SOME RECENT ADAPTATIONS AND APPLICATIONS OF QUAL-II IN THE NORTHEAST

presented at the

Stormwater and Water Quality Model Users Group Meeting
University of Florida, Gainesville, January 27-28, 1983

by

William W. Walker, Jr., Environmental Engineer
1127 Lowell Road, Concord, Massachusetts 01742

Introduction

The QUAL-II model has an extensive history which can be traced to the original work of Streeter and Phelps (1925) and has been widely used in wasteload allocations and other aspects of river basin water quality management. Several versions of the program have appeared (Texas Water Development Board, 1970, Water Resources Engineers, 1972, Meta Systems, 1979, Roesner et al., 1981). Generally, all versions provide a capability for simulating longitudinal transport and transformation of water quality components in one-dimensional, vertically-mixed systems with steady-state hydraulic conditions. This paper describes certain modifications which have been made in the model structure to improve simulations of dissolved oxygen conditions in rivers heavily impacted by photosynthesis. The code has also been adapted for use on microcomputers. The development of this version is traced to wasteload allocation studies in Vermont (Meta Systems, 1979, Vermont Department of Water Resources, 1982) and to recent studies in Maine (Walker, 1982) and Massachusetts (Walker, 1983).

Model Modifications

The simulation of nutrient cycles and algal growth kinetics tend to be more important in rivers and shallow impoundments with low velocities. In these situations, photosynthesis by suspended phytoplankton, aquatic plants, and/or periphyton may represent important components of the oxygen balance. Several alterations have been made in the QUAL-II structure to improve simulations of phytoplankton, nutrients, and oxygen under these conditions. These include:

(1) addition of detrital organic phosphorus and organic nitrogen compartments;

(2) provision for algal uptake of ammonia and/or nitrate nitrogen (vs. nitrate only in previous versions);

(3) provision for self-shading by phytoplankton; (computing light extinction coefficients as a function of chlorophyll introduces an important feedback control on peak biomass levels in nutrient-rich environments);

(4) specification of alternative (vs. multiplicative) nutrient limitation by nitrogen or phosphorus;

Control pathways are depicted in Figure 1. The addition of detrital organic nutrient compartments essentially closes the nutrient cycles and permits model calibration and testing against observed total nitrogen and total phosphorus data, as well as individual nutrient species. The other modifications are designed to reflect the kinetic formulations used in state-of-the-art phytoplankton models, as applied to lakes and estuaries (Di Torro et al., 1977). Details on the equations and functional forms are given elsewhere (Vermont Department of Water Resources, 1982, VanBenschoten and Walker, 1982).

Other additions and structural modifications used in the applications discussed below include:

(1) calculation "Apparent BOD-5" concentrations as a function of carbonaceous BOD and estimated 5-day algal respiration at 20 deg C (permits calibration and testing against observed BOD-5 data);

(2) calculation of Secchi depths from chlorophyll and non-algal light extinction coefficients (also useful in calibration and impact assessments);

(3) output of several diagnostic variables useful for identifying controlling processes, including breakdowns of oxygen sources and sinks (g/m3-day) and algal growth factors in each computational element;

(4) provision for specifying benthic sources and/or sinks for any state variable by reach in g/m2-day, including plant photosynthesis and respiration;

(5) provision for including dam reaeration at the downstream end of any reach;

(6) provision for simulating eddy-diffusive exchanges with downstream water bodies by specifying far-field concentrations and effective dispersion rate (useful for simulating fresh-water estuaries or other backwater situations where the downstream water quality boundary condition is fixed);

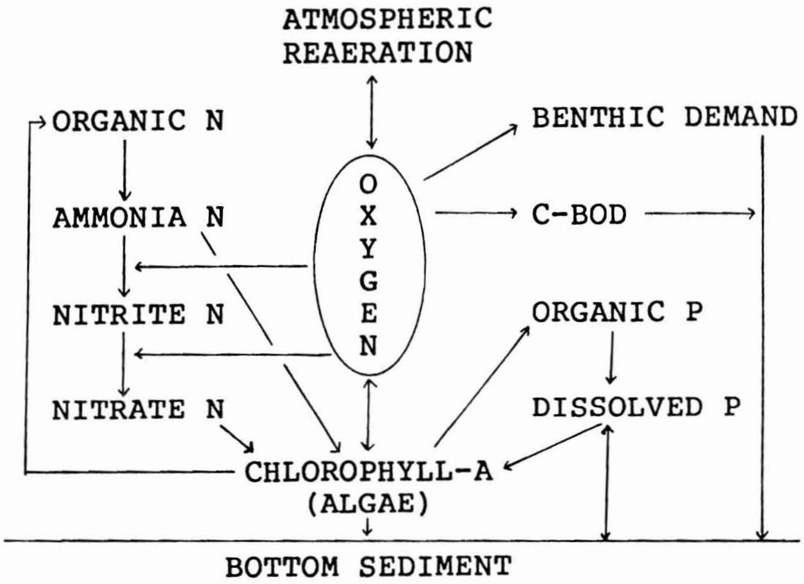
(7) provision for estimating longitudinal dispersion coefficients using a function developed by Fischer et al. (1979), reportedly more realistic than the Elder (1959) equation;

(8) provision for simulating diel oxygen fluctuations attributed to photosynthesis and respiration using an approximate formulation described by DiTorro (1968);

The last modification permits calculation of daily minimum oxygen concentrations without applying the model in a non-steady-state mode. Diel flucutations are calculated around the steady-state solution as a function of

Figure 1

Control Pathways in the Modified QUAL-II Model



reaeration rate, photosynthesis rate, and day length.

In the Vermont application, most of the above changes have been implemented by modifying certain subroutines in the EPA code and adding new subroutines for simulating detrital organic nutrients and diel oxygen variations. A SAS (SAS Institute, 1979) interface has also been developed for manipulating model output and plotting observed and predicted concentration profiles (Walker, 1980). The interface has been extremely useful in streamlining calibration, testing, and report writing.

In subsequent applications, the program code has been completely rewritten and adapted for use on a microcomputer. The micro version is written in standard FORTRAN and uses overlays to overcome storage limitations. It has also been run on mainframes. Experimentation indicated that a version written in intrepreted BASIC would be too slow and storage-limited to be practical in most applications. Application limits are determined primarily by the number of computational elements, computer memory, and the memory overhead consumed by the FORTRAN compiler, linker, and input/output operations. On a system with approximately 40K of available storage (64K less overhead), the current version can handle up to 190 computational elements. Provisions for branching or non-steady-state simulations are not included, primarily because they have not been required in applications to date. These restrictions could be lifted with additional code modifications and overlaying. The micro version has been tested against the modified EPA code using input files developed for the Vermont Winooski River application. A separate program has also been written for plotting observed and predicted profiles. Execution times for a typical problem, including printing and plotting, are on the order of ten minutes on an 8-bit, 4 mhz microcomputer equipped with a special arithmetic chip available for most systems.

Upgrading of the algal growth kinetics (especially the inclusion of self-shading) reduces the linearity of the equations has been found to pose problems for the steady-state solution algorithm, particularly in systems with long hydraulic residence times. In the current EPA code (Roesner et al., 1981), convergence is guided and tested based upon algal growth rates. In the modified code, convergence is tested based upon stability of the state variables from one iteration to the next. Certain modifications of the tri-diagonal matrix formulation have also been successful in improving convergence properties, especially in systems with long residence times or significant algal growth limitation by self-shading or nutrients.

Calibration and Testing Procedures

Model inputs may be broadly classified as (1) "boundary conditions" or (2) "system parameters". Boundary conditions include such factors as river flows, waste inputs, morphometry, and climate; these can be directly measured or independently estimated. System parameters include the fundamental rate and stoichiometric coefficients which are used in process-level simulations and which are usually difficult to measure directly. In simulating a given river system, the boundary conditions vary from one time period to another, depending upon various driving forces, while the system parameters should be relatively constant.

The development of input estimates within each category is based upon combinations of the following:

(1) direct monitoring data
(2) empirical functions (e.g. reaeration rate formulae)
(3) literature values and guidance manuals (e.g., Zison et al., 1978, NACASI, 1980)
(4) empirical adjustment ("tuning") to observed water quality profiles
(5) field reconnaissance

The calibration process would be relatively straight-forward if all inputs could be directly measured. This is generally infeasible, however, because of the complexity of the model, implicit nature of some coefficients, and limitations in monitoring resources and technology. Calibration of this type of model requires subjective judgments because the feasible ranges of most coefficients are wide and more than one set of coefficients can often be selected to fit a given set of field data. Because of these limitations, user experience and field reconnaissance are valuable assets in model applications. Sensitivity analysis should be employed to determine the importance of parametric and structural assumptions.

One test of model generality is based upon stability of the process-level parameters from one time period to another in a given river. This test involves simulating observed water quality conditions under at least two different sets of boundary conditions using a fixed set of parameters. A more severe test of generality would require parameter stability from one river to another. A model with this property, while difficult to achieve, would be extremely useful because it would ease the calibration and testing requirements for each application.

Because of the desirability of achieving generality and learning more about the strengths and weaknesses of the model structure, a relatively conservative approach involving minimal adjustment of system parameters has been taken in calibrating the model to the systems described below. Most parameter adjustments have been limited to characteristics which could logically vary from one river to another, such as benthic photosynthesis or benthic oxygen demand; these are essentially forcing functions, as opposed to system parameters. Stoichiometric coefficients (e.g., respiration equivalents, algae chlorophyll-a and nutrient contents) and many rate coefficients have been held constant at "reasonable" values, based upon literature ranges and accumulated experience with the model.

Many parameters have been estimated with the aid of published empirical relationships (e.g. reaeration rate), rather than adjusted to fit individual profiles. Direct field measurements of reaeration rate would be preferable, but are usually infeasible because of time or economic constraints. Variations in certain process-level parameters, such as algal growth rate, respiration rate, and settling velocity, from one reach to another in a given river would introduce too many degrees of freedom in the calibration process and are less defensible on a scientific basis; accordingly, reach-to-reach adjustments in these parameters are not part of the calibration procedure.

Applications

The model has been applied in studies of three river basins in the Northeast: (1) Lower Winooski River, Vermont (VanBenschoten and Walker, 1982); (2) Upper East Branch of the Sebasticook River, Maine (Walker, 1982); and (3) Sudbury/Concord Rivers, Massachusetts (Walker, 1983). While there are several unique features associated with each of these applications, all include low-velocity reaches in shallow impoundments or backwater areas with high concentrations of algae (generally greater then 30 mg chlorophyll-a/m3) during critical periods. Key parameter estimates are summarized in Table 1. Model generality is reflected by the stabilities of some parameters and instabilities of others from one system to another. Each application is described briefly below.

The Winooski River originates in the Green Mountains of Vermont and empties into Lake Champlain. In its last 32 kilometers, the river flows through the metropolitan Burlington area, where there are two hydropower dams and several industrial and municipal point sources. Violations of the 6 mg/liter dissolved oxygen standard have generally been observed near the mouth of the river, where the elevation gradient is relatively small and where maximum summer algal populations of about 30 mg/m3 are generally found. The oxygen violations are usually associated with large diel fluctuations (up to 8 mg/liter), attributed to combined effects of (1) algal photosynthesis and respiration and (2) daily fluctuations in river flow resulting from hydropower operations (typically 50 to 1200 cfs). Sustained periods of oxygen violations have also been observed at various locations under conditions of maximum temperature (> 30 degrees C) and die-off of algal blooms.

The Vermont Agency of Environmental Conservation (VAEC, 1980, 1982) conducted a wasteload allocation study in order to assess possible requirements for advanced waste treatment. The unsteady flow regimes induced by hydropower peaking operations posed several potential problems for the modeling effort. Because of the complexities and extensive data requirements involved in application of a non-steady-state hydraulic and water quality model, the Agency elected to use a steady-state model and to conduct the allocation runs under steady 7Q10 conditions, under the assumption that the utilities would be required to pass a minimum of 7Q10 during non-generating hours. The model described above was calibrated and tested against data from week-long intensive surveys conducted during two different years. With the cooperation of the power company, stable flow conditions were maintained during both surveys to provide suitable data sets for calibration and testing of a steady-state model. Observed and predicted concentration profiles for the second survey are shown in Figure 2.

The Sebasticook study (Walker, 1982) examined the impacts of a combined municipal/industrial discharge on a small stream which discharges into an inlet of Lake Sebasticook, a eutrophic lake in central Maine. The shallow inlet is characterized by high algal and aquatic plant densities and hydraulic exchanges with open lake waters are probably important in determining concentrations at the lower end. Preliminary model simulations indicate that the inlet is functioning as an oxidation pond, since oxygen turnover rates in the water column consist largely of photosynthesis and respiration by algae and aquatic plants. A detailed evaluation is hindered by lack of diurnal sampling for dissolved oxygen and limited spatial and

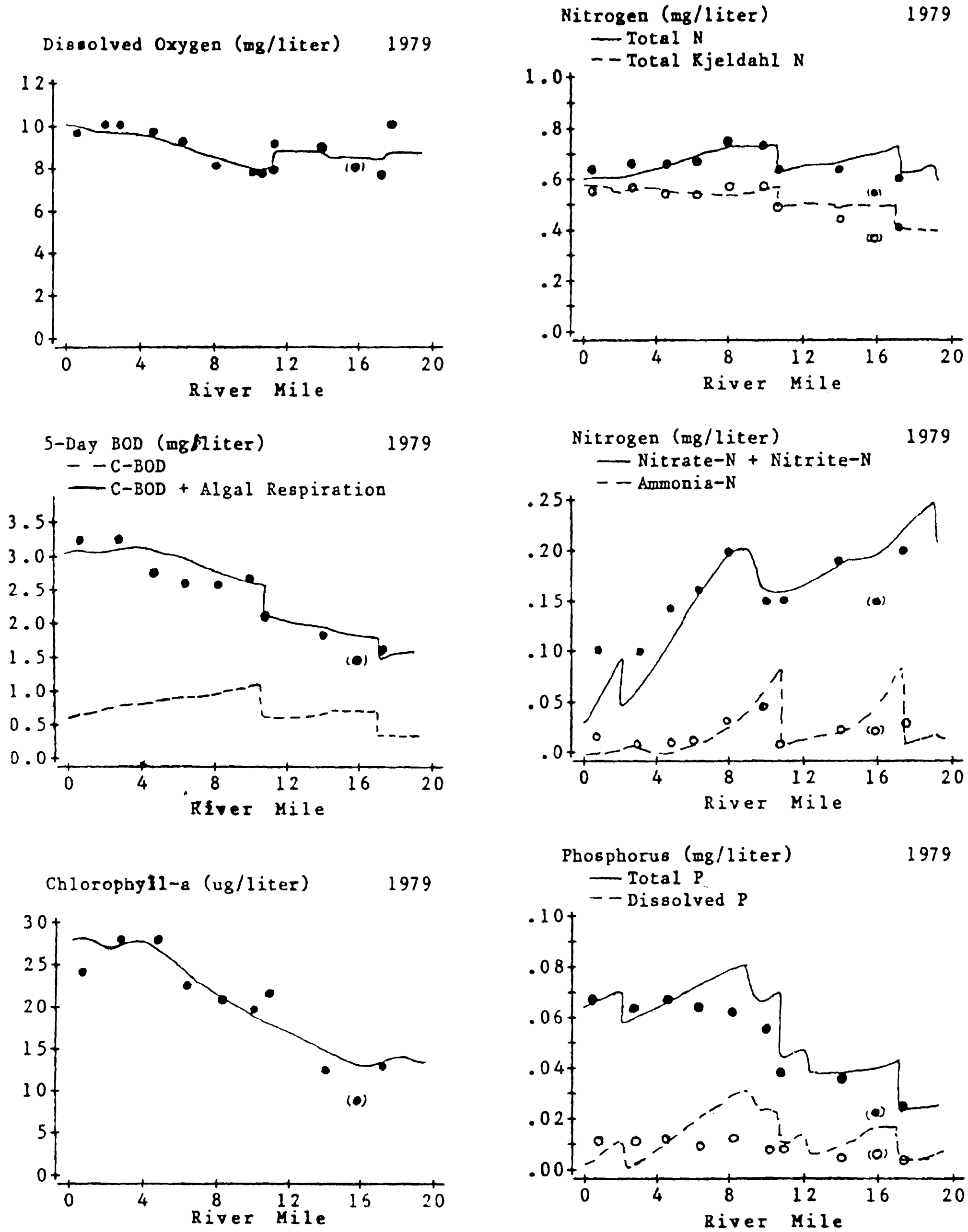
Table 1
Parameter Estimates Used in Winooski, Sebasticook, and Sudbury Applications

Parameters	Value/Comments
Reaeration Rate	O'Connor & Dobbins (1958) equation constrained to K2 > 1 / mean depth (Su)
Longitudinal Dispersion	Elder(1959) (Wi), Fischer (1979) (Se,Su)
Decay/Oxidation Rates (1/day)	
BOD-U	.2 + bed activity (Zison et al., 1978)
Ammonia N	.2 - 2 (Wi), .3 - 1 (Se), .6 (Su)
Nitrite N	2.0 (Wi,Se), 3.0 (Su)
Organic N	.1
Organic P	.1
Algal Parameters	
Maximum Growth Rate	2.3 1/day (Wi,Su), 2.5 1/day (Se)
Respiration Rate	.12 1/day
Settling Velocity	.75 m/day (Wi,Su), .60 m/day (Se)
Chlorophyll Content	.010 mg Chl-a / mg Algae
P Content	.011 mg P / mg Algae
N Content	.080 mg N / mg Algae
Light Extinction	43.2 m2/g Chl-a
Ammonia Pref. Factor	.9
Photo. Oxygen Equiv.	1.6 mg 02 / mg algae
Resp. Oxygen Equiv.	2.0 mg 02 / mg algae
Half-Saturation Constants	
Algal P Uptake	.005 g/m3
Algal N Uptake	.03 g/m3
Algal Growth vs. Light	1.5 calories/cm2-hr
Benthic Oxygen Fluxes (g/m2-day)	
Plant Photosynthesis	0 - 2 (Wi), 0 - 2 (Se), 1.5 - 10 (Su)
Plant Respiration	0 (Wi), 0 - 2 (Se), 1.5 - 10 (Su)
Other Benthic Demand	.5 (Wi), .5 (Se), 1 - 3 (Su)*
Other Benthic Fluxes (g/m2-day)	
Dissolved P Source **	0 - .005 (Se,Su)
Ammonia N Source **	0 - .025 (Su, channel)
Ammonia N Sink	.05 (Su, overbank)
Nitrate N Sink	.10 (Su, overbank)

Wi = Winooski, Se = Sebasticook, Su = Sudbury
parameters are zero in other applications if some initials are given
parameters are used in all applications if no initials are given
ranges refer to reach-specific values, all rates at 20 degrees C
* plus wetland benthic loading component
** benthic sources of phosphorus and ammonia in impounded reaches

Figure 2

Observed and Predicted Water Quality Profiles
Lower Winooski River 1979


Dissolved Oxygen (mg/liter) 1979

Nitrogen (mg/liter) 1979

5-Day BOD (mg/liter) 1979

Nitrogen (mg/liter) 1979

Chlorophyll-a (ug/liter) 1979

Phosphorus (mg/liter) 1979

temporal sampling frequencies for all water quality variables. In this application, reasonable simulation of observed chlorophyll and afternoon oxygen (between predicted daily mean and daily maximum) profiles was achieved with minor adjustments in the parameters used in the Winooski simulations.

The model has been recently applied to the Sudbury/Concord Rivers in Massachusetts (Walker, 1983), as part of an assessment of the potential environmental constraints involved in diverting waters from the upper watershed for water supply purposes. The study extends over 51 river kilometers, 44 of which consist of a shallow impoundment surrounded by wetlands, including the Great Meadows National Wildlife Refuge. Both the model and monitoring data indicate that water quality conditions are controlled largely by the hydraulic geometry and by interactions with tributary wetlands and that point sources are of minor importance. Hydraulic simulations using HEC-II and detailed channel cross-section measurements at 278 locations have been used to define hydraulic geometries in water quality model.

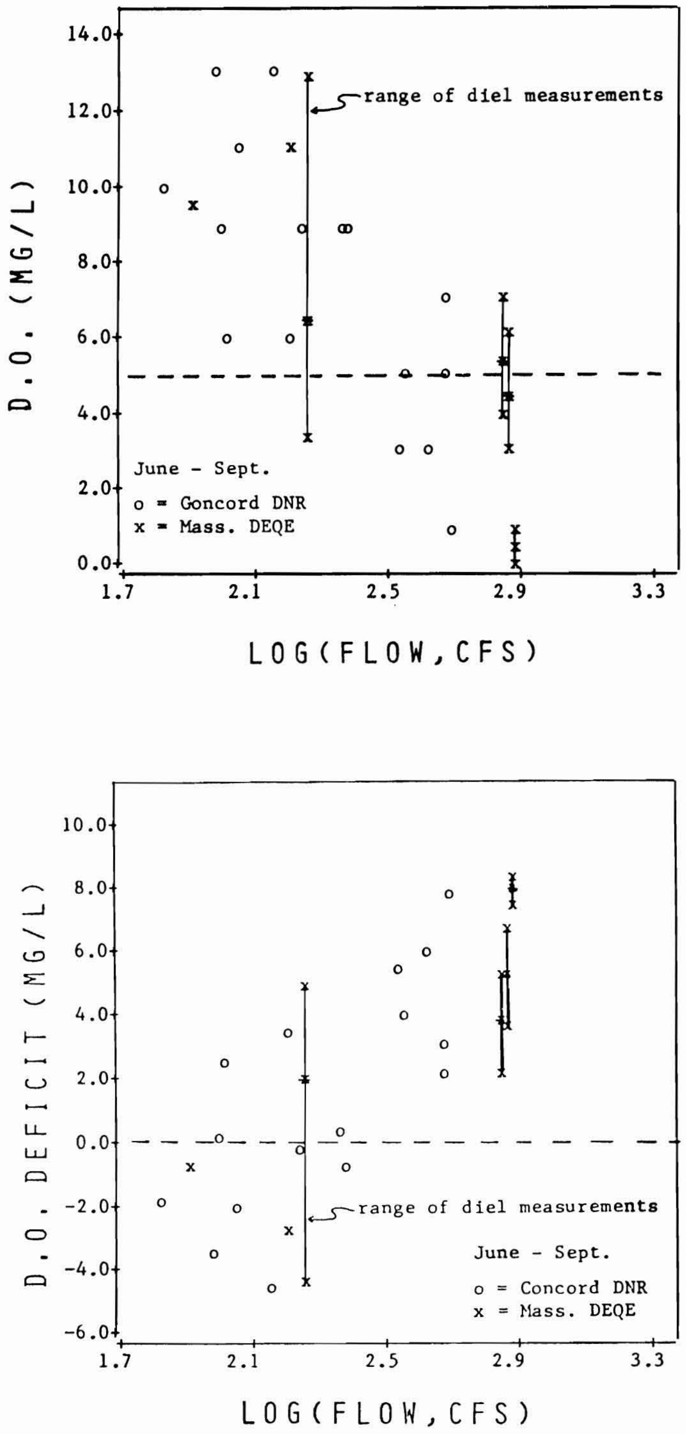
As a result of the channel and floodplain morphometry and backwater effects, the river undergoes relatively large changes in width as a function of flow in certain reaches. Bottom sediments in the channel and overbank areas are highly organic in nature and reflect the export, settling, and decay of organic materials from adjacent wetlands. Figure 3 depicts variations in dissolved oxygen and dissolved oxygen deficit as a function of river flow measured during summer months at the lower end of the impounded area most stongly influenced by adjacent wetlands. A unique aspect of this system is that dissolved oxygen levels tend to be lower (and deficits, higher) during high-flow periods. The relationships in Figure 3 reflect the combined influences of (1) higher organic loadings during high-flow periods; (2) higher benthic demands in overbank areas; (3) less algal growth because of the increased flushing rate during high-flow periods; (4) die-off and decay of wetland vegetation during infrequent summer flooding events. The last condition results in the most severe water quality conditions, including depression of oxygen levels below 2 mg/liter over most the impoundent. A significant fishkill was reported in 1938 following the largest recorded July flood.

Preliminary calibration of the net benthic oxygen demands in each model reach under high-flow and low-flow conditions indicated that demands increased with the ratio of tributary wetland area to river surface area and increased with average basin runoff. Accordingly, a simple mass balance model linking the apparent benthic demand to tributary wetland areas and runoff rate has been used to represent wetland interactions. The calibrated wetland organic export rate of .17 grams of oxygen demand per square meter per day represents only about 1.3 to 2.1 percent of the literature range for net primary productivity of freshwater emergent macrophytes on fertile sites in temperature regions (Wetzel, 1975). The remainder of the organic matter produced in the wetlands is apparently decomposed in place or flushed downstream with little decomposition. Another wetland interaction considered in the model is benthic uptake of nitrate (.1 g/m2-day) in overbank areas and is attributed to plant uptake and denitrification supported by organic substrates, as observed in other wetland systems (Kadlec and Kadlec, 1978).

The model has been calibrated and tested against data from three intensive surveys (1) August 1973, summer low-flow; (2) July 1973, summer

Figure 3

Summer Dissolved Oxygen Concentration and Deficit
at Route 117 vs. Concord River Flow at Lowell



flood; and (3) June 1979, late-spring flood. While the average flows were similar in the July 1973 and June 1979 surveys, the major hydrologic difference is that the former occurred a week after a summer storm event of about seven-year freqency, whereas flows were decreasing seasonally during the latter, when only flood-tolerant vegetation would have developed in adjacent wetlands. Over most of the impoundment, diel oxygen fluctuations were less than 1 g/m3 during the July 1973 survey, as compared with a range of 2 - 8 g/m3 for the other surveys; this reflects a suppression of plant photosynthesis associated with summer flooding.

Observed and predicted daily mean oxygen profiles for each survey are shown in Figure 4. The severe conditions during July of 1973 have been simulated by setting benthic photosynthesis rates to zero, as compared with a 1.5 - 10 g/m2-day range calibrated to various reaches for the other survey periods. All other model parameters are fixed for the three simulations. An oxygen sag attributed to high benthic demands and low velocities is apparent below river kilometer 48, the approximate upper end of the backwater effects created by the impoundment at river kilometer 7.

Observed and predicted chlorophyll-a profiles are shown in Figure 5. Using the same kinetic and stoichiometric parameters used in the Lower Winooski algal simulations, the model simulates the peak algal densities observed during the low-flow and spring-flood surveys with reasonable accuracy, especially considering that the observed points are based upon single grab samples. For the low-flow survey, the chlorophyll profile is over-predicted below the Assabet River (RKM 25). The time-of-travel through the impoundment during that survey was about 20 days and it is possible that the lower observed chlorophyll levels reflect higher flow conditions previous to the survey. Other possible explanations include effects of zooplankton predation (more likely to be important at long residence times but not simulated by the model), or shading by floating duckweed which have been observed in this portion of the river. Despite this problem, the model adequately simulates the observed chlorophyll-a profiles in the upper end of the impoundment, where the oxygen sag is located.

Conclusions

This paper has described adaptations and applications of QUAL-II to three New England river basins. Incorporation of organic nutrient compartments and updating of algal growth kinetics increase the realism and generality of the model. Interfacing the model output with SAS and plotting routines facilitates calibration, testing, and statistical analysis of observed and predicted water quality profiles. The revised code can be used on microcomputers or mainframes with FORTRAN capability.

Reasonable generality is indicated by model calibration to observed water quality profiles with minimal adjustment in key parameter estimates from one application to another, especially in those parameters which determine nutrient and algal profiles. Relatively large variations in some parameters, including nitrification rate, benthic oxygen demand, and benthic photosynthesis, reflect inherent limitations in this type of model and dictate needs for calibration and testing in each application. Modifications of the code to permit systematic sensitivity analysis (Walker, 1982a) would improve user perspectives of key processes and assumptions in a given model application.

Figure 4

Observed and Predicted Mean Dissolved Oxygen Concentrations
Sudbury/Concord Rivers

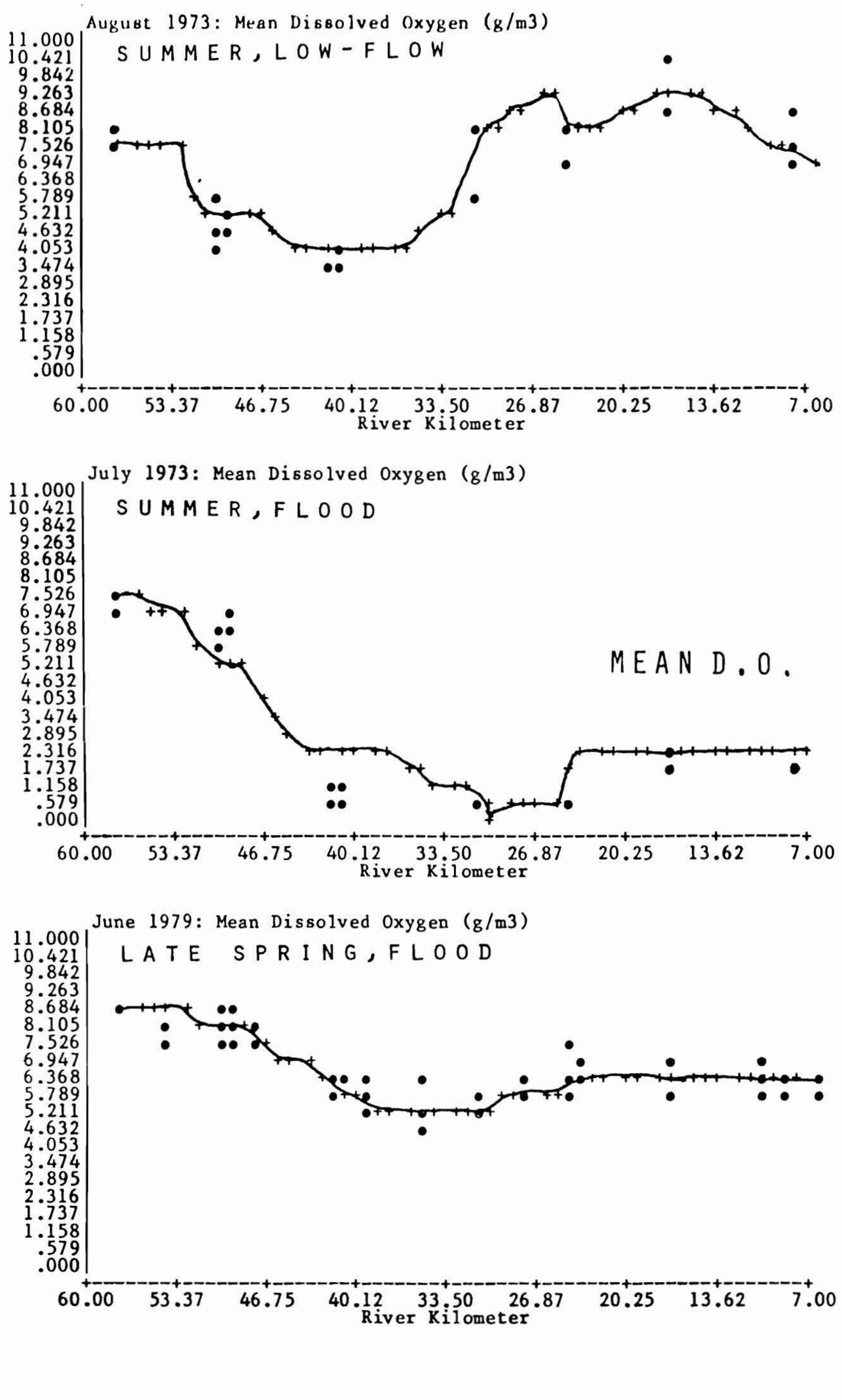
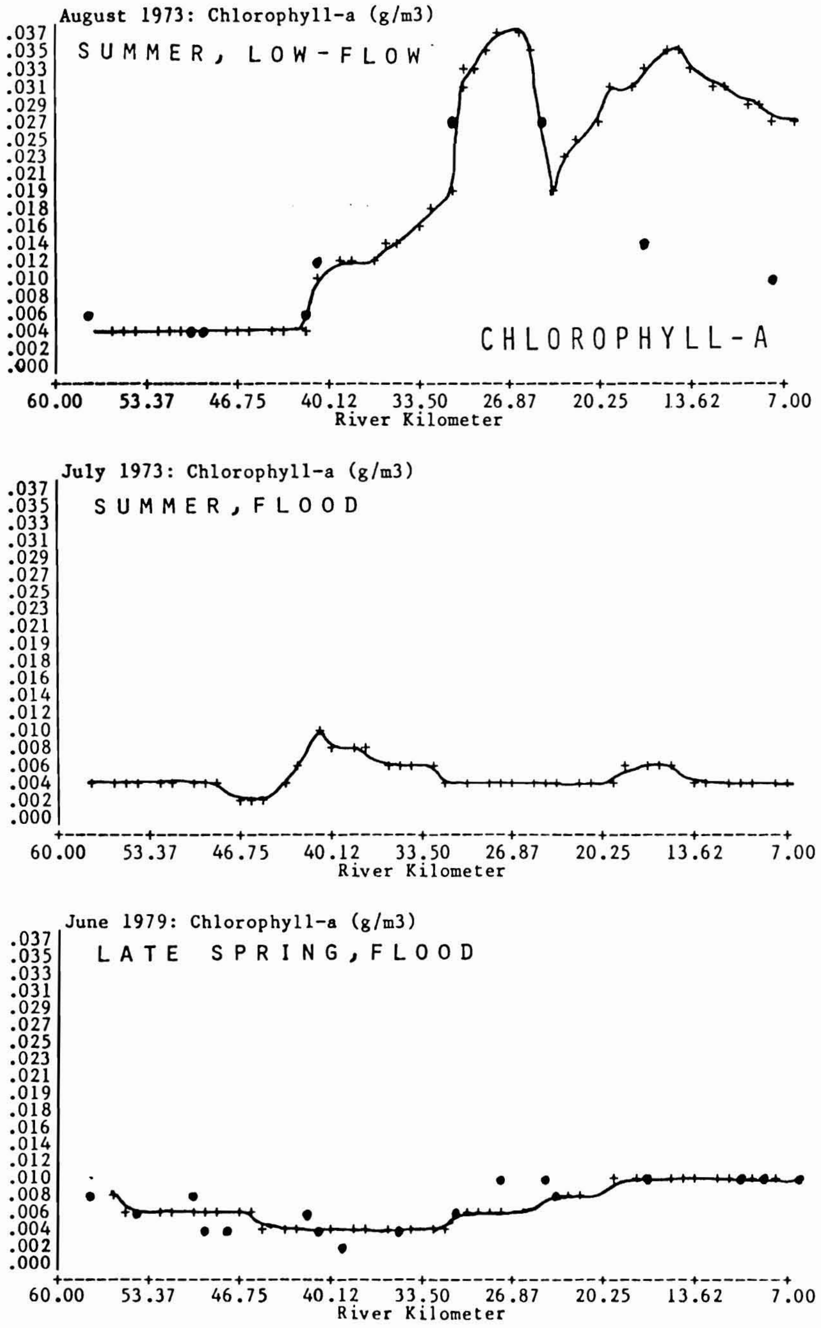


Figure 5

Observed and Predicted Chlorophyll-a Concentrations
Sudbury/Concord Rivers



References

DiTorro, D.M., "Algae and Dissolved Oxygen", in "Basic Models of Natural Systems", prepared for U.S. Environmental Protection Agency by Manhattan College, New York, 1968.

DiTorro, D.M., Thomann, R.V., O´Connor, D.J., and Mancini, J.L., "Estuarine Phytoplankton Biomass Models - Verification Analyses and Preliminary Applications", in *The Sea*, John Wiley and Sons, Inc., New York, 1977.

Elder, J.W., "The Dispersion of Marked Fluid in Turbulent Shear Flow", *Journal of Fluid Mechanics*, Vol. 5, pp. 544-560, 1959.

Fischer, H.B., E.J. List, R.C.Y. Koh, J. Imberger, and N.H. Brooks, *Mixing in Inland and Coastal Waters*, Academic Press, New York, 1979.

Kadlec, R.H. and J.A. Kadlec, "Wetlands and Water Quality", in *Wetland Functions and Values: The State of Our Understanding* , American Water Resources Association, November 1978.

Meta Systems, Inc., "Documentation for the Meta Systems Version of the QUAL-II Water Quality Simulation Model", prepared for U.S. Environmental Protection Agency, Water Planning Division, 1979.

National Council for Air and Stream Improvement, Inc., "A Review of the Mathematical Water Quality Model QUAL-II and Guidance for Its Use", Stream Improvement Technical Bulletin No. 335, 1980.

O´Connor, D.J. and W.E. Dobbins, "Mechanism of Reaeration in Natural Streams", *Trans. ASCE*, Vol. 123, 1958.

Roesner, L.A., et al., "Computer Program Documentation for Stream Quality Model (QUAL-II)", U.S. Environmental Protection Agency, Center for Water Quality Modeling, Athens Environmental Research Laboratory, Georgia, EPA-600/9-81-014, 1981.

SAS Institute Inc., "SAS Users Guide", Raleigh, NC, 1979.

Streeter, H.W. and E.B. Phelps, "A Study of the Pollution and Natural Purification of the Ohio River", U.S. Public Health Service Bulletin 146 (reprinted 1958), 1925.

Texas Water Development Board, "Simulation of Water Quality in Streams and Canals", Program Documentation and User´s Manual, 1970.

VanBenschoten, J.B. and W. W. Walker, "Calibration and Application of QUAL-II to the Lower Winooski River", draft manuscript submitted to *Water Resources Bulletin*, American Water Resources Association, August 1982.

Vermont Agency of Environmental Conservation, "Lower Winooski River Wasteload Allocation Study - Part A: Report of Data", Department of Water Resources and Environmental Engineering, Montpelier, December 1980.

Vermont Agency of Environmental Conservation, "Lower Winooski River Wasteload Allocation Study - Part B: Mathematical Modeling Report", Department of Water Resources and Environmental Engineering, Montpelier, January 1982.

Walker, W. W., "A SAS Interface for QUAL-II", prepared for U.S. Environmental Protection Agency and Vermont Agency of Environmental Conservation, 1980.

Walker, W. W., "Calibration and Application of QUAL-II to the Upper East Branch of the Sebasticook River between Corinna and Coburn", prepared for Kleinschmidt and Dutting, Inc., Pittsfield, Maine, 1982.

Walker, W.W., "A Sensitivity and Error Analysis Procedure for Lake Eutrophication Modeling", Water Resources Bulletin, American Water Resources Association, Vol. 18, No. 1, pp. 53-61, February 1982a.

Walker, W. W., "Downstream Water Quality Impacts of Diversions from Sudbury Reservoir - Model Calibration and Testing", prepared for Interdisciplinary Environmental Planning, Inc., Parsons Brinkerhoff Quade & Douglas, Inc., and Metropolitan District Commission, Commonwealth of Massachusetts, January 1983.

Water Resources Engineers, Inc., "Progress Report on Contract No. 68-01-0713, Upper Mississippi River Basin Model Project", prepared for U.S. Environmental Protection Agency, September 1972.

Wetzel, R.G., Limnology, W.B. Saunders Company, Philadelphia, 1975.

Zison, S.W., W.B. Mills, D. Deimer, C.W. Chen, "Rates, Constants, and Kinetics in Surface Water Quality Modeling", U.S. Environmental Protection Agency, Athens Environmental Research Laboratory, Georgia, EPA-600/3-78-105, December 1978.

The work described in this paper was not funded by the U.S. Environmental Protection Agency. The contents do not necessarily reflect the views of the Agency and no official endorsement should be inferred.

United States
Environmental Protection
Agency

Environmental Research
Laboratory
Athens GA 30613

EPA-600/9-83-015
September 1983

Research and Development

EPA

Proceedings of Stormwater and Water Quality Model Users Group Meeting

W. W. WALKER
1127 Lowell Road
Concord, MA. 01742

January 27-28, 1983