TENNESSEE VALLEY AUTHORITY

Resource Development
River Basin Operations
Water Resources

APPROACHES TO VERIFICATION
OF TWO-DIMENSIONAL WATER QUALITY MODELS

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TVA/WR/WQ--90/26

Chattanooga, Tennessee

November 1990

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CONTENTS

	Page
Tables.....	iv
Figures.....	v
Acknowledgements.....	viii
Executive Summary.....	xi
Introduction.....	1
Background.....	4
Statistical Tests for Model Verification.....	7
Verification of the BETTER Model.....	12
Conclusions.....	29
References.....	31
Appendix.....	33

Tables

Number	Page
1. Water Quality Sampling Variables, Locations, and Dates of Collection in Chickamauga Reservoir.....	17
2. Descriptive Statistics for Mean Residuals.....	21
3. Descriptive Statistics for Mean Relative Percent Error...	23
4. Descriptive Statistics for Standard Error of the Residuals.....	24
5. Descriptive Statistics for 95% Confidence Limit of the Residuals.....	25
6. Descriptive Statistics for Correlation Coefficient.....	27
7. Descriptive Statistics for Reliability Index.....	28

Figures

Number	Page
1. Possible Cases in Regression between Calculated and Observed Values.....	11
2. Map of Chickamaga Reservoir.....	13
3. Final Calibration using 1987 Observed Dissolved Oxygen Concentrations.....	15
4. Qualitative Verification using 1988 Observed Dissolved Oxygen Concentrations.....	16
5. Representation of Modeled Geometry for Chickamauga Reservoir at a 682 ft elevation and 1989 Sampling Locations.....	19
A1. Isopleths of the Mean Residuals for Temperature.....	34
A2. Isopleths of the Mean Relative Error for Temperature....	35
A3. Isopleths of the Standard Error for Temperature.....	36
A4. Isopleths of the 95% Confidence Limit for Temperature...	37
A5. Isopleths of the Correlation Coefficient for Temperature.....	38
A6. Isopleths of the Reliability Index for Temperature.....	39
A7. Isopleths of the Mean Residuals for Dissolved Oxygen....	40
A8. Isopleths of the Mean Relative Error for Dissolved Oxygen.....	41
A9. Isopleths of the Standard Error for Dissolved Oxygen....	42
A10. Isopleths of the 95% Confidence Limit for Dissolved Oxygen.....	43
A11. Isopleths of the Correlation Coefficient for Dissolved Oxygen.....	44
A12. Isopleths of the Reliability Index for Dissolved Oxygen.....	45
A13. Isopleths of the Mean Residuals for pH.....	46
A14. Isopleths of the Mean Relative Error for pH.....	47

A15.	Isopleths of the Standard Error for pH.....	48
A16.	Isopleths of the 95% Confidence Limit for pH.....	49
A17.	Isopleths of the Correlation Coefficient for pH.....	50
A18.	Isopleths of the Reliability Index for pH.....	51
A19.	Isopleths of the Mean Residuals for 5-day BOD.....	52
A20.	Isopleths of the Mean Relative Error for 5-day BOD.....	53
A21.	Isopleths of the Standard Error for 5-day BOD.....	54
A22.	Isopleths of the 95% Confidence Limit for 5-day BOD.....	55
A23.	Isopleths of the Correlation Coefficient for 5-day BOD..	56
A24.	Isopleths of the Reliability Index for 5-day BOD.....	57
A25.	Isopleths of the Mean Residuals for Total Organic Carbon.....	58
A26.	Isopleths of the Mean Relative Error for Total Organic Carbon.....	59
A27.	Isopleths of the Standard Error for Total Organic Carbon.....	60
A28.	Isopleths of the 95% Confidence Limit for Total Organic Carbon.....	61
A29.	Isopleths of the Correlation Coefficient for Total Organic Carbon.....	62
A30.	Isopleths of the Reliability Index for Total Organic Carbon.....	63
A31.	Isopleths of the Mean Residuals for Alkalinity.....	64
A32.	Isopleths of the Mean Relative Error for Alkalinity.....	65
A33.	Isopleths of the Standard Error for Alkalinity.....	66
A34.	Isopleths of the 95% Confidence Limit for Alkalinity....	67
A35.	Isopleths of the Correlation Coefficient for Alkalinity.....	68
A36.	Isopleths of the Reliability Index for Alkalinity.....	69
A37.	Isopleths of the Mean Residuals for Suspended Solids....	70

A38.	Isopleths of the Mean Relative Error for Suspended Solids.....	71
A39.	Isopleths of the Standard Error for Suspended Solids....	72
A40.	Isopleths of the 95% Confidence Limit for Suspended Solids.....	73
A41.	Isopleths of the Correlation Coefficient for Suspended Solids.....	74
A42.	Isopleths of the Reliability Index for Suspended Solids.....	75
A43.	Isopleths of the Mean Residuals for Orthophosphate-P....	76
A44.	Isopleths of the Mean Relative Error for Orthophosphate-P.....	77
A45.	Isopleths of the Standard Error for Orthophosphate-P....	78
A46.	Isopleths of the 95% Confidence Limit for Orthophosphate-P.....	79
A47.	Isopleths of the Correlation Coefficient for Orthophosphate-P.....	80
A48.	Isopleths of the Reliability Index for Orthophosphate-P.....	81
A49.	Isopleths of the Mean Residuals for Ammonia-N.....	82
A50.	Isopleths of the Mean Relative Error for Ammonia-N.....	83
A51.	Isopleths of the Standard Error for Ammonia-N.....	84
A52.	Isopleths of the 95% Confidence Limit for Ammonia-N.....	85
A53.	Isopleths of the Correlation Coefficient for Ammonia-N.....	86
A54.	Isopleths of the Reliability Index for Ammonia-N.....	87
A55.	Isopleths of the Mean Residuals for Nitrate-N.....	88
A56.	Isopleths of the Mean Relative Error for Nitrate-N.....	89
A57.	Isopleths of the Standard Error for Nitrate-N.....	90
A58.	Isopleths of the 95% Confidence Limit for Nitrate-N.....	91
A59.	Isopleths of the Correlation Coefficient for Nitrate-N.....	92
A60.	Isopleths of the Reliability Index for Nitrate-N.....	93

ACKNOWLEDGEMENTS

The author is sincerely grateful to Ming C. Shiao who compiled the the necessary input data from 1989 and ran the simulation for the modeled data set used in this verification. The author is obliged to Neil E. Carriker for an excellent editorial review.

EXECUTIVE SUMMARY

The verification of a water quality model is the one procedure most needed by decision makers evaluating a model predictions, but is often not adequate or done at all. The results of a properly conducted verification provide the decision makers with an estimate of the uncertainty associated with model predictions. Several statistical tests are available for quantifying the performance of a model. Six methods of verification were evaluated using an application of the BETTER two-dimensional water quality model for Chickamauga reservoir. Model predictions for ten state variables were compared to observed conditions from 1989. Spatial distributions of the verification measures showed the model predictions were generally adequate, except at a few specific locations in the reservoir. The most useful statistics were the mean and standard error of the residuals. Quantifiable measures of model performance should be calculated during calibration and verification of future applications of the BETTER model.

INTRODUCTION

The use of mathematical models that conceptualize water quality processes and relationships in streams, lakes, and reservoirs has increased dramatically over the last two decades. The models are used to develop a better understanding of the system and its responses to external stimuli, and to provide guidance to resource managers for various decisions. Due to the inherent complexities of natural systems, estimates of parameters that reflect the characteristics of the particular systems under study must be incorporated into these models. In order for results of model simulations to be useful for decision making, some measure of prediction uncertainty must be defined.

Development of a water quality model for a specific system generally progresses through three separate levels of credibility. First, the model is initialized into an operational form by compiling the required input data into the appropriate format. Initial values for model parameters are estimated using professional judgement. Initialized models can be used to explore relative differences between model simulations, but provide a limited level of confidence in the absolute predictions. The second level of credibility is to calibrate the initialized model with actual measurements of state variables from the system. Values of model parameters are adjusted to reflect actual conditions of the system from the measured results. Calibrated Models can be used with more confidence in absolute predictions within the range of measured conditions. Finally, a level of uncertainty is defined for the model predictions from actual measurements independent of the calibration data. This evaluation is commonly called model verification.

Model verification has been the subject of much debate. The term "verify" suggests that all model predictions are accurate and precise to some predefined level of uncertainty. This implies that verification is the testing of a null hypothesis at a specified alpha level. In most applications, verification provides a statement that the model adequately describes observed system behavior so that it is acceptable for making predictions. Confirmation, validation, certification, and evaluation are other terms that have been used interchangeably with verification to describe this procedure.

Models can be verified by several means. Often, the degree of verification is limited to graphical inspections of model predictions against measured observations. In these cases, the verification measure is a qualitative statement that the model is sufficient or performs reasonably. Most evaluations of model performance do not answer the basic question often asked by the decision makers: "What is the level of confidence that can be placed on the results?". To address this question, various statistical tests can be applied as part of the verification procedure.

Two factors, increasingly complex models and resource management questions, make the verification of water quality models essential. Current water quality models simulate dynamic changes of numerous state variables of a system in two or three spatial dimensions. This complexity taxes the ability of the analyst to fully comprehend the model output. In addition, the management issues may be too complex to address completely with the particular models that are available. Most model predictions are typically deterministic: a single value is determined for each state variable at each location for every specified time interval. These

predictions usually are made to determine the effects of pollution abatement strategies which often involve considerable costs. The uncertainty of these model predictions must be considered, since decisions made from "wrong" answers can be costly, both economically and environmentally.

Over the past 10 years, the Tennessee Valley Authority (TVA) has developed a dynamic two-dimensional water quality reservoir model called BETTER (Box Exchange Temperature Transport Ecology Reservoir). The model simulates numerous physical and chemical state variables using a heuristic flow movement based on matching density layers. Applications of the BETTER model to TVA reservoirs have only been qualitatively verified. The objective of this report is to evaluate different statistical approaches of verification for use with dynamic two-dimensional models, including the BETTER model.

BACKGROUND

Since the earliest beginnings of water quality modeling the need for evaluating the credibility of the model has been recognized. The work of Streeter and Phelps (1925) provided both qualitative comparisons and quantitative evaluations (relative and root mean square error) between observed and theoretical calculations of dissolved oxygen. As computer simulations became more widely used in numerous disciplines, modelers raised many philosophical questions on the factual objectivity and testability of models (Naylor and Finger, 1967).

The terminology used to describe the process of establishing model credibility varies widely. Mihram (1973) proposed a distinction between "verification" (algorithm consistency) and "validation" (reflects system reality). Miller (1974) differentiated between "external validation" (compare observations with predictions) and "internal validation" (sensitivity analysis). External validation will always be limited to the range of conditions observed in the actual system. With sensitivity analysis, the actual uncertainties in the input data are estimated and combined to produce an estimate of model prediction uncertainty. Loehle (1983) classified models into logical, theoretical, and predictive types and showed that each model type required different techniques for evaluating performance. Reckhow and Chapra (1983) argued that the terms "verification" or "validation" imply a level of truth that is unattainable. These investigators assert that statistically significant tests for goodness-of-fit are at best "confirmation", which is not truth but a measured consistency with empirical evidence.

In 1980, the U.S. Environmental Protection Agency sponsored a workshop on verification of water quality models. Many of the presentations stressed the importance of model verification and several presented statistical verification methods (Hydroscience, 1980). However, no consensus on verification guidelines were produced from the group discussions. Leggett and Williams (1981) proposed a reliability index for model verification. Thomann (1982) discussed statistical and qualitative measures of verification and provided examples for dissolved oxygen and eutrophication models. Reckhow and Chapra (1983) provided a literature review of previous model verifications and described methods for verification of both deterministic and stochastic models. Wlosinski and Collins (1985) verified the one-dimensional CE-QUAL-R1 reservoir model for 20 state variables using a reliability index (Leggett and Williams, 1981). Reckhow et al. (1990) discussed the assumptions underlying statistical verification methods and provided both parametric and nonparametric examples.

Although there are many different methods for quantitatively assessing the credibility of water quality models, models usually are verified qualitatively by inspection of observed and simulated data. Due to the expense of collecting additional independent data for verification, models frequently are used for prediction simulations after calibration only. Many of the questions that are raised during decision-making can be addressed with quantitative measures of model credibility produced during verification. However, there are several potential drawbacks associated with quantifiable measures of model verification (Thomann, 1982):

1. A tendency may be created to "curve fit" the model to data to improve verification statistics.
2. Not all of the credibility of a model is embodied in verification statistics (i.e. model error statistics may be excellent but the wrong mechanisms are included in the model).
3. Good verification statistics do not necessarily imply the ability to accurately predict future water quality.
4. Statistics are still no replacement for informed judgement in model structure, data analyses, and credibility determination.

The BETTER two-dimensional reservoir water quality model has been applied to 9 reservoirs in the Tennessee and Cumberland River Valleys. Five of these model applications were not verified and management simulations were conducted with only a calibrated version: Boone (Brown et al., 1985), Fort Loudoun (Brown et al., 1985), Gunter'sville (Bender et al., 1990), Old Hickory (Brown et al., 1986), and Pickwick (Brown et al., 1985). Three of these applications were verified with qualitative statements of model confidence made from inspection of plots of simulated and observed data: Barkley (Brown, 1989), Cherokee (Hauser et al., 1987), and Chickamauga (Butkus et al., 1990). Only one application of the BETTER model has been verified with some quantitative measure of confidence; Cheatham (Brown et al., 1989). In this application, the correlation coefficient was figured for 7 state variables at 4 locations from weekly measurements.

STATISTICAL TESTS FOR MODEL VERIFICATION

The selection of an appropriate test to quantify the reliability of a model must be based upon the needs of the decision process. There are many issues that could be addressed during decision making with the proper measure of model uncertainty. There are several questions that should be asked when selecting a measure of verification (Reckhow and Chapra, 1983):

1. Is the model intended to be primarily descriptive (identifying hypothesized cause-effect relationships) or primarily predictive? Different statistical tests are appropriate in each case.
2. What characteristics of the prediction are of interest? The important issue may require information on mean values, extreme values, seasonal variability, spatial variability, or all predicted values.
3. What is the criterion for a successful verification? In some situations the decisions must be made from predictions with a specified level of confidence. In most cases, the inherent model uncertainty is accepted and considered as a factor in the decision making process.
4. Are the assumptions of any of the statistical tests violated? The assumptions of primary concern are the distribution and independence of the data. For distributions that are not normal, nonparametric tests are available. For spatial or time series data, data reduction may be needed to eliminate autocorrelation.
5. Are all error terms quantified? Often the prediction error is underestimated because the model specification error is not evaluated.
6. Are there any peculiar features to the model application of concern? Since each application is unique, the verification method and subsequent resource management decisions must recognize any distinctive factors that might influence the results.

There are several quantitative measures that can be used to test the reliability of model predictions. Generally, these are statistical tests of the agreement between observed and simulated values. Water quality variables often contain seasonal patterns and trends that would violate the independence assumption of the statistical tests. To avoid this problem, verification should be conducted on the residuals (predicted values minus observed values). If the patterns and trends are adequately modeled, the remaining residuals should have a constant variance around zero. One null hypothesis that could be tested would be that the residuals are not significantly different from zero.

Another useful statistic that can be used for verification is the relative error, defined as absolute value of the residual divided by the observed value. This statistic can be presented as a percentage making it an easily understood measure of model adequacy. The major disadvantage of relative error as a verification statistic is that when observed values are low, small errors result in extremely high relative error values. In contrast, when observed values greatly exceed predicted values the maximum relative error is 100%. However, the statistic can be aggregated over time, space or across variables to produce an overall estimate of prediction error.

The variances of the residuals can describe the frequency and magnitude of the deviations of predicted values from observations. The variance is usually standardized by the sample size to provide the estimate of the sample distribution. Since the variance of the mean has square units, the square root is often taken to transform the value to the same units as the original values. This statistic is called the standard error. The standard error defines an interval where 68% of the values in

the distribution are closest to the sample mean. This measure of dispersion is widely used in hypothesis testing.

The Student's t distribution can be used in verification to provide information on the degree of confidence in the mean prediction over space or time. At any specified level of prediction certainty, a confidence limit can be calculated that produces an upper and lower bound on the mean model prediction. A 95% confidence limit signifies that one is 95% sure the true mean value is the sample mean plus or minus the confidence limit. The 68% confidence limit is equal to the standard error. When calculated for a residual, the sample mean is hypothesized to be zero. Thus, confidence limits for residuals describe the degree of certainty that the model predicts observed conditions.

A very helpful technique used to compare model predictions with observations is construction of a bivariate plot. Visual inspection of plots of predicted versus observed values can give additional insight to the reliability of the model. If the model accurately predicts the observed conditions, the plot will be linear with a slope of one and an intercept at the origin. The correlation coefficient (r) is a measure of the strength of the relationship between two variables. The correlation coefficient has a range from +1 (indicating a perfect positive correlation) to -1 (indicating a perfect negative correlation). As values approach zero there is less relationship between the two variables.

A similar statistic often used for verification is the coefficient of determination. This statistic is simply the square of the correlation coefficient. It describes the amount of variance in a dependent variable that is explained by an independent variable. Since both the model

predictions and measured observations are mutually independent, the coefficient of determination is not the appropriate statistic to be used for comparison. Use of the correlation coefficient as the only measure of correspondence between the predictions and observations can be misleading. A high value does not necessarily imply the model is predicting accurately. One must also examine the slope, intercept and distribution of the relationship to assess the goodness-of-fit (figure 1).

Another statistic that has been used for model verification is the reliability index (Leggett and Williams, 1981). This index incorporates information from a bivariate plot of predictions versus observations into a single measure of goodness-of-fit. Values of the index range from 1.0 (indicating a perfect prediction) to infinity. The index value describes the degree to which the predictions agree with the observations. For example, a index value of 2.0 signifies that the measured versus predicted values were within a factor of two of each other, whereas a index value of 10.0 means the comparisons are an order of magnitude apart. This index is useful in that it is intuitively easy to interpret.

This report tests these measures of verification for the Chickamauga Reservoir application of the BETTER model. Observed values collected in 1989 are independent of the data used to calibrate the Chickamauga Reservoir application. Six measures of verification are evaluated: mean residuals, mean relative error, standard error of the residuals, 95% confidence limit of the residuals, correlation coefficient, and reliability index.

Figure 1. Possible Cases in Regression between Calculated and Observed Values (from Thomann, 1980)

VERIFICATION OF THE BETTER MODEL

Although the BETTER model has been applied to nine reservoirs, in only one case has any quantitative measure of model reliability been figured (Brown et al., 1989). TVA is currently distributing the BETTER model to interested water resource professionals. However, there has been no previous work on quantifying the reliability of the model for predictive purposes. This report presents a case study of verification methods on a specific application of the BETTER model for Chickamauga Reservoir.

Chickamauga Reservoir was formed by the closure in 1940 of Chickamauga Dam at Tennessee River Mile (TRM) 471, and extends 58.9 miles from Chattanooga, Tennessee, north to Watts Bar Dam (figure 2). The reservoir has a major arm formed by the confluence with the Hiwassee River at TRM 499.4. At normal full pool, Chickamauga Reservoir has a surface area of 35,400 acres, with a volume of 735,000 acre-feet, and 810 miles of shoreline. Annual average hydraulic residence time is approximately 10 days based on the annual average flow of about 34,000 cubic feet per second. The project is managed for the primary purposes of navigation, flood control, and power production.

Due to concerns about the redistribution of dissolved oxygen (DO) caused by the thermal discharge from Sequoyah Nuclear Plant, the BETTER model was applied to Chickamauga Reservoir (Butkus et al., 1990). In previous applications of the model, calibration was conducted by matching model results with field measurements from a single year. When the Chickamauga application was developed, no single year of existing data was sufficient for complete model calibration. Therefore, three separate years (1985, 1986, and 1987) of field data were used for calibration. All

Figure 2. Map of Chickamauga Reservoir

calibration was conducted by iterative inspections of computed and observed state variable plots and changing model parameters until the dynamic patterns were matched as closely as possible (figure 3). Qualitative verification was made similarly by inspection of computed variables with field measurements from year 1988 (figure 4). No quantifiable measure of model performance was calculated for either calibration or verification.

There are four general problems with the original verification of the Chickamauga Reservoir model. First, No quantitative measure of model prediction uncertainty was derived. The purpose of the model was to predict changes in the extent and duration of DO redistribution under various management scenarios and decide the likely impact on fisheries. Some knowledge of the model prediction uncertainty could have changed the conclusions of fishery evaluation. Second, the amount of data collected in 1988 was very scant. Only three variables were measured and surveys were discontinued in May for all locations upstream of TRM 485. Third, only elevation versus time contour plots were generated. Nonconservative water quality variables do not have complete continuity from point to point over time. The two-dimensional construct of the model should be retained since reservoir water quality constituents are more nearly regionalized variables over longitudinal space. Fourth, there is no information on the interpolation method used to generate the isopleth plots in the documentation of the contouring program (Harper, 1987). Numerous different methods exist for interpolating values between known points that could change the resulting plots.

In 1989, field measurements and water quality samples were collected monthly from April to October at 19 locations throughout the reservoir (table 1). Meteorological and hydrologic conditions in 1989 were

Figure 3. Final Calibration using 1987 Observed Dissolved Oxygen Concentrations (from Butkus et al., 1990)

Figure 4. Qualitative Verification using 1988 Observed Dissolved Oxygen Concentrations
(from Butkus et al., 1990)

Table 1. Water Quality Sampling Variables, Locations, and Dates of Collection in Chickamauga Reservoir

Variable	Analysis Method	Detection Limit
Temperature	in situ Thermister	0.1 deg. Celcius
Dissolved Oxygen	in situ Electrode	0.1 mg/l
pH	in situ Electrometric	Not Applicable
BOD, 5-day	Incubation	1 mg/l
Total Organic Carbon	Oxidation - Infrared	0.2 mg/l
Alkalinity	Potentiometric Titration	1 mg/l as CaCO ₃
Suspended Solids (Total)	Nonfilterable Residue	1 mg/l
Orthophosphate-P	Auto Colormetric Ascorbic Acid	0.01 mg/l
Ammonia-N (Total)	Auto Colormetric Phenate	0.01 mg/l
Nitrate-N (Total plus Nitrite)	Auto Cadmium Reduction	0.01 mg/l

Sampling Dates (1989)

April 19, May 17, June 28, July 27, August 22, September 19

Sampling Locations (Main Channel)

Tennessee River Mile 471.2, 473.4, 475.4, 478.2, 480.4, 481.4, 482.4, 482.9, 483.4,
483.5, 484.1, 484.7, 490.5, 496.5, 506.6, 518.0, 529.9
Hiwassee River Mile 7.4, 20.0

considerably different from the previous 5 years. Flows from Chickamauga Dam in 1989 were 140% of the long term (1958-1988) average. In contrast, flows for the calibration years (1985-1987) reflected effects of a severe extended drought that began in the Tennessee Valley Region in the spring of 1984 and lasted to the winter of 1988. Thus, the water quality data collected during 1989 is ideal for verifying model performance beyond the range of data used in calibration, since the high flow conditions were quite different from the drought years used to calibrate the model.

The Chickamauga Reservoir model was rerun using the same boundary assumptions as in calibration, but with measured inflow and meteorological data for 1989. Model predictions for 10 state variables were compiled for each model cell for the days corresponding to sampling dates (Julian days 109, 137, 179, 208, 234, and 262). Measured orthophosphate-P was used for comparison with modeled biologically available-P, since only a small percentage of particulate-P is available in the short period reflective of the 10 day hydraulic residence time (Lee et al. 1980). Modeled reservoir pool elevation was essentially the same for each of these dates (682 ft above msl) resulting in the model geometry shown in figure 5.

Kriging was used to spatially interpolate measured and modeled water quality variables along the thalweg of the Tennessee and Hiwassee Rivers. Kriging is the most statistically accurate method of estimating the spatial continuity of a regionalized variable (Davis, 1986). Modeled state variables were assumed to represent a location in the middle of the downstream conveyance area in each model cell. The reservoir geometry was finely divided into grid areas representing each foot in elevation versus one-tenth a river mile (6190 total cells). The program SURFER (Golden Software, 1989) was used for estimation of the grid points using the kriging interpolation option and a 10 point octant search method.

CHICKAMAUGA RESERVOIR MODEL CELLS AND SAMPLING LOCATIONS

WATER QUALITY VARIABLES

- Temperature, Dissolved Oxygen, pH
- BOD - 5 day, Total Organic Carbon, Alkalinity, Suspended Solids, Orthophosphate-P, Ammonia-N, Nitrate-N

Figure 5. Representation of Modeled Geometry for Chickamauga Reservoir at a 682 ft elevation and 1989 Sampling Locations

Six measures of verification were figured between the observed and predicted state variables. By retaining the two-dimensional construct of the model geometry, comparisons could be made over the entire year at all locations in the reservoir. The statistics computed for this verification are: (1) mean residual, (2) mean relative error, (3) standard error, (4) 95% confidence limit, (5) correlation coefficient, and (6) reliability index. The spatial distributions of these statistics for each state variable are presented in appendix figures.

Descriptive statistics for the mean residuals of the state variables pooled spatially are shown in Table 2. Most of the mean values are at or below the variable detection limit. Alkalinity was consistently under-predicted by the model, particularly in the Hiwassee River arm (figure A31). Median values are generally similar, implying that the distribution is normal for the mean residuals. The coefficient of variation is exceedingly high for over half the state variables. This is a result of the mean residual being very close to zero, amplifying the effect of any variation. Thus, for the case where the model performs well and yields predicted values close to observed values, the coefficient of variation of residuals is not a good performance statistic.

Although the statistics of the spatially pooled state variable residuals indicate good model performance, there are a few excursions way beyond the central tendency toward a zero mean residual. These extreme values are a result of the model not predicting conditions well at specific locations. Inspection of the spatial plots of mean residual reveal the locations where these deviations occur. Knowledge of model performance at a particular place in the reservoir may be needed for the decision process.

Table 2. Descriptive Statistics for Mean Residuals

Variable	Mean	Median	Minimum	Maximum	Coefficient of Variation
Temperature (deg. C)	0.01	0.01	-3.66	4.51	8712%
Dissolved Oxygen (mg/l)	0.13	0.23	-5.71	0.93	480%
pH (standard units)	0.10	0.08	-0.18	0.57	83%
BOD, 5-day (mg/l)	0.01	0.06	-1.25	0.42	3527%
Total Organic Carbon (mg/l)	0.11	-0.02	-1.09	1.47	451%
Alkalinity (mg/l)	-5.92	-5.31	-18.05	2.05	61%
Suspended Solids (mg/l)	1.44	1.04	-3.17	11.18	217%
Orthophosphate-P (mg/l)	0.010	0.004	-0.001	0.291	2213%
Ammonia-N (mg/l)	0.003	0.004	-0.009	0.016	117%
Nitrate-N (mg/l)	0.033	0.039	-0.009	0.067	53%

The mean values for the relative percent error present a different interpretation of model performance than the mean residuals for specific state variables (table 3). Using the relative error as the only measure of model verification, alkalinity would be assessed as being predicted accurately with a mean of 14 percent. This statistic can be deceptive in that state variables with large numerical values relative to the variation result in deflated relative error statistics compared to state variables with small numerical values. However, the relative error is useful in determining where in the reservoir the model is not predicting specific state variables correctly. For example, orthophosphorus is not predicted well along the bottom of the Tennessee River or at the surface of the Hiwassee River arm of the reservoir (figure A44).

The standard error is a very useful statistic for evaluating model performance. When the standard error is determined from the residuals it provides a plus/minus uncertainty estimate of the deterministic values predicted by the model. The standard error describes this prediction uncertainty with a 68% confidence. Descriptive statistics for the standard error of the residuals pooled spatially show that the Chickamauga Reservoir model predicts each of the state variables extremely well (table 4). The 95% confidence interval is the level of uncertainty commonly used to test for significance. Values for the 95% confidence limit are about two and a half times greater than standard error estimates. Using this higher level of confidence, the model predicts state variables reasonably well (table 5).

Table 3. Descriptive Statistics for Mean Relative Percent Error

Variable	Mean	Median	Minimum	Maximum	Coefficient of Variation
Temperature	3.5	2.6	0.8	21.9	66%
Dissolved Oxygen	12.7	12.1	2.8	82.0	48%
pH	2.7	2.7	1.4	7.7	25%
BOD, 5-day	38.4	35.2	12.7	140.5	48%
Total Organic Carbon	24.2	18.1	3.1	114.1	81%
Alkalinity	14.1	10.9	5.8	43.6	65%
Suspended Solids	130.4	84.4	21.2	1664.7	116%
Orthophosphate-P	173.7	112.8	40.5	3696.3	156%
Ammonia-N	124.2	86.7	21.7	2319.7	120%
Nitrate-N	19.7	18.6	10.4	116.2	30%

Table 4. Descriptive Statistics for Standard Error of the Residuals

Variable	Mean	Median	Minimum	Maximum	Coefficient of Variation
Temperature (deg. C)	0.26	0.25	0.08	0.79	37%
Dissolved Oxygen (mg/l)	0.42	0.40	0.13	0.86	39%
pH (standard units)	0.09	0.08	0.04	0.208	34%
BOD, 5-day (mg/l)	0.18	0.18	0.09	0.33	26%
Total Organic Carbon (mg/l)	0.16	0.16	0.03	0.50	39%
Alkalinity (mg/l)	2.0	2.0	0.6	4.0	39%
Suspended Solids (mg/l)	1.5	1.1	0.5	5.9	59%
Orthophosphate-P (mg/l)	0.005	0.003	0.001	0.142	203%
Ammonia-N (mg/l)	0.011	0.005	0.0001	0.315	196%
Nitrate-N (mg/l)	0.012	0.011	0.005	0.036	36%

Table 5. Descriptive Statistics for 95% Confidence Limit of the Residuals

Variable	Mean	Median	Minimum	Maximum	Coefficient of Variation
Temperature (deg. C)	0.67	0.63	0.21	2.03	37%
Dissolved Oxygen (mg/l)	1.07	1.03	0.33	2.21	39%
pH (standard units)	0.22	0.20	0.10	0.53	34%
BOD, 5-day (mg/l)	0.46	0.48	0.22	0.85	26%
Total Organic Carbon (mg/l)	0.42	0.40	0.08	1.30	39%
Alkalinity (mg/l)	5.3	5.1	1.7	11.2	39%
Suspended Solids (mg/l)	3.8	2.9	1.2	15.2	59%
Orthophosphate-P (mg/l)	0.012	0.007	0.002	0.366	203%
Ammonia-N (mg/l)	0.030	0.014	0.001	0.810	196%
Nitrate-N (mg/l)	0.032	0.029	0.014	0.093	36%

The correlation coefficient is a verification measure that quantifies the strength of the linear relationship between modeled and measured state variables. The Chickamauga Reservoir model appears to show extremely good model performance using this statistic (table 6). The Cheatham Reservoir model does not appear to predict conditions quite as accurately. The relatively high values for Chickamauga probably are an artifact of the kriging method used to interpolate modeled and observed values spatially. This interpolation increases the sample size of the comparison resulting in higher correlation coefficients. The estimation of values between known points was necessary since observations were not taken at all the conveyance areas of the modeled cells. Thus, the correlation coefficient is not an acceptable measure of model performance with spatially interpolated data.

The reliability index of Leggett and Williams (1981) provides a measure of verification that describes the model predictions as a multiplicative factor of the measured observations. The Chickamauga Reservoir model predicts most state variables within a factor of 2 (table 7). However, the range of index values for both 5-day BOD and orthophosphate are quite high (maximum 851 and 115, respectively). Inspection of the spatial plots reveal that the model does not accurately predict the 5-day BOD at the reservoir inflows nor orthophosphate in the hypolimnion of the reservoir lacustrine zone. Although the reliability index is intuitively easy to interpret, it is of limited value for decision making due to the small range of values for each state variable.

Table 6. Descriptive Statistics for Correlation Coefficient

Variable	Mean	Median	Minimum	Maximum	Coefficient of Variation	Mean Values for Cheatham Reservoir (Brown et al. 1989)
Temperature	0.9995	0.9997	0.9972	0.9999	0.03%	0.9938
Dissolved Oxygen	0.9915	0.9931	0.6910	0.9994	1%	0.9166
pH	0.9996	0.9997	0.9983	0.9999	0.02%	0.4710
BOD, 5-day	0.9446	0.9455	0.3084	0.9902	3%	0.6654
Total Organic Carbon	0.9820	0.9876	0.8573	0.9995	2%	-----
Alkalinity	0.9948	0.9966	0.9782	0.9997	1%	-----
Suspended Solids	0.9008	0.9084	0.7409	0.9949	6%	0.5166
Orthophosphate-P	0.8419	0.8661	0.3076	0.9725	12%	0.6514
Ammonia-N	0.8922	0.9130	0.4737	0.9981	9%	0.5056
Nitrate-N	0.9901	0.9948	0.8461	0.9987	1%	-----

Table 7. Descriptive Statistics for Reliability Index

Variable	Mean	Median	Minimum	Maximum	Coefficient of Variation
Temperature	1.043	1.034	1.010	1.236	3%
Dissolved Oxygen	1.166	1.151	1.036	8.980	16%
pH	1.031	1.031	1.016	1.088	1%
BOD, 5-day	1.881	1.545	1.155	851.300	623%
Total Organic Carbon	1.329	1.282	1.040	2.783	18%
Alkalinity	1.206	1.134	1.089	1.833	15%
Suspended Solids	2.133	2.003	1.323	4.618	27%
Orthophosphate-P	2.475	2.169	1.541	115.228	82%
Ammonia-N	2.128	1.908	1.298	6.192	33%
Nitrate-N	1.247	1.216	1.110	2.399	8%

CONCLUSIONS

If water quality models are to be useful for making water resource management decisions, some level of confidence must be placed on the model predictions. Although qualitative comparison of measured and modeled data can provide some insight into model performance, quantitative measures can answer the basic question required by decision makers: "What is the level of confidence that can be placed on the results?". When using goodness-of-fit measures to evaluate model performance, the modeler must be cautious not to "curve fit" the model to the data just to improve the statistics. Statistics merely augment, not replace informed professional judgement in model structure, data analysis, and credibility determination. Good verification statistics do not necessarily imply the ability to accurately predict future water quality. However, quantifiable measures of verification can assist water resource managers in assessing model credibility.

Many statistical methods are available for measuring model performance. Selection of the proper measure of verification depends partly on how the model predictions are to be used. If the model is primarily be used for descriptive purposes, a sensitivity analysis may be all that is required. Models used for predictive purposes may only require specific information, such as mean or extreme values. The particular test chosen for verification must not violate any of the statistical assumptions, such as the distribution or independence of the data.

Several verification measures were evaluated for the BETTER model application of Chickamauga Reservoir. The mean and standard error of the residuals appear to be the most useful statistics to evaluate model performance. The mean residual provides information on the magnitude and spatial distribution of the differences between predictions and observations. The standard error of the residual provides a plus/minus estimate of model prediction uncertainty. By retaining the two-dimensional construct of the model and evaluating the predictions over time, model uncertainty can be estimated at any location within the reservoir. Knowledge of this spatial uncertainty can help identify locations where the model does not accurately reflect actual reservoir conditions. These measures of verification can also be used for other two-dimensional models, such as air or ground water quality models. The following recommendations are offered:

1. Retain the two-dimensional construct of the BETTER model when evaluating model performance. This allows the estimation of quantifiable measures of uncertainty at specific locations in the reservoir.
2. Verification of future applications of the BETTER model should use the mean and standard error of the residuals to evaluate model performance.
3. Calculate the mean and standard error of the residuals with the calibration data set. This should be done independently of the actual calibration process to avoid influencing informed judgement in selecting model parameters.

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APPENDIX

TEMPERATURE: MEAN RESIDUAL (deg. C)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.01 deg. C

Median = 0.01 deg. C

Minimum = -3.66 deg. C

Maximum = 4.51 deg. C

Figure A1. Isopleths of the Mean Residuals for Temperature

TEMPERATURE: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 3.5%
 Median = 2.6%
 Minimum = 0.8%
 Maximum = 21.9%

Figure A2. Isopleths of the Mean Relative Error for Temperature

TEMPERATURE: STANDARD ERROR (deg. C)

RESERVOIR WIDE

Mean = 0.26 deg. C
 Median = 0.25 deg. C
 Minimum = 0.08 deg. C
 Maximum = 0.79 deg. C

Figure A3. Isopleths of the Standard Error for Temperature

TEMPERATURE: 95% CONFIDENCE LIMIT (deg. C)

RESERVOIR WIDE

Mean = 0.67 deg. C

Median = 0.63 deg. C

Minimum = 0.21 deg. C

Maximum = 2.03 deg. C

Figure A4. Isopleths of the 95% Confidence Limit for Temperature

TEMPERATURE: CORRELATION COEFFICIENT

RESERVOIR WIDE

Mean = 0.9995

Median = 0.9997

Minimum = 0.9972

Maximum = 0.9999

Figure A5. Isopleths of the Correlation Coefficient for Temperature

TEMPERATURE: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 1.043

Median = 1.034

Minimum = 1.010

Maximum = 1.2367

Figure A6. Isopleths of the Reliability Index for Temperature

DISSOLVED OXYGEN: MEAN RESIDUAL (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

RESERVOIR WIDE

Mean = 0.13 mg/l

Median = 0.23 mg/l

Minimum = -5.71 mg/l

Maximum = 0.93 mg/l

Figure A7. Isopleths of the Mean Residuals for Dissolved Oxygen

DISSOLVED OXYGEN: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 12.7%
 Median = 12.1%
 Minimum = 2.8%
 Maximum = 82.0%

Figure A8. Isopleths of the Mean Relative Error for Dissolved Oxygen

DISSOLVED OXYGEN: STANDARD ERROR (mg/l)

RESERVOIR WIDE

Mean = 0.42 mg/l
 Median = 0.40 mg/l
 Minimum = 0.13 mg/l
 Maximum = 0.86 mg/l

Figure A9. Isopleths of the Standard Error for Dissolved Oxygen

DISSOLVED OXYGEN: 95% CONFIDENCE LIMIT (mg/l)

RESERVOIR WIDE

Mean = 1.07 mg/l
 Median = 1.03 mg/l
 Minimum = 0.33 mg/l
 Maximum = 2.21 mg/l

Figure A10. Isopleths of the 95% Confidence Limit for Dissolved Oxygen

DISSOLVED OXYGEN: CORRELATION COEFFICIENT

RESERVOIR WIDE

Mean = 0.9915
 Median = 0.9931
 Minimum = 0.6910
 Maximum = 0.9994

Figure A11. Isopleths of the Correlation Coefficient for Dissolved Oxygen

DISSOLVED OXYGEN: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 1.166
 Median = 1.151
 Minimum = 1.036
 Maximum = 8.980

Figure A12. Isopleths of the Reliability Index for Dissolved Oxygen

pH: MEAN RESIDUAL

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

RESERVOIR WIDE

Mean = 0.10
 Median = 0.08
 Minimum = -0.18
 Maximum = 0.57

Figure A13. Isopleths of the Mean Residuals for pH

pH: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 2.7%

Median = 2.7%

Minimum = 1.4%

Maximum = 7.7%

Figure A14. Isopleths of the Mean Relative Error for pH

pH: STANDARD ERROR (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.085
 Median = 0.076
 Minimum = 0.038
 Maximum = 0.208

Figure A15. Isopleths of the Standard Error for pH

pH: 95% CONFIDENCE LIMIT

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.22

Median = 0.20

Minimum = 0.10

Maximum = 0.53

Figure A16. Isopleths of the 95% Confidence Limit for pH

pH: CORRELATION COEFFICIENT

CHICKAMAUGA RESERVOIR -- TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.9996

Median = 0.9997

Minimum = 0.9983

Maximum = 0.9999

Figure A17. Isopleths of the Correlation Coefficient for pH

pH: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 1.031
 Median = 1.031
 Minimum = 1.016
 Maximum = 1.088

Figure A18. Isopleths of the Reliability Index for pH

BOD-5: MEAN RESIDUAL (mg/l)

RESERVOIR WIDE

Mean = 0.01 mg/l
 Median = 0.06 mg/l
 Minimum = -1.25 mg/l
 Maximum = 0.42 mg/l

Figure A19. Isopleths of the Mean Residuals for 5-day BOD

BOD-5: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 38.4%

Median = 35.2%

Minimum = 12.7%

Maximum = 140.5%

Figure A20. Isopleths of the Mean Relative Error for 5-day BOD

BOD-5: STANDARD ERROR (mg/l)

RESERVOIR WIDE

Mean = 0.18 mg/l

Median = 0.18 mg/l

Minimum = 0.09 mg/l

Maximum = 0.33 mg/l

Figure A21. Isopleths of the Standard Error for 5-day BOD

BOD-5: 95% CONFIDENCE LIMIT (mg/l)

RESERVOIR WIDE

Mean = 0.46 mg/l

Median = 0.48 mg/l

Minimum = 0.22 mg/l

Maximum = 0.85 mg/l

Figure A22. Isopleths of the 95% Confidence Limit for 5-day BOD

BOD-5: CORRELATION COEFFICIENT

RESERVOIR WIDE

Mean = 0.9446

Median = 0.9455

Minimum = 0.3084

Maximum = 0.9902

Figure A23. Isopleths of the Correlation Coefficient for 5-day BOD

BOD-5: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 1.881
 Median = 1.545
 Minimum = 1.155
 Maximum = 851.3

Figure A24. Isopleths of the Reliability Index for 5-day BOD

TOTAL ORGANIC CARBON: MEAN RESIDUAL (mg/l)

RESERVOIR WIDE

Mean = 0.11 mg/l

Median = -0.02 mg/l

Minimum = -1.09 mg/l

Maximum = 1.47 mg/l

Figure A25. Isopleths of the Mean Residuals for Total Organic Carbon

TOTAL ORGANIC CARBON: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 24.2%

Median = 18.1%

Minimum = 3.1%

Maximum = 114.1%

Figure A26. Isopleths of the Mean Relative Error for Total Organic Carbon

TOTAL ORGANIC CARBON: STANDARD ERROR (mg/l)

RESERVOIR WIDE

Mean = 0.16 mg/l
 Median = 0.16 mg/l
 Minimum = 0.03 mg/l
 Maximum = 0.50 mg/l

Figure A27. Isopleths of the Standard Error for Total Organic Carbon

TOTAL ORGANIC CARBON: 95% CONFIDENCE LIMIT (mg/l)

RESERVOIR WIDE

Mean = 0.42 mg/l
 Median = 0.40 mg/l
 Minimum = 0.08 mg/l
 Maximum = 1.30 mg/l

Figure A28. Isopleths of the 95% Confidence Limit for Total Organic Carbon

TOTAL ORGANIC CARBON: CORRELATION COEFFICIENT

RESERVOIR WIDE

Mean = 0.9820

Median = 0.9876

Minimum = 0.8573

Maximum = 0.9995

Figure A29. Isopleths of the Correlation Coefficient for Total Organic Carbon

TOTAL ORGANIC CARBON: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 1.329

Median = 1.282

Minimum = 1.040

Maximum = 2.783

Figure A30. Isopleths of the Reliability Index for Total Organic Carbon

ALKALINITY: MEAN RESIDUAL (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = -5.92 mg/l
 Median = -5.31 mg/l
 Minimum = -18.05 mg/l
 Maximum = 2.05 mg/l

Figure A31. Isopleths of the Mean Residuals for Alkalinity

ALKALINITY: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 14.1%
 Median = 10.9%
 Minimum = 5.8%
 Maximum = 43.6%

Figure A32. Isopleths of the Mean Relative Error for Alkalinity

ALKALINITY: STANDARD ERROR (mg/l)

RESERVOIR WIDE

Mean = 2.0 mg/l
 Median = 2.0 mg/l
 Minimum = 0.6 mg/l
 Maximum = 4.0 mg/l

Figure A33. Isopleths of the Standard Error for Alkalinity

ALKALINITY: 95% CONFIDENCE LIMIT

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 5.3 mg/l

Median = 5.1 mg/l

Minimum = 1.7 mg/l

Maximum = 11.2 mg/l

Figure A34. Isopleths of the 95% Confidence Limit for Alkalinity

ALKALINITY: CORRELATION COEFFICIENT

RESERVOIR WIDE

Mean = 0.9948

Median = 0.9966

Minimum = 0.9782

Maximum = 0.9997

Figure A35. Isopleths of the Correlation Coefficient for Alkalinity

ALKALINITY: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 1.206

Median = 1.134

Minimum = 1.089

Maximum = 1.833

Figure A36. Isopleths of the Reliability Index for Alkalinity

SUSPENDED SOLIDS: MEAN RESIDUAL (mg/l)

RESERVOIR WIDE

Mean = 1.44 mg/l
 Median = 1.04 mg/l
 Minimum = -3.17 mg/l
 Maximum = 11.18 mg/l

Figure A37. Isopleths of the Mean Residuals for Suspended Solids

SUSPENDED SOLIDS: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 130.4%

Median = 84.4%

Minimum = 21.2%

Maximum = 1664.7%

Figure A38. Isopleths of the Mean Relative Error for Suspended Solids

SUSPENDED SOLIDS: STANDARD ERROR (mg/l)

RESERVOIR WIDE

Mean = 1.5 mg/l

Median = 1.1 mg/l

Minimum = 0.5 mg/l

Maximum = 5.9 mg/l

Figure A39. Isopleths of the Standard Error for Suspended Solids

SUSPENDED SOLIDS: 95% CONFIDENCE LIMIT (mg/l)

RESERVOIR WIDE

Mean = 3.8 mg/l
 Median = 2.9 mg/l
 Minimum = 1.2 mg/l
 Maximum = 15.2 mg/l

Figure A40. Isopleths of the 95% Confidence Limit for Suspended Solids

SUSPENDED SOLIDS: CORRELATION COEFFICIENT

RESERVOIR WIDE

Mean = 0.9008

Median = 0.9084

Minimum = 0.7409

Maximum = 0.9949

Figure A41. Isopleths of the Correlation Coefficient for Suspended Solids

SUSPENDED SOLIDS: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 2.133
 Median = 2.003
 Minimum = 1.323
 Maximum = 4.618

Figure A42. Isopleths of the Reliability Index for Suspended Solids

ORTHO-PHOSPHATE: MEAN RESIDUAL (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.010 mg/l

Median = 0.004 mg/l

Minimum = -0.001 mg/l

Maximum = 0.291 mg/l

Figure A43. Isopleths of the Mean Residuals for Orthophosphate-P

ORTHO-PHOSPHATE: MEAN RELATIVE ERROR (%)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 173.7%

Median = 112.8%

Minimum = 40.5%

Maximum = 3696.3%

Figure A44. Isopleths of the Mean Relative Error for Orthophosphate-P

ORTHO-PHOSPHATE: STANDARD ERROR (mg/l)

RESERVOIR WIDE

Mean = 0.005 mg/l
 Median = 0.003 mg/l
 Minimum = 0.001 mg/l
 Maximum = 0.142 mg/l

Figure A45. Isopleths of the Standard Error for Orthophosphate-P

ORTHO-PHOSPHATE: 95% CONFIDENCE LIMIT (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.012 mg/l
 Median = 0.007 mg/l
 Minimum = 0.002 mg/l
 Maximum = 0.366 mg/l

Figure A46. Isopleths of the 95% Confidence Limit for Orthophosphate-P

ORTHO-PHOSPHATE: CORRELATION COEFFICIENT

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.8419

Median = 0.8661

Minimum = 0.3076

Maximum = 0.9725

Figure A47. Isopleths of the Correlation Coefficient for Orthophosphate-P

ORTHO-PHOSPHATE: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 2.475

Median = 2.169

Minimum = 1.541

Maximum = 115.2

Figure A48. Isopleths of the Reliability Index for Orthophosphate-P

AMMONIA: MEAN RESIDUAL (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.003 mg/l
 Median = 0.004 mg/l
 Minimum = -0.009 mg/l
 Maximum = 0.016 mg/l

Figure A49. Isopleths of the Mean Residuals for Ammonia-N

AMMONIA: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 124.2%

Median = 86.7%

Minimum = 21.7%

Maximum = 2319.7%

Figure A50. Isopleths of the Mean Relative Error for Ammonia-N

AMMONIA: STANDARD ERROR (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

RESERVOIR WIDE

Mean = 0.011 mg/l
 Median = 0.005 mg/l
 Minimum = 0.0001 mg/l
 Maximum = 0.315 mg/l

Figure A51. Isopleths of the Standard Error for Ammonia-N

A topographic map of the Chickamauga Reservoir area. The vertical axis on the left is labeled 'ELEVATION (FT)' and ranges from 610 to 690 in increments of 10. The horizontal axis at the bottom is labeled 'TENNESSEE RIVER MILE' and ranges from 470 to 530 in increments of 10. The map shows the reservoir's shoreline and several elevation contours. Contours are labeled with values such as 0.01, 0.02, 0.03, and 1.00. A prominent contour labeled '0.01' is located in the upper right portion of the reservoir. Another contour labeled '0.02' is visible in the lower left. The Tennessee River is shown as a winding line at the bottom of the map, with several points labeled '0.02' and '0.03'. A small rectangular area in the upper right corner contains a detailed inset showing a close-up of the river's course and surrounding terrain, with labels '0.02' and '0.03'.

Mean = 0.030 mg/l
Median = 0.014 mg/l
Minimum = 0.001 mg/l
Maximum = 0.810 mg/l

Figure A52. Isopleths of the 95% Confidence Limit for Ammonia-N

AMMONIA: CORRELATION COEFFICIENT

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.8922

Median = 0.9130

Minimum = 0.4737

Maximum = 0.9981

Figure A53. Isopleths of the Correlation Coefficient for Ammonia-N

AMMONIA: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 2.128

Median = 1.908

Minimum = 1.298

Maximum = 6.192

Figure A54. Isopleths of the Reliability Index for Ammonia-N

NITRATE: MEAN RESIDUAL (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

RESERVOIR WIDE

Mean = 0.033 mg/l
 Median = 0.039 mg/l
 Minimum = -0.009 mg/l
 Maximum = 0.067 mg/l

Figure A55. Isopleths of the Mean Residuals for Nitrate-N

NITRATE: MEAN RELATIVE ERROR (%)

RESERVOIR WIDE

Mean = 19.7%

Median = 18.6%

Minimum = 10.4%

Maximum = 116.2%

Figure A56. Isopleths of the Mean Relative Error for Nitrate-N

NITRATE: STANDARD ERROR (mg/l)

CHICKAMAUGA RESERVOIR - TENNESSEE RIVER

HIWASSEE RIVER ARM

RESERVOIR WIDE

Mean = 0.012 mg/l
 Median = 0.011 mg/l
 Minimum = 0.005 mg/l
 Maximum = 0.036 mg/l

Figure A57. Isopleths of the Standard Error for Nitrate-N

NITRATE: 95% CONFIDENCE LIMIT (mg/l)

RESERVOIR WIDE

Mean = 0.032 mg/l
 Median = 0.029 mg/l
 Minimum = 0.014 mg/l
 Maximum = 0.093 mg/l

Figure A58. Isopleths of the 95% Confidence Limit for Nitrate-N

NITRATE: CORRELATION COEFFICIENT

Figure A59. Isopleths of the Correlation Coefficient for Nitrate-N

NITRATE: RELIABILITY INDEX

RESERVOIR WIDE

Mean = 1.247
 Median = 1.216
 Minimum = 1.110
 Maximum = 2.399

Figure A60. Isopleths of the Reliability Index for Nitrate-N

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01 / 29 / 91