This report describes the application of a two-dimensional, laterally averaged, hydrodynamic and water quality model (CE-QUAL-W2) to DeGray Lake, Arkansas. The model successfully predicted spatial and temporal variations in dissolved oxygen concentrations and other water quality variables over the stratification cycle. The application and testing of the model are described.
PREFACE

This report was sponsored by the Office, Chief of Engineers (OCE), US Army, as part of the Environmental and Water Quality Operational Studies (EWQOS) Program, Work Unit 31595 (IC.2), entitled "Develop and Evaluate Multidimensional Reservoir Water Quality and Ecological Predictive Techniques." The OCE Technical Monitors for EWQOS were Mr. Earl Eiker, Dr. John Bushman, and Mr. James L. Gottesman.

This report describes the application and testing of CE-QUAL-W2, a two-dimensional, laterally averaged model of hydrodynamics and water quality, to DeGray Lake, Arkansas.

The study was conducted and the report prepared by Dr. James L. Martin of the Water Quality Modeling Group (WQMG), Ecosystem Research and Simulation Division (ERSD), Environmental Laboratory (EL), US Army Engineer Waterways Experiment Station (WES), under the direct supervision of Mr. Mark S. Dortch, Chief, WQMG, and under the general supervision of Mr. Donald L. Robey, Chief, ERSD, and Dr. John Harrison, Chief, EL. Program Manager for EWQOS was Dr. J. L. Mahloch, EL. Reviews and contributions by Dr. Robert Kennedy, Aquatic Processes and Effects Group, ERSD, and Dr. Stephen Schreiner and Mr. Dortch, WQMG, are gratefully acknowledged. This report was prepared for publication by Ms. Jessica S. Ruff of the WES Information Products Division.

COL Allen F. Grum, USA, was the previous Director of WES. COL Dwayne G. Lee, CE, is the present Commander and Director. Dr. Robert W. Whalin is Technical Director.

This report should be cited as follows:

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APPENDIX A: COMPUTATION OF THE RELIABILITY INDEX A1
1. A two-dimensional (2-D), laterally averaged hydrodynamic and water quality model, CE-QUAL-W2, has been developed by the Environmental and Hydraulics Laboratories of the US Army Engineer Waterways Experiment Station (WES), as a tool for water resources management. The model was developed to allow simulation of water bodies where resolution of longitudinal as well as vertical gradients in water quality over time is required.

2. This report documents the application of CE-QUAL-W2 to DeGray Lake, Arkansas. This reservoir has been extensively studied by the Corps of Engineers and is known to exhibit seasonal variations in water quality along both longitudinal and vertical axes. The application served a number of purposes including analysis and refinement of the code, location and correction of errors in the code and data sets, sensitivity analyses, and other tests of the code as well as comparisons of model predictions with data collected. Descriptions of the application and testing follow an overview of the basic features of CE-QUAL-W2. Detailed descriptions of the model is available in its user's manual (Environmental and Hydraulics Laboratories 1986).
PART II: MODEL DESCRIPTION

3. CE-QUAL-W2 is a 2-D model that describes vertical and longitudinal distributions of hydrodynamics, thermal energy, and selected biological and chemical materials in a water body through time. The model is based upon the Generalized Longitudinal-Vertical Hydrodynamics and Transport (GLVHT) model of rivers, reservoirs, and estuaries (Buchak and Edinger 1984), earlier versions of which were known as the Laterally Averaged Reservoir Model (LARM) (Buchak and Edinger 1982). The GLVHT model has been under development since 1975 by WES and J. E. Edinger and Associates of Wayne, Pa. GLVHT has been previously used to simulate temperature distributions and circulation patterns in water bodies and has been applied to a variety of systems (Buchak and Edinger 1984). Primary modifications to the GLVHT model resulting in CE-QUAL-W2 included addition of algorithms to simulate water quality constituents. These modifications were made relying heavily upon the established structure of GLVHT, and the basic programming and solution techniques remain intact.

4. CE-QUAL-W2 is based upon the finite difference solution of the laterally averaged equations of fluid motion including: (a) the free water surface, (b) hydrostatic pressure, (c) horizontal momentum, (d) continuity, (e) constituent transport, and (f) an equation of state relating density and constituents including temperature and solids concentrations (dissolved and suspended). Unknowns include the water surface elevations, pressures, densities, horizontal and vertical velocity, and constituent concentrations. By solving for the water surface elevation implicitly, the restrictive Courant surface gravity wave criterion is removed, allowing simulation of reasonable time frames for field applications, such as entire stratification cycles. An explicit scheme is then used to transport heat and chemical/biological constituents. The model has the capability of including head or flow boundary conditions, branches, multiple withdrawals, and other features which allow its application to a variety of situations. A number of statistical and graphical aids are available to assist in interpretation of results.
5. Some of the basic features of the model are summarized below:
   a. Two-dimensional (laterally averaged) simulations of temperatures, constituents, and flow fields.
   b. Hydrodynamic computations influenced by variable water density caused by temperature and dissolved and suspended solids.
   c. Simulation of the interactions of numerous biological/chemical factors influencing water quality.
   d. Allowance for multiple inflow loadings and withdrawals from tributaries, point and nonpoint loadings, precipitation, branch inflows, and outflows from a dam.
   e. Allowance for multiple branches.
   f. Allowance for ice cover computations.
   g. Allowance for multiple time steps.
   h. Allowance for flow or head boundary conditions, making it applicable for reservoir or estuarine modeling.
   i. Simulation of circulation patterns.
   j. Restart capability.
   k. Inclusion of evaporation in water balance.
   l. Heat transfer computations.
   m. Variety of output options.

6. The simulation of biological and chemical constituents affecting water quality is a major attribute of CE-QUAL-W2. The model simulates the interactive dynamics of physical factors (such as flow and temperature regimes), chemical factors (such as nutrients), and an algal assemblage. The model structure allows for the simulation of up to 20 water quality constituents in addition to temperature, density, and circulation patterns. Hydrodynamics and water temperatures can be simulated independently of, or in conjunction with, other water quality constituents.

7. The water quality constituents are arranged in four levels of complexity as shown below:
8. The first level includes either conservative materials or those which do not interact with other constituents in that level. The second level allows simulation of the interactive dynamics of algae-dissolved oxygen-nutrients. The third level allows simulation of pH and carbonate species. The fourth level, which currently contains algorithms for predicting concentrations of total iron, is included to allow simulation of iron and nutrient interactions and to allow future additions of other anaerobic constituents.

9. The levels are generally intended to be run in tandem, rather than separately. For example, the prediction of pH variations requires that the effects of algal respiration, decomposition, and other factors affecting inorganic carbon concentrations be simulated. Any of the constituents listed may be omitted from simulations at the discretion of the user. This allows considerable flexibility in model applications. For example, it may be possible to simulate dissolved oxygen (DO) variations in some systems using only the dissolved organic matter and
DO compartments, similar to typical biochemical oxygen demand DO modeling. Simulations of conservative tracers or coliform bacteria may also not be required for an application. However, it is very important that the user be completely familiar with the model structure and study requirements as well as the biology and chemistry of the study system before omitting a particular water quality variable.

10. A simplified description of the kinetic interactions between constituents is provided in Table 1. A detailed description of kinetics is provided in the CE-QUAL-W2 User's Manual (Environmental and Hydraulics Laboratories 1986). The pH and distribution of carbonate species are determined from predicted alkalinity and inorganic carbon concentrations using standard carbonate relationships. Kinetic interactions listed, with the exception of advection and diffusion, are computed in separate subroutines for each constituent. Transport, as well as loadings and withdrawals, are computed in the main body of the source code and updated every computational time step. However, provisions are made to allow sources and sinks due to decomposition, photosynthesis, etc., to be updated at different frequencies than hydrodynamics. This is consistent with the generally coarser time scale required to resolve biological/equilibrium chemical interactions and allows a considerable savings in computation time.

11. The majority of interactions are also influenced by temperature, and temperature rate multipliers are used to modify reaction kinetics. Options are also included to allow updating of temperature rate multipliers at different frequencies than hydrodynamics. For example, stability requirements may limit steps to less than 0.5 hr for a simulation. However, temperature variations occurring during this short a time span may have a negligible effect on biological and chemical processes. Thus, it may be possible to update temperature rate multipliers less frequently than hydrodynamics without appreciably affecting the processes of importance.
Table 1

Internal Process Interactions for Variables in CE-QUAL-W2

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NOTES:
- SS = suspended solids
- TDS = total dissolved solids
- DOM = dissolved organic matter
- (L) = labile
- (R) = refractory
- F = diffusion and advection
- Y = settling, diffusion, advection
- D = decay, decomposition, release
- M = mortality
- R = respiration
- P = photosynthesis
- S = settling
- A = adsorption
- X = exchange at air/water interface
PART III: RESERVOIR CHARACTERISTICS

12. DeGray Lake is a warm monomictic Corps of Engineer reservoir created during 1969-1970 by the impoundment of the Caddo River in south-central Arkansas (Figure 1). The reservoir is used for power generation, flood control, and recreation. At conservation pool (124.4 m NGVD), DeGray Lake has a volume of $8.08 \times 10^8$ m$^3$ and a surface area of 54.3 km$^2$. The 32-km-long reservoir has a mean depth of 14.9 m with a maximum depth of 60 m. The shoreline development ratio of 12.8 reflects the dendritic shape of DeGray Lake. Average monthly residence time varied from 0.28 year in April to 3.51 years in November 1979, while in 1980 mean residence times varied from 0.72 year in May to 7.57 years in October (Ford and Stein 1984).

13. An extensive data base is available for DeGray Lake. The reservoir has been the site of field studies since impoundment began in
1969. This data base includes vertical profiles for a number of constituents, taken twice a month. Data from three sampling stations were used for this study, including one located near the upper end of the reservoir (Station 12, Figure 1), near its midpoint (Station 10), and near the dam (Station 4). Stations 10 and 12 best represented the transition zone and Station 4 the lacustrine zone of the heuristic model of Thornton et al. (1980).

14. DeGray Lake exhibits seasonal patterns of DO and nutrient dynamics which are common in many CE reservoirs. Following the onset of stratification, DO depletions first occur in the upstream hypolimnion and then gradually progress in a downstream direction. During summer months of the early years following impoundment, anoxic conditions occurred in the hypolimnion throughout the reservoir. In later years, the general trend has been to observe higher hypolimnetic DO concentrations in the lacustrine zone (Kennedy and Nix 1986). The distance to which hypolimnetic anoxia extends down the reservoir has varied from year to year; however, the trend for early oxygen depletion in the upstream hypolimnion has been observed from 1970 through 1981 (Nix 1986). A metalimnetic DO minimum has also been observed each year.

15. The seasonal pattern of DO depletions is evident in DO isopleths for two sampling stations for 1979 (Figure 2). Anoxic conditions occurred at the upstream station (Station 12) beginning shortly after the onset of stratification and extending until late fall. Similar conditions occurred at the midpoint station (Station 10), and anoxic conditions extended to near the surface during summer months. The hypolimnion of the lacustrine zone did not become anoxic; however, a metalimnetic DO minimum developed by early summer and persisted throughout the remainder of the year. The depth of the metalimnetic minimum increased during the latter part of the year, corresponding to the deepening of the thermocline (Figure 2). However, destratification did not result in removal of the metalimnetic minimum until early the following year. This seasonal pattern of anoxia also occurred during 1980, although the development of the metalimnetic minima occurred nearly 2 months later in the year.
Figure 2. Observed 1979, DO variations at DeGray Lake (concentrations in mg/l)
PART IV: MODEL APPLICATION

16. Observed water quality patterns in DeGray Lake indicated that both vertical and longitudinal gradients occurred, and intensive field studies indicated that lateral variations were generally small (Thornton et al. 1982), making application of a 2-D model appropriate. A yearly time frame was chosen for the application to allow assessment of the predictive capability of the model for the complete stratification cycle.

Geometry

17. DeGray Lake was idealized by a finite difference grid consisting of a single main branch with 32 segments \((I = 1 \text{ to } 32)\) nearly 1 km in length \((DLX)\) along the longitudinal \((x)\) axis and 36 \((k = 1 \text{ to } 36)\) vertical \((z)\) axis layers 2 m \((h)\) in depth (Figure 3) with each model
cell having an assigned cell width. The number of active cells in the computational grid varied with predicted water surface elevations and averaged nearly 608 cells. The grid structure established by Johnson et al. (1981) for an application of the LARM model to DeGray was used for this application.

18. A table of elevations and their associated reservoir volumes and surface areas is provided in model output for comparisons with known relationships. The area-capacity curves for the known system and the imposed geometry should compare favorably. This comparison was made for the DeGray application and, although some discrepancies occurred between actual and predicted volumes at given elevations, they were considered insufficient to require modification of the grid.

**Boundary Conditions**

19. CE-QUAL-W2 requires boundary condition data including head or flows, constituent concentrations, and meteorological conditions. Flow boundary conditions were used in this application, with a single inflow at the upstream end of the reservoir and downstream outflow from the dam.

20. Daily inflows and water temperatures and constituent concentrations measured every 2 weeks were available from a station located on the Caddo River at the crossing of Highway 84 (Figure 1) near Amity, Ark. For practical purposes, this inflow may be assumed to enter DeGray Lake just above the backwater at normal pool elevation (Ford and Stein 1984). Inflows varied considerably between 1979 and 1980, with 1979 being characterized by a series of high-flow events during the spring (Figure 4). A period of low inflows occurred during the summer months of both 1979 and 1980, and a relatively high inflow occurred late in both years.

21. Inflow concentrations for all simulated constituents were available with the exception of dissolved organic matter (DOM) and phytoplankton. Inflow concentrations were available for dissolved organic carbon, which were converted to DOM by dividing by the coefficient 0.45,
Figure 4. Inflows into DeGray Lake
assuming that organic matter is composed of approximately 45 percent carbon (dry weight). This percentage is consistent with carbon/biomass ratios for algae and numerous other organisms reported by Jorgensen (1979). DOM was further subdivided into labile and refractory components, and it was assumed that 70 percent of inflow organic matter was refractory. Wetzel (1975) and others have indicated that the bulk of organic matter is composed of compounds resistant to degradation. Inflow concentrations of phytoplankton were assumed to be zero. Inflow temperatures exhibited little variation between 1979 and 1980 (Figure 5), while inflow constituent concentrations varied considerably. For example, inflow concentrations of ammonia-nitrogen were generally lower and exhibited less variation in 1979 than in 1980 (Figure 6), while the opposite was true for phosphate-phosphorus (Figure 7) and total dissolved solids (Figure 8).

22. Inflow concentrations represented "snapshot" measurements rather than daily averages and were assumed to remain constant between periods of updating. Since flows were updated daily and constituent concentrations every 2 weeks, errors may have resulted in material loadings, particularly during storm events since significantly more materials enter a lake during storm events than during base flow (Perrier, Westerdahl, and Nix 1977). Additionally, flows from the Caddo River were increased by 47 percent and 68 percent for 1979 and 1980, respectively, to account for ungauged inflows, following Ford and Stein (1984). This method assumes that all material loadings are equal in concentration to the Caddo River, which may not have been the case. Thus, errors may have occurred in material loadings used in model simulations.

23. Outflow magnitudes were obtained from operating records, as were water surface elevations. Outflows varied considerably between 1979 and 1980, being higher during the spring of 1979 corresponding to the periods of high inflows. The project is equipped with a multilevel outlet structure. During the early portion of 1979, waters were released from outlets near the surface, after which the outlet location was lowered approximately 12 m.
Figure 5. Inflow temperatures into DeGray Lake
Figure 6. Inflow ammonia-nitrogen concentrations into DeGray Lake
Figure 7. Inflow phosphate-phosphorus concentrations into DeGray Lake
Figure 8. Inflow total dissolved solids concentrations into DeGray Lake
24. Meteorological data were obtained from the Little Rock, Ark., National Oceanic and Atmospheric Administration station, located approximately 100 km from the reservoir. Daily average equilibrium temperatures, solar radiation, and coefficients of heat exchange were computed from meteorological data using a modified version of the US Army Engineer District, Baltimore (1977), program.

**Computer Requirements**

25. All computations were conducted on a VAX 11/750 minicomputer. Hydrodynamics and temperature simulations were found to require approximately 0.0022 sec per model cell per time iteration. This time requirement was increased by approximately 10 percent for each water quality constituent included in simulations, if updated every time iteration. This application required 2.1 megabytes of virtual memory at runtime.
26. CE-QUAL-W2 was applied to DeGray Lake using data collected during 1979 and 1980. Data collected during 1979 were used for calibration and testing while data from 1980 were used for model verification. Graphical and statistical comparisons were made between model predictions and measured values. Following recommendations by Wlosinski (1984), the Reliability Index (RI) of Leggett and Williams (1981) was used as the primary statistic for comparison of predicted and measured values. The RI becomes larger as measured and observed values diverge, with an RI of 1.0 indicating a perfect prediction. The computation of the RI is discussed in Appendix A.

27. For some model variables, flux values were also computed. Fluxes, as used here, refer to the mass rate of transfer between state variables (after Patten 1971), as represented by the source/sink terms of the transport equation, integrated over time. Flux values have been shown by Wlosinski (1985) to be of utility in assessing model predictions by providing information on factors causing predicted concentrations. Unless indicated otherwise, all results presented in this section are from verification simulations.

**Time Steps**

28. Upon completion of the compilation of data sets and an initial run to check for errors in setup, simulations were conducted to determine the time steps required to maintain numerical stability. Provisions are included to allow users to specify up to 50 time step/iteration pairs, allowing reduced time steps during highly dynamic conditions, such as storm period, and increased time steps during more quiescent conditions, thereby saving computation time. The time step determination was accomplished by conducting simulations for 1979 and 1980 using a constant time step of 360 sec and examining water velocity snapshots for each day of simulation. Time steps were then estimated using internal Courant conditions (see Environmental and Hydraulics
Laboratories 1986). These estimates were found to be reasonably accurate during dynamic events such as storm periods; however, they extremely overestimated the time step that could be used during other periods.

29. The maximum time step that could be used during any period was 1,500 sec, while calculations using internal Courant conditions often yielded time step estimates an order of magnitude greater. Estimates of time steps were made using other criteria and while continuously searching the grid for the most limiting estimate. However, no single criterion was found that could reliably estimate the time step for use. Therefore, while time steps during dynamic conditions may be estimated using Courant conditions, it may be necessary to determine maximum time steps for particular applications by trial and error.

30. A total of eight time step/iteration pairs were identified for 1979 simulations, ranging from 360 to 1,500 sec, while only a single time step, 1,500 sec, was required of 1980. The use of multiple time steps for 1979 simulations reduced computation time to approximately 35 percent of that where a single time step was used.

Water Budget

31. A water balance, accounting for the various components of water entering or leaving DeGray Lake, was performed in studies by Ford and Stein (1984). Their computations indicated that residual errors occurred in the water balance which were attributed to ungauged flows. They suggested the use of a simple correction factor to adjust gauged inflows to account for the ungauged flow and achieve a year-by-year balance. Correction factors for 1974 to 1980 were computed. This approach was employed in this study, and gauged inflows were multiplied by 1.47 and 1.68 for the years 1979 and 1980, respectively, to achieve a water balance. This represents a relatively large error in flows. The approach further assumes that loadings from all sources are the same as those from the Caddo River, which may not be the case.
32. Comparisons were made between predicted and observed water surface elevations. Some discrepancies were noted, particularly in the latter part of the 1979 simulations, where predicted and observed water surface elevations differed by nearly 1 m. The discrepancy can be attributed, in part, to differences between actual and imposed geometries, as noted earlier. The differences, while relatively large, were considered insufficient to require modification of the spatial grid given the purposes of this application.

Hydrodynamics and Water Temperature

33. An option is provided CE-QUAL-W2 to allow simulation of hydrodynamics and temperatures independently of water quality constituents. This option was utilized to calibrate the model against measured temperature data. CE-QUAL-W2 predicts the average temperature of each cell using input data for surface heat exchanges, solar radiation, inflows, and outflows. Results can then be compared with measured data in order to assess the predictive capability of the model. Temperature predictions were compared with field data taken from DeGray Lake during 1979 for model calibration, using both the RI and graphical aids. Temperature was also utilized essentially as a "tracer" to allow evaluation of predicted circulation patterns.

34. Initial simulations yielded poor agreement between measured and predicted vertical temperature predictions. Predicted water temperatures were found to decrease uniformly with depth in a nearly exponential manner, while measured temperatures indicated development of a thermocline during summer months. Vertical temperature predictions were observed to be largely affected by the sheltering coefficient, which is used essentially to reduce wind speeds due to sheltering effects. However, setting the sheltering coefficient equal to zero, which effectively removed wind-driven mixing from computations, did not appreciably improve model predictions. The predicted temperature distributions
indicated that vertical mixing was being overestimated. This was also evidenced in tests involving conservative tracers. A tracer concentration placed in the layer corresponding to the observed thermocline was quickly eroded. A metalimnetic oxygen minimum commonly develops in DeGray Lake during summer months. The predicted excessive vertical mixing was sufficient to prevent the establishment of large gradients in this region.

35. The predicted excessive vertical mixing was attributed to two factors. The first factor was rounding errors. Tests were conducted with all flows and surface exchanges set equal to zero. In the absence of any driving force, it would be expected that no velocity field would develop. However, appreciable velocities were generated. The predicted velocities were found to remain at zero only if all real variables were double-precisioned (using 64-bit arithmetic in computations). Additional tests failed to reveal any single variable or group of variables that could be double-precisioned and achieve the same results. All real variables were then double-precisioned in all subsequent simulations. The addition of double-precisioning was found to increase computation times by approximately 50 percent. Ingram, Dent, and Radhakrishnan (1983) stated that single-precision arithmetic should be avoided when using a VAX minicomputer for scientific and engineering applications. Thus, the need for double-precision arithmetic may not be universal among computer systems and may not be required in applications with appreciable vertical mixing.

36. A second factor believed to have contributed to overestimations of vertical mixing resulted from differences in vertical diffusive heat transport between bottom and other model cells in the presence of a sloping bottom of the water body. Test simulations were conducted to identify factors contributing to vertical mixing in the absence of any external driving force. Simulations conducted without thermal stratification did not result in artificial velocities being generated. Simulations conducted with a stratified system produced only small velocities when the water body bottom was flat and widths were either constant or varied with depth. However, if the bottom was sloped, such as in the
DeGray spatial grid (Figure 3), relatively large velocities were generated. These artificial velocities were found to increase as the horizontal dispersion coefficient approached zero.

37. CE-QUAL-W2 models the bottom slope as a series of stairsteps, as demonstrated in Figure 3. In the absence of any external forces or velocity gradients, vertical diffusion occurs at a minimum specified rate (0.14 mm² sec⁻¹). Diffusion cannot occur through the water body bottom, restricting diffusive transport to the top face for bottom cells. Diffusion occurs through both top and bottom faces of all other model cells. For a stratified water body with a sloping bottom, the imbalance in diffusive transport results in slight temperature differences between model cells in a given layer since some are and some are not bottom cells. The temperature differences result in horizontal pressure gradients which ultimately induce velocities. As transport cannot occur through the side of the cells at the stairstep, additional temperature imbalances occur. As velocities are generated, the velocity gradient results in increased vertical diffusion, and a snowball effect is created. Increasing the longitudinal dispersion coefficient was found to decrease the artificial velocities. This is attributed to their reducing horizontal pressure gradients by essentially smearing the artificially introduced temperature differences.

38. Since the artificially induced velocities were found to decrease as the longitudinal dispersion coefficient was increased, additional simulations were conducted to estimate the minimum value that would allow resolution of the pronounced vertical gradients observed in DeGray Lake. It was found that the artificially introduced velocities did not allow pronounced vertical gradients to become established when the longitudinal dispersion coefficient was less than 10 m² sec⁻¹. Simulations with a longitudinal dispersion coefficient of 10 m² sec⁻¹ did not result in artificial velocities being generated for the case of a stratified system with a sloping bottom. This value was then retained for all subsequent simulations. The addition of double-precision arithmetic and increasing the longitudinal dispersion term for heat were found to dramatically improve model predictions.
39. Tests were then conducted to assess the impact of increased longitudinal dispersion coefficients on longitudinal gradients in predicted temperatures. For example, a test was conducted using a high-temperature inflow (77° C) of constant flow rate (11.33 m$^3$ sec$^{-1}$) to assess differences in the downstream extent of thermal plumes. After a steady-state temperature distribution was achieved, comparisons were made between longitudinal differences in isotherms. Differences of only approximately 1 km (one model segment = 0.997 km) were noted between predicted isotherms at 32° C or higher for longitudinal dispersion coefficients for heat of 1 m$^2$ sec$^{-1}$ and 10 m$^2$ sec$^{-1}$; this indicated that excessive smearing of longitudinal gradients did not occur. Additional testing may be required for applications where strong longitudinal gradients in temperature are expected. A separate longitudinal dispersion coefficient is utilized for all other constituents to allow different rates of longitudinal dispersion for heat and water quality variables.

40. CE-QUAL-W2 allows the specification of outlets from multiple layers at the dam. Each outlet is assigned a layer location and a flow. If the present surface layer is below the outlet layer, outflows from that layer do not occur. For outlets below the predicted water surface, the zones from which water is withdrawn are computed through the solution of the equations of motion. The computed withdrawal zones are accurately represented for line sinks* or outlets whose widths approach the width of the reservoir. However, for point sinks, where the outlet widths are only a small fraction of the total width of the reservoir, withdrawal zones may not be adequately represented.* This is a direct consequence of lateral averaging. To correct for this in this application, steady-state simulations were conducted using the SELECT mathematical withdrawal model (Bohan and Grace 1973) for several stratification and flow conditions. The total outflow was then proportioned among vertical layers of the 2-D model until the predicted withdrawal zones closely matched those predicted by SELECT.

* Personal Communication, 1986, Mark S. Dortch, Hydraulic Engineer, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
41. Additional testing of the model was conducted in relation to the thermal budget. CE-QUAL-W2 utilizes the equilibrium temperature approach (Edinger, Brady, and Geyer 1974) to predict surface heat exchange. The computation of equilibrium temperatures, solar radiation, and coefficients of heat exchange are performed in external programs and provided as data inputs. Temperature predictions were found to be sensitive to the windspeed function used to compute evaporative heat loss. The use of the windspeed function based upon studies by Harbeck, Koberg, and Hughes (1959) was found to improve water temperature predictions. Further comparisons were made between the equilibrium temperature approach and a full heat balance as is used in the one-dimension (1-D) model, CE-QUAL-R1 (Environmental Laboratory 1982). A full heat balance was incorporated into CE-QUAL-W2, and temperature predictions were compared with those obtained using the equilibrium temperature approach. Differences between model predictions were slight (less than 0.5°C in surface waters), and the equilibrium temperature approach was retained for use in the model. The equilibrium approach has the advantage that factors affecting surface heat exchange may be computed by preprocessor programs and provided as data in simulations, allowing a savings in computation time.

42. The model allows inclusion of wind direction effects relative to the water body orientation (relative to north) on wind-driven mixing. However, time-varying data on wind direction were not available for the DeGray application. The effect of changing wind direction and seasonal variations in sheltering were included in simulations by using varying wind sheltering coefficients for different times of the year. The sheltering coefficient was varied from 0.7 in the early spring to 0.3 during the late summer, based upon average wind direction information from Ford and Stein (1984) and sheltering due to surrounding topography. The inclusion of a variable sheltering coefficient improved temperature predictions. However, this approach did not allow evaluation of formulations in CE-QUAL-W2 to predict cross wind shear effects on surface mixing.
43. Simulations were also conducted varying the Chezy resistance coefficient, used in the computation of bottom shear. Model predictions were found to be relatively insensitive to variations in the Chezy coefficient, in the range of 50 to 90 m$^{1/2}$ sec$^{-1}$. Hydraulic parameters used in final calibration and verification simulations are provided in Table 2.

44. Simulations for both 1979 and 1980 indicated that, prior to thermal stratification, inflows to the reservoir generally occurred as overflows, with plunging flows near the dam and strong upstream return flows at middepths (Figure 9). The overflows resulted from inflows being warmer and less dense than reservoir waters. Following stratification, inflows generally were predicted to enter as interflows with associated flow reversals both at the water surface and below the interflow. Velocities during the summer months were generally small due to the low magnitude of inflows and outflows. During the fall, additional storm events contributed to mixing, but the dominant mixing mechanism was convective as surface waters cooled. Convection did not result in complete mixing of the reservoir by the end of the calibration or verification simulations, which was consistent with field observations.

45. Vertical profiles of predicted and measured temperatures for two sampling stations on DeGray over the verification year are shown in Figure 10. As can be seen, model predictions closely match measured data, although the depth of the thermocline was consistently overestimated. The seasonal variations in stratification are also correctly predicted. The RI for water temperature predictions over the verification year varied from 1.12 to 1.16 (Table 3) for the three stations as compared with 1.11 for the DeGray application of the 1-D model CE-QUAL-R1 (Wlosinski and Collins 1985).

**Biological/Chemical Predictions and Comparisons**

46. Upon completion of calibration of the physical components of the system, calibration of biological/chemical constituents began. The major objective of the application of CE-QUAL-W2 was to assess its
Table 2
Partial Listing of Coefficients and Constants Used in the 
DeGray Application of CE-QUAL-W2

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Unit*</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic parameters</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Longitudinal dispersion of momentum</td>
<td>$m^2/\text{sec}$</td>
<td>10.0</td>
</tr>
<tr>
<td>Longitudinal dispersion of heat</td>
<td>$m^2/\text{sec}$</td>
<td>10.0</td>
</tr>
<tr>
<td>Longitudinal dispersion of constituents</td>
<td>$m/\text{sec}$</td>
<td>1.0</td>
</tr>
<tr>
<td>Chezy coefficient</td>
<td>$m^{1/2}/\text{sec}$</td>
<td>70.0</td>
</tr>
<tr>
<td>Radiation absorbed in surface layer</td>
<td>$m/\text{sec}$</td>
<td>0.45</td>
</tr>
<tr>
<td>Light attenuation coefficient</td>
<td>$m$</td>
<td>0.40</td>
</tr>
<tr>
<td>Attenuation coefficient for inorganic Suspended solids</td>
<td>$m/\text{g}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Attenuation coefficient for organic Suspended solids</td>
<td>$m/\text{g}$</td>
<td>0.10</td>
</tr>
<tr>
<td>Suspended solids settling rate</td>
<td>$m/\text{day}$</td>
<td>2.0</td>
</tr>
<tr>
<td>DOM</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Labile DOM decay rate</td>
<td>$\text{day}^{-1}$</td>
<td>0.12</td>
</tr>
<tr>
<td>Transfer rate (labile to refractory)</td>
<td>$\text{day}^{-1}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Refractory DOM decay rate</td>
<td>$\text{day}$</td>
<td>0.001</td>
</tr>
<tr>
<td>Phytoplankton</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maximum growth rate</td>
<td>$\text{day}^{-1}$</td>
<td>1.1</td>
</tr>
<tr>
<td>Settling rate</td>
<td>$m/\text{day}$</td>
<td>0.14</td>
</tr>
<tr>
<td>Phosphorus half-saturation constant</td>
<td>$\text{mg}^{1/2}/\text{L}$</td>
<td>0.009</td>
</tr>
<tr>
<td>Nitrogen half-saturation constant</td>
<td>$\text{mg}^{1/2}/\text{L}$</td>
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</tr>
<tr>
<td>Saturation light intensity</td>
<td>$W/\text{m}^2$</td>
<td>150.0</td>
</tr>
<tr>
<td>Dark respiration rate</td>
<td>$\text{day}^{-1}$</td>
<td>0.017</td>
</tr>
<tr>
<td>Photorespiration rate</td>
<td>$\text{day}^{-1}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Mortality rate</td>
<td>$\text{day}$</td>
<td>0.01</td>
</tr>
<tr>
<td>Detritus</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Decay rate</td>
<td>$\text{day}^{-1}$</td>
<td>0.06</td>
</tr>
<tr>
<td>Settling rate</td>
<td>$m/\text{day}$</td>
<td>0.35</td>
</tr>
<tr>
<td>Nitrogen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ammonia decay (nitrification) rate</td>
<td>$\text{day}^{-1}$</td>
<td>0.12</td>
</tr>
<tr>
<td>Nitrate reduction rate</td>
<td>$\text{day}$</td>
<td>0.12</td>
</tr>
<tr>
<td>Sediment release rate</td>
<td>$g/\text{m}^2/\text{day}$</td>
<td>0.08, 0.02**</td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>$m/\text{g}$</td>
<td>1.0</td>
</tr>
</tbody>
</table>

* Note that units of per day given here are converted to units of per second in simulations.

** Higher value refers to the transition zone and lower value to the lacustrine zone.

(Continued)
<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Unit*</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phosphorus</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sediment release rate</td>
<td>g m⁻²day⁻¹</td>
<td>0.015, 0.004**</td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>m⁻¹g⁻¹</td>
<td>1.2</td>
</tr>
<tr>
<td>Dissolved oxygen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sediment oxygen demand</td>
<td>g m⁻²day⁻¹</td>
<td>1.0, 0.25**</td>
</tr>
<tr>
<td>Total iron</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sediment release rate</td>
<td>g m⁻²day⁻¹</td>
<td>0.5, 0.125**</td>
</tr>
<tr>
<td>Settling rate</td>
<td>m⁻¹day⁻¹</td>
<td>2.0</td>
</tr>
<tr>
<td>Stoichiometric coefficients</td>
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<td></td>
</tr>
<tr>
<td>Phosphorus</td>
<td></td>
<td>0.011</td>
</tr>
<tr>
<td>Carbon</td>
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<td>0.45</td>
</tr>
<tr>
<td>Nitrogen</td>
<td></td>
<td>0.08</td>
</tr>
<tr>
<td>Oxygen</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ammonia</td>
<td></td>
<td>4.57</td>
</tr>
<tr>
<td>Detritus</td>
<td></td>
<td>1.40</td>
</tr>
<tr>
<td>Algal respiration</td>
<td></td>
<td>1.10</td>
</tr>
<tr>
<td>Photosynthesis</td>
<td></td>
<td>1.40</td>
</tr>
</tbody>
</table>
Figure 9. Predicted circulation patterns for three periods during the 1980 verification simulations. Vector lengths are scaled for a certain number of hours (specified at the top of each section) where the same vector length represents a greater velocity magnitude as the scale becomes smaller.
Figure 10. Predicted and observed water temperatures for the 1980 DeGray Lake verification simulations (Continued)
LEGEND

--- SIMULATION

X OBSERVED

b. Lacustrine zone (Station 4)

Figure 10. (Concluded)
Table 3
Reliability Index for Calibration and Verification Simulations of Selected Constituents

<table>
<thead>
<tr>
<th>Constituent</th>
<th>1979 Calibration</th>
<th>1980 Verification</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Station 4</td>
<td>Station 12</td>
</tr>
<tr>
<td>Temperature</td>
<td>1.14</td>
<td>1.16</td>
</tr>
<tr>
<td></td>
<td>1.15</td>
<td>1.12</td>
</tr>
<tr>
<td>DOM</td>
<td>1.29</td>
<td>1.44</td>
</tr>
<tr>
<td></td>
<td>1.51</td>
<td>1.68</td>
</tr>
<tr>
<td>Phosphate-phosphorus</td>
<td>2.93</td>
<td>3.44</td>
</tr>
<tr>
<td></td>
<td>4.43</td>
<td>2.43</td>
</tr>
<tr>
<td>Ammonia-nitrogen</td>
<td>6.20</td>
<td>4.15</td>
</tr>
<tr>
<td></td>
<td>3.66</td>
<td>3.16</td>
</tr>
<tr>
<td>Nitrate-nitrogen</td>
<td>2.18</td>
<td>4.47</td>
</tr>
<tr>
<td></td>
<td>2.40</td>
<td>3.97</td>
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<tr>
<td>DO</td>
<td>1.53</td>
<td>1.85</td>
</tr>
<tr>
<td></td>
<td>1.62</td>
<td>1.78</td>
</tr>
<tr>
<td>TDS</td>
<td>1.74</td>
<td>2.33</td>
</tr>
<tr>
<td></td>
<td>2.26</td>
<td>1.79</td>
</tr>
<tr>
<td>Algae</td>
<td>3.93</td>
<td>--</td>
</tr>
<tr>
<td></td>
<td>8.83</td>
<td>--</td>
</tr>
<tr>
<td>Total iron</td>
<td>10.80</td>
<td>1.25</td>
</tr>
<tr>
<td></td>
<td>6.19</td>
<td>4.78</td>
</tr>
</tbody>
</table>
capability to simulate water quality in both the vertical and longitudinal directions over time. An additional objective was to determine the minimum resolution, in terms of constituents, required to adequately describe the system. This analysis resulted in the number and arrangement of constituents described earlier. This exercise also revealed errors and deficiencies in the coding which were corrected. Biological/chemical predictions and comparisons are discussed separately for each of the major constituents. Values of various model parameters resulting from model calibration are provided in Table 2. The values of model parameters were well within ranges reported in the literature, as summarized in the model user's manual (Environmental and Hydraulics Laboratories 1986). The parameter values were initially taken from a previous application of the 1-D model CE-QUAL-R1 (Wlosinski and Collins 1985) for those processes in common for the two models. Many of the values, including temperature and stoichiometric coefficients, were not changed in the application of CE-QUAL-W2.

47. Table 3 presents the computed RI's for calibration and verification simulations at Stations 4 and 12 (see Figure 1). The RI for water temperature is relatively low and is comparable between stations and simulation years. For other constituents which exhibit a greater degree of variability, the RI is generally larger and less comparable between stations and simulation years. The RI's provide an overall indication of the model's performance. However, it must be realized that poorer RI's must be expected for constituents such as phosphate-phosphorus, which can vary several orders of magnitude in concentration.

Temperature effects

48. Most biological and chemical rates are temperature dependent. The temperature effects on biological/chemical processes in CE-QUAL-W2 are computed using the formulation of Thornton and Lessem (1978). The formulation describes, in general, how biological/chemical processes exhibit an optimum range and diminish (asymmetrically) at higher and lower temperatures. The required temperature values and rate coefficients were obtained from a previous application of the 1-D reservoir
model, CE-QUAL-R1, to DeGray Lake (Wlosinski and Collings 1985) and were used without modification.

49. The temperature rate multipliers are computed in a separate subroutine in the source code. Temperature rate multipliers are produced for each process using predicted temperatures for each model cell. The resulting number of rate multipliers that must be computed makes this subroutine the most expensive, in terms of computation time, of the process descriptions. However, the temperature variations that occur over typically short computation intervals may have a negligible effect on biological/chemical rates. Therefore, provisions were made to allow temperature rate multipliers to be updated only after a selected number of time iterations, thereby allowing savings in computation time. Updates were keyed to a number of time iterations rather than elapsed time to allow for frequent updates during more dynamic periods, such as storm events, which require a smaller time step for stability. Simulations were conducted to determine the effect of varying the update interval, and no observable differences in model predictions were observed for up to 24 time steps between updates. This update frequency was then retained for all subsequent simulations and corresponded to updating temperature rate multipliers every 10 hr or less of simulation.

Update Intervals

50. The constituent sources and sinks are separated into two parts in CE-QUAL-W2—those due to boundary loadings (such as inflows) and those due to constituent reactions (such as decomposition). The boundary loadings are provided as input data and were updated each day for flow and temperature and every 2 weeks for other constituents (see Section Boundary Conditions, PART IV). The sources and sinks due to constituent reactions are computed in a series of subroutines which, if called every computational time step, may significantly add to the computational cost of performing simulations. However, the driving forces causing changes in the computed source/sink terms may be small between the time steps required for computing hydrodynamics (which varied from 6 to 25 min in this application). For example, the process descriptions are affected by water temperatures, but variations in computed water
temperatures may be small between time steps. Thus, it may often be possible to update the source/sink terms due to reactions (by making calls to subroutines) less frequently than hydrodynamics.

51. An option is included to allow updating of constituent sources and sinks due to reactions at different frequencies than hydrodynamics. Simulations were conducted to determine the effects of varying reaction update frequencies on model predictions and the resulting savings in computation time. Tests consisted of varying the reaction update interval and computing and comparing the predicted concentrations and model fluxes (factors causing variations in concentrations). For the conditions simulated, updating constituent sources and sinks (due to reactions) only every 12 iterations had no effect on model predictions and resulted in over a 30-percent savings of computation time. Increasing the number of iterations between updates beyond this point did not result in appreciable additional savings. This update frequency (updating every 12 iterations) was used in all final calibration and verification simulations. However, in test simulations where meteorological conditions were updated at hourly intervals, setting the update frequency for constituent source and sink reactions to greater than two iterations per update did result in differences in model predictions; this was due to the approximately 0.5-hr time steps used during parts of 1979 and all of 1980. Thus, updating constituent source and sink reactions less frequently than hydrodynamics can result in a considerable savings in computation time, but care should be exercised in selecting update frequencies. For example, the selection of the frequency for updating reactions should consider the frequency of updating boundary conditions. Additionally, the values for constituent rates (such as settling velocities) should be considered in order to avoid errors. Initial simulations should be conducted with frequent updating for comparisons with simulations using less frequent updates to determine if errors are introduced.

Tracer

52. An arbitrary conservative material was included in the model to allow simulation of tracer studies and to facilitate testing and
calibration of flow regimes. The tracer was used to evaluate the effects of mixing on material distributions and the capability of the model to predict overflows, interflows, and underflows. The tracer was found to be a valuable tool in assessing hydrodynamic predictions.

53. Johnson et al. (1981) performed studies of storm events on DeGray using LARM, a precursor of the GLVHT model on which CE-QUAL-W2 is based, by simulating conservative materials and comparing results with field measurements. They indicated that LARM correctly predicted inflow placements, travel times, and dilutions and provided a valuable tool in evaluating impacts of storm events.

**Inorganic suspended solids**

54. Inorganic suspended solids were included in the model primarily because of their importance in the sorption of nutrients and toxic materials. Inorganic suspended solids effects are also included in formulations for computing water density and the extinction coefficient for light, thereby affecting temperature, water movement, and algal growth.

55. Inorganic suspended solids are affected only by transport and settling and are obtained only through allochthonous sources. Settled inorganic solids are not accumulated, and no provisions are made for resuspension. The apparent settling velocity used in CE-QUAL-W2 may be somewhat higher than that of one-dimensional or compartment (box type) models since transport effects are explicitly described.

56. Simulations indicated that predictions of inorganic suspended solids concentrations were sensitive to variations in settling velocities. The effect of increased settling velocities was to cause solids to be settled in upper regions of the reservoir during quiescent periods. Relatively high concentrations of inorganic suspended solids were predicted to extend downreservoir only during storm events. Therefore, inorganic suspended solids effects on predicted light and nutrient availability were greatest within the transition zone. No field data were available specifically for inorganic suspended solids. Total solids and dissolved solids were measured, providing a measurement of total suspended solids (combined organic and inorganic components).
Additionally, no data were available for suspended solids at Station 4 for 1979 calibration year, and data were limited at other stations. Therefore, no rigorous attempt was made to estimate inorganic suspended solids or to calibrate and verify inorganic suspended solids predictions.

**Coliform bacteria**

57. The capability of simulating coliform bacteria is essential due to their wide use as indicators of contamination and as the basis for water quality standards. Coliforms are derived only from allochthonous sources and are affected only by transport and mortality. Model formulations allow simulation of effects of die-off and dilution on laterally averaged coliform concentrations.

58. Johnson et al. (1981) evaluated coliform predictions during storm events at DeGray using LARM (upon which CE-QUAL-W2 is based). They determined that coliform distributions and die-off could be correctly predicted. This constituent was further tested in this application, but no rigorous attempt was made to verify predictions against field data. However, simulations indicated that coliforms were generally removed within the transition zone of the reservoir, which was consistent with field data.

**Total dissolved solids**

59. Total dissolved solids (TDS) affect water density and its ionic strength, thereby affecting water movement, pH, and the distribution of carbonate species. TDS are treated as a conservative constituent and are affected only by transport. An option is included for the use of salinity (parts per thousand) rather than TDS (parts per million) in simulations, and this choice is also reflected in calculations of density and ionic strength. Only TDS were used in this application.

60. Model predictions (Figure 11) indicated that TDS remained relatively constant over the verification year, while measured values varied considerably, particularly at Station 12. This variability is further evidenced in the relatively high computed RI values for TDS (Table 3). Wide TDS variations over relatively short time periods were evident in data collected during both 1979 and 1980. It is not known if
Figure 11. Predicted and observed TDS concentrations for the 1980 DeGray Lake verification simulations (Continued)

LEGEND

--- SIMULATION

X OBSERVED

a. Transition zone (Station 12)
b. Lacustrine zone (Station 4)

Figure 11. (Concluded)
these variations result from some phenomena not considered in model formulations or if they represent errors in the data set.

**Dissolved organic matter**

61. DOM in this study was estimated by dividing measured concentrations of dissolved organic carbon by the coefficient 0.45, assuming that 45 percent of organic matter is composed of carbon (dry weight). The DOM was then further subdivided into labile and more refractory components. It was assumed that all of the DOM initially in the reservoir and 70 percent of the inflow DOM consisted of refractory compounds. This partitioning was based on previous modeling studies* and model calibration, and was somewhat arbitrary since few data were available for fractioning organic matter. However, specifying a higher percentage of labile components in initial DOM resulted in excessive losses of both DOM and DO. This study indicated the importance of separating DOM into different groups.

62. Model predictions were found sensitive to variations in decay rates of both labile and more refractory components of DOM. The decay rates used in final calibration and verification simulations of DOM are provided in Table 2.

63. Measured and predicted total DOM (labile + refractory) compared favorably, as demonstrated by time series of vertical profiles (Figure 12) and the computed RI values (Table 3). Both predicted and observed total DOM remained relatively constant. This was consistent with the assumption that the majority of DOM was refractory. Labile DOM was derived from inflows and algal photorespiration and mortality, and exhibited the greatest variability in surface waters and in the transition zone. The majority of inflow labile DOM was predicted to degrade within the transition zone (Figure 13) and had greatest impacts upon DO and nutrient dynamics in that region.

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* Personal Communication, 1986, J. H. Wlosinski, Aquatic Biologist, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.
Figure 12. Predicted and observed total DOM concentrations for the 1980 DeGray Lake verification simulations (Continued)
b. Lacustrine zone (Station 4)

Figure 12. (Concluded)
Algae

64. Predicted algal populations are affected by growth, mortality, photorespiration, dark respiration, and settling. Algal growth is computed from a maximum growth rate which is modified by water temperature, light, and nutrient availability. Photorespiration is affected by light and water temperature. Dark respiration is affected by water temperature. Algal mortality reflects both natural and predator mortality. Rate constants for these processes used in final calibration and verification simulations are provided in Table 2. Algal mortality and photorespiration serve as a source for labile DOM and detritus, with 80 percent of mortality being assigned to detritus. Algal growth affects predicted DO, inorganic carbon, and nutrient concentrations, while dark respiration affects DO and inorganic carbon. Algal populations, as well as detritus and inorganic suspended solids, affect light availability, allowing simulation of self-shading.

65. Predicted algal populations were found to sensitive to growth rates, particularly in the timing of blooms. The respiration, settling, and mortality rates also affected predicted algal concentrations.
Populations were also found sensitive to predicted phosphorus concentrations of surface waters, and phosphorus was the primary factor limiting growth. Predictions where phosphorus was overestimated resulted in higher predicted algal populations than observed, particularly in the fall following the introduction of phosphorus into surface waters by increased mixing. Efforts to predict reasonable fall algal concentrations resulted in populations at other times of the year being slightly low. This difficulty was attributed to deficiencies in descriptions of phosphorus dynamics (see subsection, Phosphate-phosphorus), and additional work may be required in this area.

66. Problems associated with predicting algal populations were also a consequence of the simplified descriptions of algal dynamics. Only a single algal compartment was provided and, in this study, all rate terms were assumed to apply over the entire year. In future applications, specification of different rate terms reflecting dominant forms of phytoplankton present may be required as seasonal changes occur in population structure.

67. Predicted fluxes, or factors causing variations in predicted concentrations, were computed for 1979 simulations (Martin and Wlosinski 1985). Predicted gross primary production for the reservoir was computed to be $0.44 \times 10^{10}$ g DO. Net primary production was $0.32 \times 10^{10}$ g DO compared with estimates from field data of $0.66 \times 10^{10}$ g DO for 1979 (calculated from Gaugush and Downing 1986). The differences in observed and predicted net productivity were not considered unreasonable considering the difficulties in obtaining accurate estimates of whole lake net primary productivity. Field data also indicated that net productivity averaged 38 percent higher in the transition zone than the lacustrine zone; the model predictions averaged 20 percent higher in the transition zone than the lacustrine zone. Predicted algal respiration for the reservoir during 1979 was 26 percent of gross primary productivity as compared with averages of 20 to 30 percent for temperate lakes (Wetzel 1975). Whittaker (1975) indicated that algal respiration averages 30 to 40 percent of gross primary productivity.
68. A time series of predicted vertical profiles for algae at Station 12 and a comparison between predicted and observed concentrations at Station 4 for the verification year are provided in Figure 14. Note that some of the predicted algal populations early in the year are essentially zero. As can be seen, predicted and observed data compared favorably at Station 4. However, productivity was underestimated, and sufficient differences occurred between predicted and observed values to result in a relatively poor RI index for both calibration and verification simulations (Table 3). No verification data were available for Station 12.

Detritus

69. Detritus refers to particulate (nonliving) organic matter. Detritus is derived from boundary loadings and algal mortality and is lost through decomposition and settling. Decomposition of detritus releases nutrients and inorganic carbon and depletes DO. Model predictions indicated that detritus occurred primarily in surface waters during the springtime, and peak concentrations occurred in subsurface waters during other times of the year. The effects of detritus on predictions of other constituents were generally small. For example, detritus decay contributed only 4 percent of total DO depletions over the reservoir for 1979 simulations.

70. No calibration or verification data were available for detritus. Data were collected during 1979 for particulate organic carbon, which can be converted to particulate organic matter by dividing by 0.45, assuming that dry organic matter is 45-percent carbon. This estimate of particulate organic matter provided an upper bound for detritus. Predicted detritus concentrations for 1979 remained within this upper bound. Further estimates of detritus could be obtained by decreasing particulate organic matter by observed phytoplankton concentrations. Since detection limits varied and the two parameters were estimated using different techniques, this calculation often resulted in negative detritus predictions. These estimates were considered to have only limited value and are not presented. However, the comparisons
Figure 14. Predicted and observed algal concentrations for the 1980 DeGray Lake verification simulations (Continued)
Figure 14. (Concluded)
between predicted and calculated detritus concentrations did indicate that predicted concentrations were not unrealistic.

71. The settling and decay rates for detritus (Table 2) were within ranges reported in the literature as provided in the CE-QUAL-W2 user's manual (Environmental and Hydraulics Laboratories 1986), although a wide range of values is reported depending upon detrital characteristics.

**Phosphate-phosphorus**

72. The phosphate-phosphorus compartment in CE-QUAL-W2 is intended to simulate primarily soluble reactive phosphorus which is available for algal utilization. Particulate phosphorus (organic and inorganic) is implicitly simulated using algal and detritus groups as well as adsorption onto solids (inorganic suspended solids, iron, detritus, and algae). Algal dark respiration and the decay or decomposition of DOM, detritus, and sediments serve as sources for phosphorus while phosphorus is lost due to algal uptake and adsorption and settling. Sediment phosphorus release is allowed to occur only if DO falls below a specified minimum value (0.5 in the application). The various coefficients and constants used in final calibration and verification simulations which affected phosphorus predictions are provided in Table 2.

73. Phosphorus concentrations largely controlled predicted algal production in the surface waters of DeGray. Simulations of phosphorus indicated that two areas require further attention in future modeling studies. One area is the interaction between iron and phosphorus. Soluble iron is released under anoxic conditions and rapidly becomes insoluble under oxic conditions. The adsorption of phosphorus onto iron in oxic waters and its subsequent settling is a major mechanism for phosphorus removal. This effect was particularly important in the lacustrine zone of DeGray due to the low concentrations of other suspended solids.

74. Kennedy, Montgomery, and James (1983) emphasized the importance of algae and iron complexes in the sedimentation of phosphorus in DeGray. However, difficulties were encountered in simulating
phosphorus-iron interactions. The result was that while adsorption and sedimentation did allow phosphorus removal, it prevented sufficient phosphorus from reaching the photic zone to sustain observed levels of algal production. Simulations conducted without iron or using low partition coefficients allowed higher productivity during summer months but resulted in excessive algal growth in the fall when mixing introduced phosphorus accumulated in anoxic waters. Simulations were conducted using varying settling rates, partition coefficients, or introducing soluble and particulate phosphorus as state variables; however, these changes did not resolve the problem.

75. The second problem requiring further attention involves the kinetics of phosphorus adsorption and desorption. This process was assumed to be at equilibrium, with phosphorus adsorbed in oxic waters and desorbed under anoxic conditions. This assumption led to relatively high phosphorus concentrations extending into the region of the metalimnetic DO minimum of the lacustrine zone, which was contrary to field observations. It was hypothesized that adsorbed phosphorus settling through the relatively thin oxygen-depleted metalimnion may not have been retained sufficiently long for desorption to occur.* Thus, phosphorus was probably removed from the metalimnetic zone as it was mixed out of the zone, became associated with particulates, and settled through the zone without becoming completely desorbed. This effect was simulated by not allowing desorption in the lacustrine zone, which allowed observed trends to be adequately characterized. However, this approach lacks generality, and additional work is required to identify and incorporate mechanistic descriptions of these phenomena.

76. Sediment release under anoxic conditions was a major source of predicted phosphorus concentrations in the transition zone of DeGray. Predicted elevated concentrations occurred following the onset of anoxic and remained until the introduction of oxygen during fall mixing, as is demonstrated by Figure 15. This trend was consistent with field

* Personal Communication, 1986, J. M. Brannon, Research Chemist, US Army Engineer Waterways Experiment Station, Vicksburg, Miss.

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Figure 15. Shaded contours of predicted phosphorus concentrations for the 1980 DeGray Lake verification simulations (concentrations in milligrams per litre)
observations, and Kennedy, Montgomery, and James (1983) indicated that anoxic sediments were a major source of phosphorus during summer months. Sediments of the upper end of DeGray appeared phosphorus-enriched as compared with the low end, as evidenced by nutrient ratios (Gunkel et al. 1984), and the majority of the material loadings occurred during fall, winter, and spring storm events (Kennedy, Montgomery, and James 1983). Phosphorus that accumulated in the anoxic hypolimnetic waters of the transition zone appeared to be a major source of phosphorus for algal growth, as evidenced by higher predicted productivity in the transition zone than in the lacustrine zone, which was consistent with field observations.

77. The importance of internal loadings in the phosphorus dynamics of DeGray was further evidenced by simulations where phosphorus was removed from inflows. The removal of phosphorus from inflows did not result in any discernible differences in model predictions. Thus, for this system, complete phosphorus removal from inflows may have little impact on nutrient dynamics as long as sediments serve as a major source.

78. The specified sediment release rate for phosphorus was dependent upon sediment oxygen demand (SOD). The SOD was mapped into two zones in the reservoir (see subsection, Dissolved oxygen), resulting in a phosphorus release rate of 0.015 g m\(^{-2}\) day\(^{-1}\) in the transition zone and 0.0038 g m\(^{-2}\) day\(^{-1}\) in the lacustrine zone, for a reservoir-wide average release rate of approximately 0.01 g m\(^{-2}\) day\(^{-1}\). The phosphorus release rates specified in this application were greater than the computed release rate of 0.001 in the application of the 1-D model CE-QUAL-R1 (Wlosinski and Collins 1985). Chamber studies of sediments collected at DeGray Lake by Chen, Brannon, and Gunnison (1984) did not detect sediment phosphorus release.

79. Observed and predicted phosphorus concentrations are compared graphically in Figure 16, and computed RI values are provided in Table 3. Variations in the vertical distribution of phosphorus over time were adequately characterized both in the transition (Station 12) and lacustrine (Station 4) zones.

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Figure 16. Predicted and observed phosphorus concentrations for the 1980 DeGray Lake verification simulations (Continued)
b. Lacustrine zone (Station 4)

Figure 16. (Concluded)
Ammonia-nitrogen

80. Ammonia-nitrogen is affected by nitrate reduction and nitrification in addition to the processes affecting phosphorus. The coefficients and constants affecting ammonia predictions are provided in Table 2. As with phosphorus, sediment release under anoxic conditions in the transition zone was a major source of predicted ammonia concentrations. Elevated ammonia concentrations were predicted to occur following the onset of anoxia and remain until the introduction of oxygen during fall mixing, as is demonstrated in Figure 17. Predicted concentrations in the anoxic zone were much higher than phosphorus concentrations, as would be expected from their stoichiometry. As with phosphorus, elevated concentrations were restricted to the anoxic hypolimnion of the transition zone and did not extend into the lacustrine zone.

81. The sediment release rate for ammonia-nitrogen was based upon SOD. SOD was mapped into two zones in the reservoir (see subsection Dissolved oxygen), resulting in a sediment release rate for ammonia-nitrogen of $0.08 \text{ g m}^{-2} \text{ day}^{-1}$ in the transition zone and $0.02 \text{ g m}^{-2} \text{ day}^{-1}$ in the lacustrine zone, for a reservoir-wide average of approximately $0.05 \text{ g m}^{-2} \text{ day}^{-1}$. The average value was greater than the computed sediment release rate of $0.01 \text{ g m}^{-2} \text{ day}^{-1}$ from the DeGray application of the 1-D model CE-QUAL-R1 (Wlosinski and Collins 1985) and the release rate of $0.02 \text{ g m}^{-2} \text{ day}^{-1}$ determined in chamber studies of DeGray lake sediments (Chen, Brannon, and Gunnison 1984).

82. Predicted and observed vertical profiles for a number of observation dates are provided in Figure 18, and computed RI values are provided in Table 3. Seasonal variations in ammonia concentrations were considered to be adequately characterized.

Nitrate-nitrogen

83. This model variable represents both nitrate and nitrite-nitrogen and is affected by nitrate reduction under low DO conditions (below or equal to $0.5 \text{ mg l}^{-1}$ in this study) and nitrification of ammonia-nitrogen under oxic conditions (above $0.5 \text{ mg l}^{-1}$) as well as by
Figure 17. Shaded contours of predicted ammonia-nitrogen concentrations for the 1980 DeGray Lake verification simulations (concentrations in milligrams per litre)
Figure 18. Predicted and observed ammonia-nitrogen concentrations for the 1980 DeGray Lake verification simulations (Continued)
b. Lacustrine zone (Station 4)

Figure 18. (Concluded)
algal uptake. Coefficients and constants affecting predicted nitrate-nitrogen concentrations are provided in Table 2.

84. The effect of algal uptake on nitrate concentrations is demonstrated by observed and predicted surface concentrations (Figure 19) at Stations 4 and 12. Complete uptake was not predicted in the verification year due to the slightly low predicted algal productivity. Where productivity was higher, such as in 1979 simulations, depletion of nitrates from surface waters was predicted. The effect of nitrate reduction was evidenced by vertical profiles at Station 12, where nitrates are removed after the onset of anoxia. Predicted concentrations remained low until the introduction of oxygen during fall mixing, after which they increased to near the initial conditions due to nitrification of the pool of ammonia-nitrogen accumulated under anoxic conditions.

**Dissolved oxygen**

85. Dissolved oxygen is a fundamental water quality parameter, and evaluating model capabilities in predicted DO variations and identifying factors affecting those predictions were of major emphasis in this research. Reaeration and photosynthesis serve as sources of DO, while algal respiration and the decay or decomposition of ammonia-nitrogen, detritus, sediments, and DOM deplete DO. Coefficients and constants affecting DO are provided in Table 2. Inflows remained a source of DO, and outflows, a sink for all simulations.

86. Dissolved oxygen predictions were found to be very sensitive to variations in SOD. In this study, SOD was modeled exclusively by specifying zeroth-order decay rates (in units of mass area$^{-2}$ time$^{-1}$). The reservoir was mapped into two zones, with a rate of 1.0 g m$^{-2}$ day$^{-1}$ for the transpiration zone and 0.25 g m$^{-2}$ day$^{-1}$ for the lacustrine zone. This mapping was based on studies by Gunkel et al. (1984) which indicated an abrupt change in sediment particle size 12 to 13 km above the dam, reflecting differences between the inundated soils of the lower end and postimpoundment deposition in the upper end.

87. The SOD value in the lacustrine zone was similar to computed SOD (0.27 g m$^{-2}$ day$^{-1}$) in the application of a 1-D model to DeGray by
Figure 19. Predicted and observed nitrate-nitrogen concentrations for the 1980 DeGray Lake verification simulations (Continued)
LEGEND

SIMULATION
X OBSERVED

b. Lacustrine zone (Station 4)

Figure 19. (Concluded)
Wlosinski (1985), and was less than the value of 0.373 g m\(^{-2}\) day\(^{-1}\) determined from chamber studies by Chen, Brannon, and Gunnison (1984). The reservoir-wide average of SOD in the 1979 CE-QUAL-W2 simulations was near 0.6 g m\(^{-2}\) day\(^{-1}\). Variations in SOD had greatest effect in the lacustrine zone, and increasing the specified SOD from only 0.25 to 0.3 resulted in excessive DO depletions in the hypolimnion. This demonstrated the strong influence of SOD on DO dynamics in the hypolimnion of the lacustrine zone. The SOD and transport (advective and diffusive) along accounted for 90 percent of the predicted DO variations in this region.

88. The predicted DO dynamics of DeGray were also found to be sensitive to other factors, such as decay and decomposition. Predicted algal populations were only found to appreciably impact DO directly when populations were high. However, indirect effects through production of DOM and detritus did impact DO dynamics.

89. Cumulative DO fluxes were computed on a reservoir-wide basis for each process affecting DO variations for the 310-day simulation period ending on 12 December 1979 (Figure 20). Greatest sources of DO were found to be, in decreasing order of importance, reaeration, inflows, and gross primary productivity. Greatest sinks were found to be, in decreasing order of importance, SOD, outflow, labile DOM decay, decay of more refractory DOM (R-DOM) components, algal respiration, ammonia decay (nitrification), and detritus decay. Transport, reaeration, SOD, and DOM decomposition alone accounted for over 80 percent of the total DO variation in the reservoir. However, simulations conducted with only these processes resulted in poor resolution of DO variations. Thus, while the reservoir-wide impact of some factors affecting DO are relatively small, they should be included in simulations due to their effects on the distribution of DO in both space and time.

90. The predicted hydrodynamics also had a great impact on DO predictions, as would be expected. In turn, DO simulations aided in calibration of hydrodynamics as well as in identifying and correcting problems in hydrodynamic predictions. The DO dynamics were only adequately represented after hydrodynamics were properly characterized.
Figure 20. Predicted DO fluxes accumulated on a reservoir-wide basis over the 310-day simulation period in 1979.

TOTAL POSITIVE FLUX = 2.22 x 10^{10} G
TOTAL NEGATIVE FLUX = 2.61 x 10^{10} G
91. Predicted DO variations in DeGray are clearly demonstrated by a time series of shaded contours (Figure 21). DO first became depleted near the bottom of the transition zone. The zone enlarged as the season progressed, gradually extending into the metalimnetic region of the lacustrine zone. During the fall deepening of the thermocline, erosion of the depleted zone occurred. Complete mixing did not occur by the end of the simulation year, which was consistent with field observations. The pattern of DO depletions suggested that the metalimnetic DO minimum was influenced by anoxic conditions in the upper portion of the reservoir. Flux computations indicated that over 50 percent of the predicted metalimnetic DO depletion was due to transport of DO-depleted waters. This is consistent with observations by Nix (1981) on the effects of advective transport on the observed metalimnetic DO minimum at DeGray Lake.

92. Predicted and observed DO concentrations are compared in Figure 22. The development of the anoxic hypolimnion in the transition zone (Station 12) and the metalimnetic minimum in the lacustrine zone (as represented by Station 4) were adequately characterized, as was also evidenced by computed RI values (Table 3). The predicted metalimnetic minimum was consistently deeper than that observed, and its fall deepening was predicted to occur earlier than observed, following the pattern of water temperature predictions.

Total iron

93. Total iron is included primarily due to its importance in nutrient cycling. Iron is known to affect nutrient dynamics in many systems, and Kennedy, Montgomery, and James (1983) indicated the importance of iron in the phosphorus dynamics of DeGray Lake. In model formulations, iron is released from sediments when DO falls below a specified minimum value (0.5 mg L\(^{-1}\) in the application) and settles when DO is at or above this value. Iron is released from sediments at a specified rate (in units of grams per square metre per day) which is affected by water temperature, sediment area, and SOD; thus, the higher SOD in the transition zone resulted in higher iron release. Release and settling rates for iron are provided in Table 2. Simulating only total
Figure 21. Shaded contours of predicted DO concentrations for the 1980 DeGray Lake verification simulations (concentrations milligrams per litre) (Continued)
LONGITUDINAL SEGMENT NO., DELTA-X = 1.0 KM

16 SEPTEMBER 1980

LONGITUDINAL SEGMENT NO., DELTA-X = 1.0 KM

14 OCTOBER 1980

LONGITUDINAL SEGMENT NO., DELTA-X = 1.0 KM

11 NOVEMBER 1980

LONGITUDINAL SEGMENT NO., DELTA-X = 1.0 KM

25 NOVEMBER 1980

Figure 21. (Concluded)
Figure 22. Predicted and observed DO concentrations for the 1980 DeGray Lake verification simulations (Continued)
b. Lacustrine zone (Station 4)

Figure 22. (Concluded)
iron did not allow predictions of DO depletions due to the oxidation of its reduced forms.

94. Predicted iron dynamics closely followed those of phosphorus and ammonia, as demonstrated in Figure 23. Sediment release under anoxic conditions was the major source of iron loadings. Nix (1986) also observed that elevated iron concentrations did not occur in DeGray until an anoxic zone developed near the bottom and suggested the origin of iron was bottom sediments. Instantaneous inflow loadings did not appear important, and no discernible differences in model predictions were noted when iron was removed from inflows, as was the case for phosphorus. Comparisons of predicted and observed concentrations (Figure 24) indicated that iron dynamics were adequately characterized.
Figure 23. Shaded contours of predicted total iron concentrations for the 1980 DeGray Lake verification simulations (concentrations in milligrams per litre).
Figure 24. Predicted and observed total iron concentrations for the 1980 DeGray Lake verification simulations (Continued)
b. Lacustrine zone (Station 4)

Figure 24. (Concluded)
PART VI: CONCLUSIONS

95. The application of CE-QUAL-W2 to DeGray Lake, Arkansas, served a number of purposes, including an analysis and refinement of process descriptions for modeled variables, as well as locating and correcting errors in the code prior to its release. The application was also intended to test the model's capability to predict water quality variations in two dimensions.

96. Model simulations adequately characterized variations in the water quality in DeGray Lake over the entire stratification cycle, as graphically demonstrated for the verification simulations and by the computed RI values. The onset of anoxia in the upstream regions was correctly characterized as well as sediment release of iron and nutrients under anoxic conditions. The establishment of a metalimnetic DO minimum was also predicted in the lower regions of the reservoir. The fall deepening of the thermocline was adequately characterized, as were the effects of the introduction of oxygen on anaerobic materials.

97. The importance of sediments in the transition zone to the overall DO and nutrient dynamics of DeGray Lake was demonstrated. Sediment oxygen demand was determined to be the major factor affecting DO depletions on a reservoir-wide basis. Sediment release of phosphorus and nitrogen under anoxic conditions largely controlled nutrient cycling.

98. The transition zone of DeGray, while comprising only approximately 20 percent of its total volume, had a large effect on the predicted DO and nutrient dynamics of the reservoir. Flux computations indicated that this region was much more dynamic than the lacustrine zone. The model showed that the metalimnetic DO minimum in the lacustrine zone was largely affected by the transport of DO-depleted waters from the transition zone in density currents along the thermocline.

99. The model application indicated several areas which require additional attention, including means of identifying and quantifying labile and refractory components of DOM, the descriptions of iron and phosphorus interactions, and the kinetics of phosphorus adsorption and
desorption. The algorithms to predict inorganic carbon, alkalinity, pH, and carbonate species as well as sediments (as a compartment which accumulates and decays organic matter) were not completely tested in this application and also require further attention.

100. While the model requires further applications to different systems to fully assess its capabilities, the initial application indicated that a realistic representation of water quality variations in two dimensions could be achieved. The initial application to DeGray Lake further demonstrated that a coupled hydrodynamic and water quality model could be economically used to simulate long-term variations in water quality in two dimensions on a minicomputer.

101. CE-QUAL-W2 is suitable for applications where resolution of longitudinal as well as vertical gradients of water quality is required, and where lateral variations are small. The model may be a valuable tool for obtaining insights into factors affecting hydrodynamic and water quality variations in the modeled systems. CE-QUAL-W2 should also provide a valuable assessment and management/planning aid by allowing an economic means for assessing the relative impacts of changes in operation or project modifications on water quality variations in reservoirs and other water bodies.
REFERENCES


APPENDIX A: COMPUTATION OF THE RELIABILITY INDEX

1. The Reliability Index was proposed by Leggett and Williams (1981) as a general test that can be used to evaluate the correspondence, or goodness of fit, between predicted values from mathematical models and observed data. Thus, the test allows inference of a model’s predictive capability. An interpretation of the index is that it indicates, in some sense, the degree to which predictions and observations agree. An RI of 1.0 indicates a perfect agreement, and the RI increases as predicted and observed values diverge. The RI is computed from

\[
RI = \frac{\left(1 + \frac{1}{N} \sum_{t=1}^{T} \sum_{n=1}^{N} \frac{1}{1 + \left(\frac{Y_{tn}}{X_{tn}}\right)^2}\right)^{1/2}}{1 + \frac{1}{N} \sum_{t=1}^{T} \sum_{n=1}^{N} \frac{1}{1 + \left(\frac{Y_{tn}}{X_{tn}}\right)^2}}
\]

where \(y\) represents the observed value, \(x\) the model predicted value, \(N\) the number of \(x, y\) pairs for a specific sampling period, and \(T\) the number of sampling periods.

2. Some caution must be exercised interpreting the RI since it is affected by variability in observations as well as the degree of correspondence between observed and predicted values. It is a measure of the model's capabilities only to the degree to which the observed data are considered "true." However, comparisons between simulations with a given model, or different models, which result in a smaller RI for the same observed data would generally indicate an improvement. The RI was compared to other commonly used statistical tests by Wlosinski (1984) and was considered the best statistic for aggregating model results.