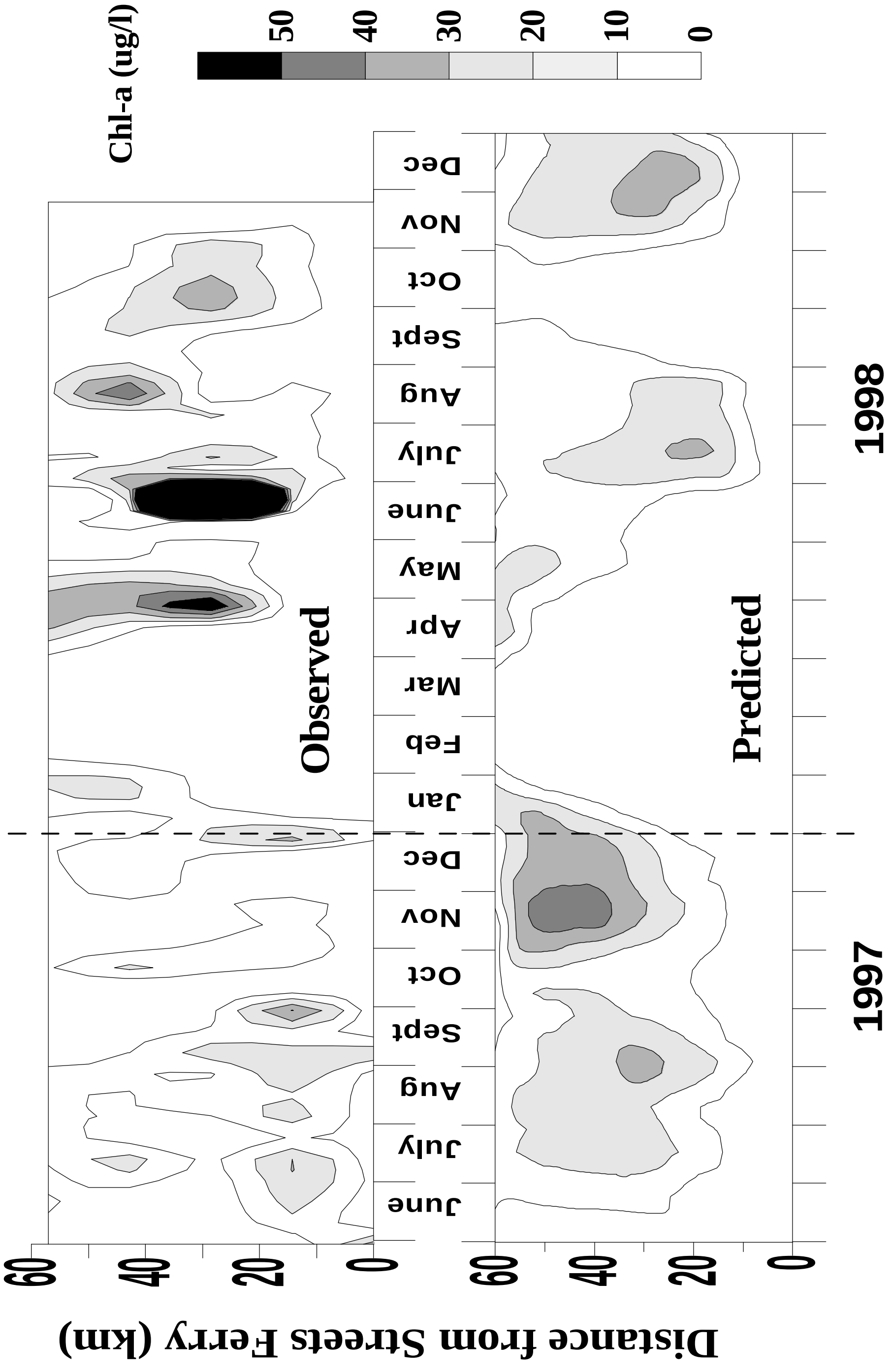

Figure 3. Observed and Predicted Surface Chlorophyll-a Concentrations in the Neuse River Estuary

located farther upstream. Late in 1997, chlorophyll-a concentrations increase in the lower estuary until the high flows of early 1998 lower residence time sufficiently to limit phytoplankton accumulation (Figure 3), even though nitrate concentrations at this time are very high throughout the estuary (Leuttich et al., in press). Predicted chlorophyll-a concentrations show this same seasonal pattern (Figure 3). Comparisons of chlorophyll-a model predictions against observations at a single location indicate that although the model predicts the overall seasonality of the chlorophyll-a distributions reasonably well, it generally misses the timing of the peak by at least a month (Figure 3, Figure 4).

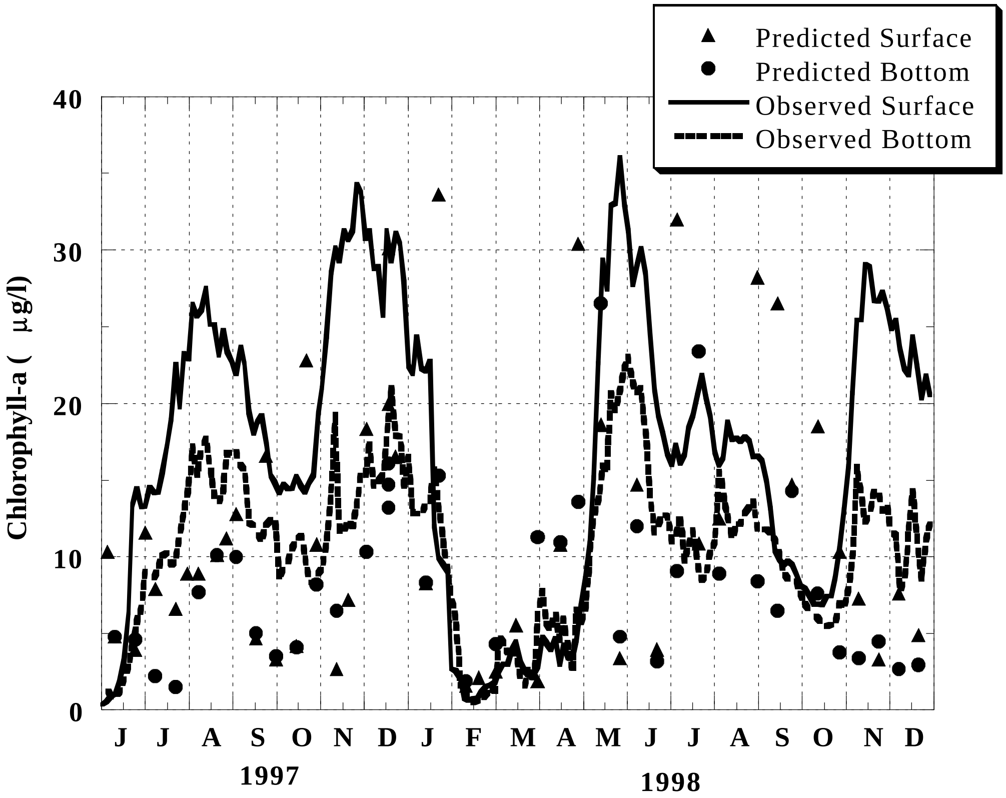

Figure 4. Observed (symbols) and Predicted (lines) Chorophyll-a Concentrations in the Neuse River Estuary near Cherry Point, North Carolina

Quantitative comparisons between observed and predicted concentrations indicate that the degree of model fit varies widely between key water quality parameters. Correlation r^2 values ranged from a high of 86.5% for salinity to a low of 6.6% for chlorophyll-a (Table 2). These values correspond to correlation coefficients of 0.93 for salinity, 0.77 for nitrite-nitrate, 0.69 for dissolved oxygen, and 0.25 for chlorophyll-a. Other quantitative calibration measures followed a similar pattern, with salinity predictions showing the smallest errors, chlorophyll-a the highest, and dissolved oxygen and nitrate-nitrite falling somewhere in between (Table 2).

Table 2. Summary of Model Calibration Performance

Calibration Statistic	Constituent			
	Salinity (PSU)	**Nitrite-Nitrate (mg/l)**	**Dissolved Oxygen (mg/l)**	**Chl-a (µg/l)**
Mean Error (P - O)	-0.86	0.15	-1.00	0.26
Root Mean Square Error	2.08	0.24	2.53	12.42
Mean Absolute Error	1.36	0.17	1.75	6.60
Normalized Mean Absolute Error (%)	28.7	63.0	24.7	84.3
Correlation r^2 (%)	86.5	59.7	48.0	6.6

From a regulatory perspective, the ability of the model to predict the timing and location of extreme values is less important than the ability to properly capture the statistical distribution of observed values. Chlorophyll-a cumulative frequency distributions for model predictions and observations were compared to examine the model's performance in this regard. Over nearly the entire range of cumulative frequencies, the model predictions agreed with the observations to within a factor of two (Figure 5). The model generally under predicted concentrations in the lower cumulative frequency range and over predicted concentrations in the upper frequency range, but it was only the most infrequent, bloom events that were badly under predicted by the model. For these cases, having probabilities of less than 1% (cumulative frequencies greater than 99%) the model predictions leveled off at approximately 45 µg/l while the observations continued increasing with decreasing probability to well over 100 µg/l (Figure 5).

Discussion

While the water quality model's predicted chlorophyll-a frequency distribution matched the observations over much of the frequency range, it badly under predicted the peak chlorophyll-a concentrations. Furthermore, the shape of two distributions was distinctly different. The observed frequency distribution looked approximately log-normal (linear distribution when plotted log-c vs. normal probability), while the model predictions had a distinct upper bound (Figure 5). Clearly some of this difference could

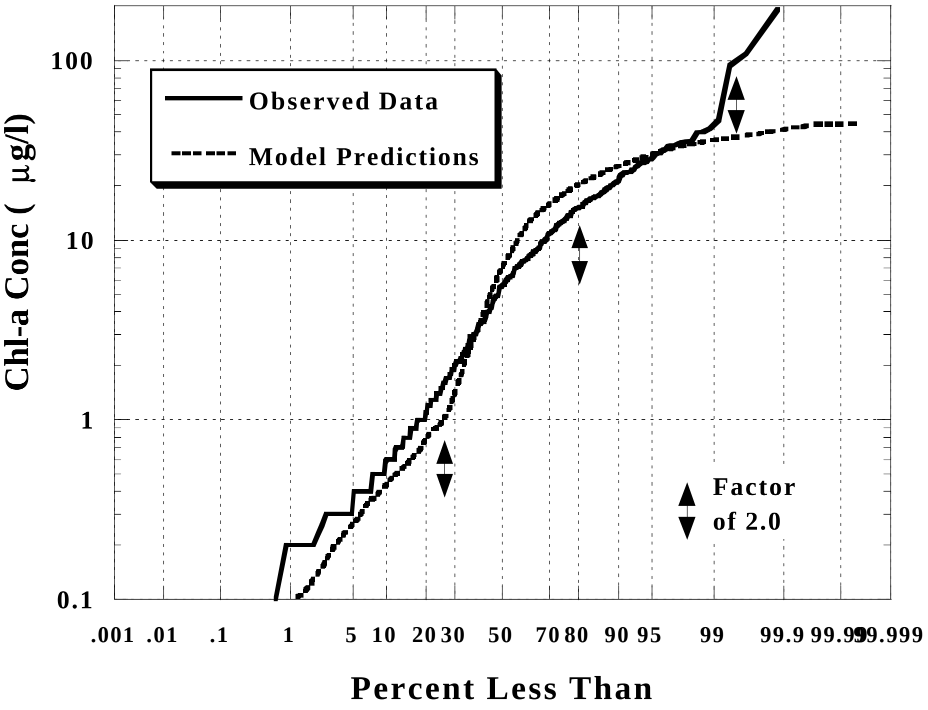

Figure 5. Cumulative Frequency Distributions of Predicted and Observed Chlorophyll-a Concentrations in the Neuse River Estuary from June 1, 1997 through December 31, 1998

be attributed to differences in the intrinsic spatial averaging of model predictions versus the observed data. The observations are grab samples of approximately one liter, while

the model's predictions can be considered averages over the much larger segment volumes. Nonetheless, the comparison raises the following question: Could the model's peak chlorophyll-a predictions be increased by varying the existing algal growth rate parameters in the model? A numerical experiment was conducted to investigate this question.

A sensitivity analysis was performed to see how model predictions of peak chlorophyll-a concentrations would be increased by changes in algal growth rate parameters. A related question of interest was how the changes in growth parameters might change the shape of the cumulative frequency distributions. Four additional model runs were conducted, each using an alternate set of algal growth parameters designed to increase algal growth rate or decrease algal losses from the water column. In each case, parameters were varied by a similar amount (50%), and all three algal groups (diatoms and dinoflagellates, chlorophytes and cryptophytes, blue-green algae) were changed in a like manner. Algal growth was quickened by: 1) increasing the maximum, unlimited growth rate, 2) decreasing the nitrogen half-saturation constant for growth, and 3) decreasing the light requirement for growth. In a fourth case, algal water column losses were decreased by lowering the algal settling velocity.

Only one of the four cases, when tested against the earlier base case model prediction and the observed data, had a significantly higher predicted peak chlorophyll-a concentration. Increasing the maximum, unlimited growth rate increased the peak value from about 45 µg/l to just over 50 µg/l (Figure 6). The other three test cases did not increase the peak predicted chlorophyll concentration at all, although there were some minor increases in concentrations at lower cumulative frequencies. Of these test cases, the lower light requirement case seemed to have the largest impact (Figure 6). In addition, the shape of the predicted frequency distribution was identical in every model test case. As before, each model run was characterized by a concave downward frequency distribution, whereas the data appeared to be log-normally distributed (Figure 6).

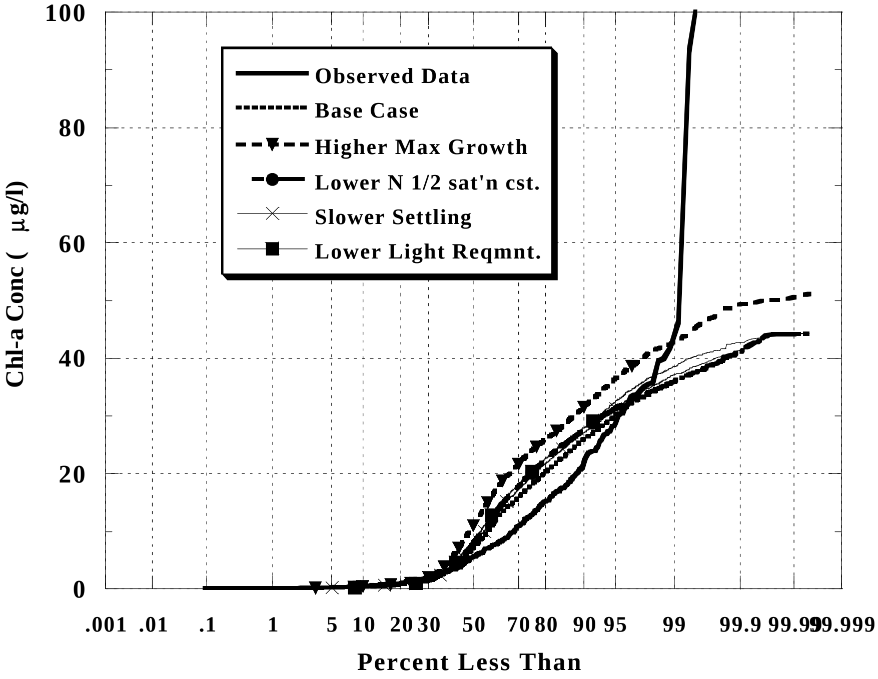

Figure 6. Cumulative Frequency Distributions of Observed Chlorophyll-a Concentrations and Predicted Concentrations for Five Model Runs with Various Algal Growth Parameterizations.

The fact that the only way to increase predicted chlorophyll-a maximum was to increase maximum growth rate suggests that limitation of biomass accumulation is controlled by factors other than light and nutrient availability or settling. This is reasonable in instances where blooms occur during periods of high nutrients, temperature, and light, such as in the upper estuary in Spring and Summer. In this case, peak concentrations are probably mostly dependent on water residence time, rather than growth limitation. Blooms that occur in Fall and Winter in the lower estuary may be more dependent on light, nutrients, and temperature limitation, but these blooms generally don't reach concentrations as high as those in Spring and Summer up-estuary.

The concave downward cumulative frequency distribution is a persistent feature of these and other eutrophication model predictions of chlorophyll-a concentrations (e.g. Hydroqual and Normandeau 1995). Whether this is due to the inherent spatial averaging of these models is unclear at this time. If so, then spatial averaging of the observed data set might be warranted. On the other hand, since eutrophication models are often used in a regulatory context, it may be inadvisable to spatially average monitoring data if this averaging would not be done when determining compliance to water quality standards. In either case, the discrepancy between the observed and predicted distributions is an important issue with regard to the calibration and use of eutrophication models, and justifies further research.

Conclusions

We conclude from this investigation that eutrophication model calibration performance can be a mixed bag. Prediction of the time and place of algal blooms is problematic. Predictions of typical concentrations and seasonality of response match observed patterns quite well. Prediction of the magnitude of blooms fails for only the rarest of events, but for these cases, model underpredictions can be severe. Because of the wide variations in model skill, use of these models for environmental management should be accomplished in a thoughtful and selective fashion.

References

Bales, J.D. and Robbins, J.C. 1999. A dynamic water-quality modeling framework for the Neuse River Estuary, North Carolina. U.S. Geological Survey, Water-Resources Investigations Report 99-4017.

Bowen, J. D., and Hieronymus, J. In press. The Neuse River Estuary's response to reduced nutrient loading: Predictions and an uncertainty analysis using a mechanistic eutrophication model. UNC Water Resources Research Institute Technical Report Series, N. C. State Univ., Raleigh, NC.

Boyer, J.N., Christian, R.R., and Stanley, D.W. 1993. Patterns of phytoplankton primary productivity in the Neuse River estuary, North Carolina, USA. *Mar. Ecol. Prog. Ser.*, 97, pp. 287-297.

Burkholder, J.M., Hobbs, C.W., and Glasgow, H.B. Jr. 1995. Distribution and environmental conditions for fish kills linked to a toxic ambush-predator dinoflagellate. *Mar. Ecol. Prog. Ser.* 124, pp. 43 -61.

Christian, R.R., Boyer, J.N., and Stanley, D.W. 1991. Multi-year distribution patterns of nutrients within the Neuse River Estuary, North Carolina. *Mar. Ecol. Prog. Ser.*, 71, pp. 259-274.

Cole, T.M., and Buchak, E.M. 1995. *CE-QUAL-W2: A two-dimensional, laterally averaged hydrodynamic and water quality model, version 2.0, Draft User Manual*. Instruction Report EL-95-1, Waterways Experiment Station, Vicksburg, MS.

Giese, G.L, Wilder, H.B., and Parker, G.G. Jr. 1985. Hydrology of major estuaries and sounds of North Carolina. U.S.G.S. water-supply paper 2221, 105 pp.

Hobbie, J.E., and Smith, N.W. 1975. Nutrients in the Neuse River Estuary. University of North Carolina Sea Grant Program. Report UNC-SG-75-21. Raleigh, NC. 183 pp.

Hydroqual and Normandeau. 1995. *A water quality model for Massachusetts and Cape Cod Bays: Calibration of the Bays Eutrophication Model (BEM*. MWRA Enviro. Quality Dept. Tech. Rpt. Series No. 95-8. Massachusetts Water Resources Authority, Boston, MA., 402 pp.

Luettich, R.A. Jr., McNinch, J.E., Pinckney, J.L. Alperin, M., Martens, C.S., Paerl, H.W., Peterson, C.H., and Wells, J.T. In press. Neuse River Estuary MODeling and MONitoring Project: Monitoring Phase - 12/31/98. UNC Water Resources Research Institute Technical Report Series, N. C. State Univ., Raleigh, NC.

Lung, W.S. 1988. The role of estuarine modeling in nutrient control. *Water Sci. and Technol.*, 20(6/7), pp. 243-252.

Mallin, M.A., and Paerl, H.W. 1994. Planktonic trophic transfer in an estuary: Seasonal, diel, and community structure effects. *Ecology*, 75(8), pp. 2168-2184.

North Carolina Division of Water Quality (NC DWQ), Water Quality Section, Environmental Sciences Branch. 1998. Neuse River Internal Nutrient Loading Studies, 1996-1997. Internal Report, North Carolina Division of Water Quality, Raleigh, NC, 50 pp.

Paerl, H.W. 1987. Dynamics of blue-green algal blooms in the lower Neuse river, NC: Causative factors and potential controls. Report No. 229, Water Resources Research Institute, UNC, Raleigh, NC.

Paerl, H.W., Mallin, M.A., Donahue, C.A., Go, M., and Peirls, B.L. 1995. Nitrogen loading sources and eutrophication of the Neuse River estuary, North Carolina: direct and indirect roles of atmospheric deposition. Report No. 291, UNC Water Resources Research Institute, N. C. State Univ., Raleigh, NC.

Paerl, H.W., and Pinckney, J.W. 1996. Hypoxia, anoxia and fish kills in relation to nutrient loading in the Neuse River estuary: Why was 1995 a "bad" year? *Water Wise*, 4(2), May 1996. UNC Sea Grant Program, Raleigh, NC.

Robbins, J.C., and Bales, J.D. 1995. Simulation of hydrodynamics and solute transport in the Neuse River estuary, North Carolina. U.S. Geological Survey Open-File Report 94-511, Raleigh, NC. 85 pp.

Rudek, J., Paerl, H.W., Mallin, M.A., and Bates, P.W. 1991. Seasonal and hydrological control of phytoplankton nutrient limitation in the lower Neuse River Estuary. *Mar. Ecol. Prog. Ser.*, 75, pp. 133-142.