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THE ENHANCED STREAM WATER QUALITY MODELS QUAL2E AND QUAL2E-UNCAS:
DOCUMENTATION AND USER MANUAL

by

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient management tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact and control of environmental contaminants, the Assessment Branch develops management or engineering tools to help pollution control officials achieve water quality goals.

The stream water quality model QUAL2E is widely used for waste load allocations, discharge permit determinations, and other conventional pollutant evaluations in the United States. Since the introduction of QUAL-II in 1970, several different versions of the model have evolved. This manual presents the most recent modifications in the form of enhanced state-of-the-art models called QUAL2E and QUAL2E-UNCAS. Both models have been developed over the past three years through cooperative agreements between the National Council for Air and Stream Improvement (NCASI), the Department of Civil Engineering at Tufts University, and EPA. Distribution and maintenance of the QUAL2E and QUAL2E-UNCAS computer programs, and training and assistance to model users, will be provided by EPA's Center for Water Quality Modeling at this Laboratory.

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ABSTRACT

This manual is a major revision to the original QUAL2E Program Documentation (EPA/600/3-85/065) released in 1985. It includes a description of the recent modifications and improvements to the widely used water quality models QUAL-II and QUAL2E. The enhancements to QUAL-II that led to QUAL2E incorporated improvements in eight areas: (1) algal, nitrogen, phosphorus, and dissolved oxygen interactions; (2) algal growth rate; (3) temperature; (4) dissolved oxygen; (5) arbitrary non-conservative constituents; (6) hydraulics; (7) downstream boundary concentrations; and (8) input/output modifications. These are fully documented in this manual. The enhancements to QUAL2E, described for the first time in this report, include (1) an extensive capability for uncertainty analysis with the model QUAL2E-UNCAS, (2) an option for reach-variable climatology input for steady state temperature simulation, and (3) an option for plotting observed dissolved oxygen data on the line printer plots of predicted dissolved oxygen concentrations.

QUAL2E, which can be operated either as a steady-state or as a dynamic model, is intended for use as a water quality planning tool. The model can be used, for example, to study the impact of waste loads on instream water quality or to identify the magnitude and quality characteristics of nonpoint waste loads as part of a field sampling program. The user also can model effects of diurnal variations in meteorological data on water quality (primarily dissolved oxygen and temperature) or examine diurnal dissolved oxygen variations caused by algal growth and respiration.

QUAL2E-UNCAS is an enhancement to QUAL2E that allows the user to perform uncertainty analysis. Three uncertainty options are available: sensitivity analysis, first order error analysis, and monte carlo simulation. With this capability, the user can assess the effect of model sensitivities and of uncertain input data on model forecasts.

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ACKNOWLEDGMENT

Over the years, many investigators have contributed to the development of what has become QUAL2E. The foundation upon which the model has been built was laid by the Texas Water Development Board in the late 1960s in the QUAL-I model. Many versions of the model emerged in the 1970s. The lineage of QUAL2E can be traced to work done for the Southeast Michigan Council of Governments (SEMCOG) by Water Resources Engineers, Inc. (now Camp, Dresser, McKee Inc.). QUAL-II/SEMCOG was chosen for distribution by the Center for Water Quality Modeling (CWQM) in the late 1970s and began to receive wide use in water quality modeling and wasteload allocation programs.

QUAL-II/SEMCOG was thoroughly reviewed, tested, and documented by the National Council of the Paper Industry for Air and Stream Improvement, Inc. (NCASI), as discussed in NCASI Technical Bulletin No. 391. Changes arising from this review were incorporated in a model called QUAL-II/NCASI, which was adopted for distribution by the Center for Water Quality Modeling. Because of a mutual interest in the program, CWQM partially sponsored an NCASI review of other versions of the QUAL-II computer program and incorporated useful features of these versions in the program called QUAL2E.

Appendix A of this documentation report, the QUAL2E users manual, is modeled after NCASI Technical Bulletin No. 457, "Modifications to the QUAL-2 Water Quality Model and User Manual for QUAL2E Version 2.2." We express our appreciation to NCASI for permission to use and modify this material in this report.

The QUAL2E program also has been made available for IBM PC-compatible microcomputer. The microcomputer installation of this program was performed by Mr. Bruce Bartell and Mr. David Disney of Computer Sciences Corporation, Inc. and was made possible through the support of Mr. King Boynton of the U.S. EPA's Office of Water and through an agreement with the US-Spain Joint Committee for Scientific and Technical Cooperation.

The current release of the program incorporates modifications to the 1985 release to accommodate large elevation differences along a river funded through an agreement with the US-Spain Joint Committee for Scientific and Technical Cooperation. The major extension to the program documented herein, the uncertainty analysis capability, was begun by the first author while on a sabbatical year (1984) from Tufts University at the Athens Environmental Research Laboratory and completed on his return to academic work.

1. INTRODUCTION

QUAL2E is a comprehensive and versatile stream water quality model. It can simulate up to 15 water quality constituents in any combination desired by the user. Constituents which can be simulated are:

1. Dissolved Oxygen
2. Biochemical Oxygen Demand
3. Temperature
4. Algae as Chlorophyll a
5. Organic Nitrogen as N
6. Ammonia as N
7. Nitrite as N
8. Nitrate as N
9. Organic Phosphorus as P
10. Dissolved Phosphorus as P
11. Coliforms
12. Arbitrary Nonconservative Constituent
13. Three Conservative Constituents

The model is applicable to dendritic streams that are well mixed. It assumes that the major transport mechanisms, advection and dispersion, are significant only along the main direction of flow (longitudinal axis of the stream or canal). It allows for multiple waste discharges, withdrawals, tributary flows, and incremental inflow and outflow. It also has the capability to compute required dilution flows for flow augmentation to meet any prespecified dissolved oxygen level.

Hydraulically, QUAL2E is limited to the simulation of time periods during which both the stream flow in river basins and input waste loads are essentially constant. QUAL2E can operate either as a steady-state or as a dynamic model, making it a very helpful water quality planning tool. When operated as a steady-state model, it can be used to study the impact of

waste loads (magnitude, quality and location) on instream water quality and also can be used in conjunction with a field sampling program to identify the magnitude and quality characteristics of nonpoint source waste loads. By operating the model dynamically, the user can study the effects of diurnal variations in meteorological data on water quality (primarily dissolved oxygen and temperature) and also can study diurnal dissolved oxygen variations due to algal growth and respiration. However, the effects of dynamic forcing functions, such as headwater flows or point loads, cannot be modeled in QUAL2E.

QUAL2E-UNCAS is a recent enhancement to QUAL2E which allows the modeler to perform uncertainty analysis on the steady state water quality simulations. Three uncertainty options are available: sensitivity analysis, first order error analysis, and monte carlo simulations. With this capability, the user can assess the effect of model sensitivities and of uncertain input data on model forecasts. Quantifications of the uncertainty in model forecasts will allow assessment of the risk (probability) of a water quality variable being above or below an acceptable level. The uncertainty methodologies provide the means whereby variance estimates and uncertainty prediction can become as much a part of water quality modeling as estimating expected values is today. An evaluation of the input factors that contribute most to the level of uncertainty will lead modelers in the direction of most efficient data gathering and research. In this manner the modeler can assess the risk of imprecise forecasts, and recommend measures for reducing the magnitude of that imprecision.

1.1 QUAL2E DEVELOPMENT

1.1.1 Current Release

The current release of QUAL2E (Version 3.0) was developed under a cooperative agreement between Tufts University, Department of Civil Engineering and the EPA Center for Water Quality Modeling (CWQM), Environmental Research Laboratory, Athens, GA. It includes modifications to prior releases of QUAL2E (Version 2.2, Brown and Barnwell, 1985) as well as an extensive capability for uncertainty analysis (UNCAS) of its steady state simulation output. This release of QUAL2E and its companion program for uncertainty analysis, QUAL2E-UNCAS, is intended to supercede all prior releases of QUAL2E and QUAL-II.

1.1.2 History

The original QUAL-II model was an extension of the stream water quality model QUAL-I developed by F. D. Masch and Associates and the Texas Water Development Board (1971) and the Texas Water Development Board (1970). In 1972, Water Resources Engineers, Inc. (WRE) under contract to the U.S. Environmental Protection Agency, modified and extended QUAL-I to produce the first version of QUAL-II. Over the next 3 years, several different versions of the model evolved in response to specific user needs. In March 1976, the Southeast Michigan Council of Governments (SEMCOG) contracted with WRE to make further modifications and to combine the best features of the existing

versions of QUAL-II into a single model. The significant modifications made in the SEMCOG version by WRE (Roesner et al., 1981a and b) were:

- Option of English or metric units on input data
- Option for English or metric output--choice is independent of input units
- Option to specify channel hydraulic properties in terms of trapezoidal channels or stage-discharge and velocity-discharge curves
- Option to use Tsivoglou's computational method for stream reaeration
- Improvement in output display routines
- Improvement in steady-state temperature computation routines

The SEMCOG version of QUAL-II was later reviewed, documented, and revised (NCASI, 1982). The revised SEMCOG version has since been maintained and supported by the EPA Center for Water Quality Modeling (CWQM). In 1983, EPA, through the CWQM, contracted with NCASI to continue the process of modifying QUAL-II to reflect state-of-the-art water quality modeling. Extensive use of QUAL-II/SEMCOG had uncovered difficulties that required corrections in the algal-nutrient-light interactions. In addition, a number of modifications to the program input and output had been suggested by users. The enhanced QUAL-II model was renamed QUAL2E (Brown and Barnwell, 1985) and incorporated improvements in eight areas. These enhancements are fully documented in this report and summarized as follows:

1. Algal, nitrogen, phosphorus, dissolved oxygen interactions
 - Organic nitrogen state variable
 - Organic phosphorus state variable
 - Nitrification inhibition at low DO
 - Algal preference factor for NH₃
2. Algal growth rate
 - Growth rate dependent upon both NH₃ and NO₃ concentrations
 - Algal self-shading
 - Three light functions for growth rate attenuation
 - Three growth rate attenuation options
 - Four diurnal averaging options for light
3. Temperature
 - Link to algal growth via solar radiation
 - Default temperature correction factors
4. Dissolved Oxygen (DO)
 - 16th Edition Standard Methods DO saturation function

- Traditional SOD units (g/m²-day or g/ft²-day)
 - Dam reaeration option
5. Arbitrary non-conservative constituent
 - First order decay
 - Removal (settling) term
 - Benthic source term
 6. Hydraulics
 - Input factor for longitudinal dispersion
 - Test for negative flow (i.e., withdrawal greater than flow)
 - Capability for incremental outflow along reach
 7. Downstream boundary
 - Option for specifying downstream boundary water quality constituent concentrations
 8. Input/output modifications
 - Detailed summary of hydraulic calculations
 - New coding forms
 - Local climatological data echo printed
 - Enhanced steady-state convergence
 - Five part final summary including components of DO deficit and plot of DO and BOD

1.1.3 Enhancements to QUAL2E

Since the first release of QUAL2E in 1985, enhancements to the model have continued. The modifications, listed below, are designed to improve the computational efficiency of the code, as well as to assist the user in model calibration and verification. The reach variable climatology modifications were added in response to applications of QUAL2E to the river network in Madrid, Spain. In that system, large changes in elevation presented difficulties in calibrating QUAL2E for temperature and dissolved oxygen. The major addition to the current release of QUAL2E is the uncertainty analysis capability. Inclusion of this feature resulted from a project which investigated various methodologies for incorporating uncertainty analysis as an integral part of the water quality modeling process. The QUAL2E model was chosen for this application because it is a general purpose computer code, widely used by consultants and state regulatory agencies in waste load allocation and other planning activities.

Enhancements to QUAL2E in the current release include:

1. Option for reach variable climatology input for steady state temperature simulation.
2. Option for including observed dissolved oxygen data on the line printer plots of predicted dissolved oxygen concentrations.
3. Changing the steady state convergence criterion for algal, nitrification, and dissolved oxygen simulations from an absolute error to a relative error.
4. Updating the formulation for estimating reaeration effects of water flowing over a dam.

Capabilities of the uncertainty analysis model, QUAL2E-UNCAS, include the following:

1. Sensitivity analysis--with an option for factorially designed combinations of input variable perturbations.
2. First order error analysis--with output consisting of a normalized sensitivity coefficient matrix, and a components of variance matrix.
3. Monte carlo simulation--with summary statistics and frequency distributions of the output variables.

1.1.4 Information Sources

Major sources of information for this revised documentation are:

1. Roesner, L. A., Giguere, P. R. and Evenson, D. E. Computer Program Documentation for Stream Quality Modeling (QUAL-II). U.S. Environmental Protection Athens, GA. EPA-600/9-81-014, February 1981.
2. JRB Associates. Users Manual for Vermont QUAL-II Model. Prepared for U.S. Environmental Protection Agency, Washington, DC. June 1983.
3. National Council for Air and Stream Improvement. A Review of the Mathematical Water Quality Model QUAL-II and Guidance for its Use, NCASI, New York, NY, Technical Bulletin No. 391, December 1982.
4. Brown, L. C. and T. O. Barnwell, Jr., Computer Program Documentation for the Enhanced Stream Water Quality Model QUAL2E. U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA, EPA/600-3-85/065, August 1985.

This documentation of QUAL2E updates the report distributed with the prior version of the model (Brown and Barnwell, 1985) and consolidates material from these and other sources into a single volume. The basic

theory and mechanics behind the development of QUAL2E are described in this volume. The two appendices contain user manuals for QUAL2E and QUAL2E-UNCAS and provide a detailed description of input data requirements, as well as sample input coding forms. This report, a copy of the QUAL2E and QUAL2E-UNCAS computer code, and sample input/output data files are available from the Center for Water Quality Modeling, U.S. Environmental Protection Agency, Environmental Research Laboratory, Athens, GA 30613.

1.1.5 Organization of this Report

The general program structure, specifications, and limitations of QUAL2E are discussed in the remainder of this chapter. Chapter 2 describes the conceptual and functional representation of QUAL2E as well as the hydraulic characteristics of the model. The mathematical basis of the water quality constituent formulations is presented in Chapter 3. Chapter 4 presents the framework for modeling temperature. With the exception of Section 4.8, it is extracted essentially verbatim from Roesner *et al.*, 1981. Chapter 5 describes the computational representation of the model and the numerical solution algorithm.

The uncertainty analysis capabilities of QUAL2E-UNCAS are documented in Chapter 6.

Appendix A contains a user manual complete with revised input coding forms for the current release (Version 3.0) of QUAL2E. Appendix B is the user manual for QUAL2E-UNCAS. Appendix C describes an example application of QUAL2E-UNCAS.

For the convenience of the majority of users, all of the units specifications are given in the English system of measurement. QUAL2E, however, will recognize either English or metric units.

1.2 QUAL2E COMPUTER MODEL

1.2.1 Prototype Representation

QUAL2E permits simulation of any branching, one-dimensional stream system. The first step in modeling a system is to subdivide the stream system into reaches, which are stretches of stream that have uniform hydraulic characteristics. Each reach is then divided into computational elements of equal length. Thus, all reaches must consist of an integer number of computational elements.

There are seven different types of computational elements:

1. Headwater element
2. Standard element
3. Element just upstream from a junction

4. Junction element
5. Last element in system
6. Input element
7. Withdrawal element

Headwater elements begin every tributary as well as the main river system, and as such, they must always be the first element in a headwater reach. A standard element is one that does not qualify as one of the remaining six element types. Because incremental flow is permitted in all element types, the only input permitted in a standard element is incremental flow. A type 3 element is used to designate an element on the main stem just upstream of a junction. A junction element (type 4) has a simulated tributary entering it. Element type 5 identifies the last computational element in the river system; there should be only one type 5 element. Element types 6 and 7 represent inputs (waste loads and unsimulated tributaries) and water withdrawals, respectively. River reaches, which are aggregates of computational elements, are the basis of most data input. Hydraulic data, reaction rate coefficients, initial conditions, and incremental flows data are constant for all computational elements within a reach.

1.2.2 Model Limitations

QUAL2E has been designed to be a relatively general program; however, certain dimensional limitations have been imposed during program development. These limitations are:

- Reaches: a maximum of 25
- Computational elements: no more than 20 per reach or a total of 250
- Headwater elements: a maximum of 7
- Junction elements: a maximum of 6
- Input and withdrawal elements: a maximum of 25

QUAL2E incorporates features of ANSI FORTRAN 77 that allow these limitations to be easily changed.

1.2.3 Model Structure and Subroutines

QUAL2E is structured as one main program supported by 51 different subroutines. Figure I-1 illustrates the functional relationships between the main program and the subroutines. New state variables can be added or modifications to existing relationships can be made with a minimum of model restructuring through the simple addition of appropriate subroutines.

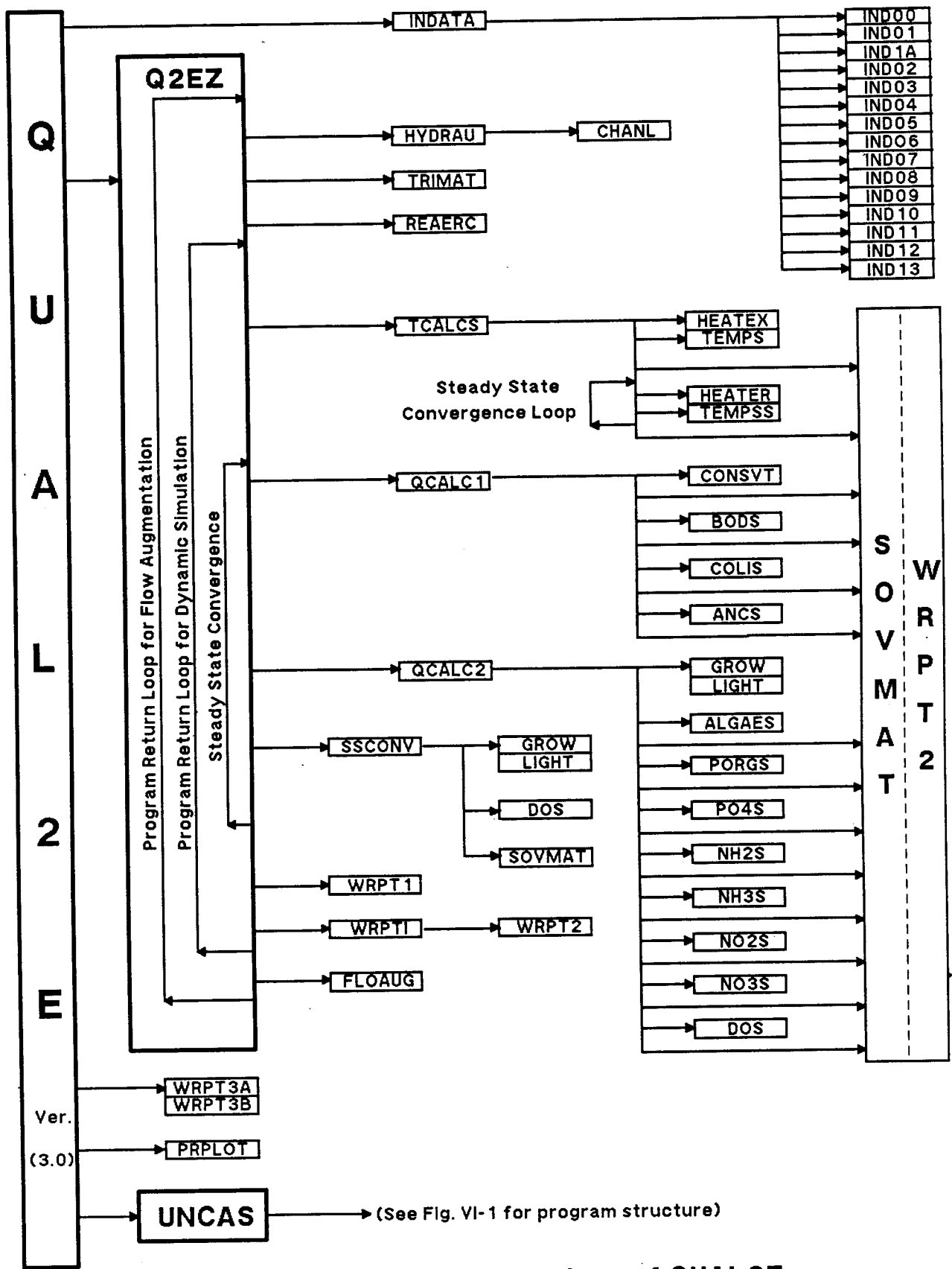


Figure I-1 General Structure of QUAL2E

The structural framework of QUAL2E has been modified from prior versions of QUAL-II. The large MAIN program and subroutine INDATA have been divided into smaller groups of subroutines, each with a more narrowly defined task. The new subroutines in QUAL2E include the algal light functions (GROW/LIGHT), the steady state algal output summary (WRPT1), the organic nitrogen and phosphorus state variables (NH2S, PORG), and the line printer plot routine (PRPLOT). This reorganization of QUAL2E into smaller programmatic units is the first step in adapting the model to micro and minicomputers that have limited memory.

QUAL2E Version 3.0 retains this modular program structure. QUAL2E may be obtained with or without the UNCAS capability. The program structure and subroutine descriptions for UNCAS are described in Chapter 6 of this report.

1.2.4 Program Language and Operating Requirements

QUAL2E is written in ANSI FORTRAN 77 and is compatible with mainframe and personal computer systems that support this language. QUAL2E typically requires 256K bytes of memory and uses a single system input device (cards or disk file) and the system's line printer (or disk file) as the output device.

If the system's normal FORTRAN input device unit is not unit 1 or the output unit is not unit 7, then the variables "NI" and "NJ" in the main program (files Q2E3P0 or Q2U3P0) should be changed to reflect the system's I/O unit identifiers.

2. GENERAL MODEL FORMULATION

2.1 INTRODUCTION

The primary objective of any stream water quality model development is to produce a tool that has the capability for simulating the behavior of the hydrologic and water quality components of a stream system. The development of this tool to simulate prototype behavior by applying a mathematical model on a digital computer proceeds through three general phases (Water Resources Engineers, Inc., 1967):

1. Conceptual representation
2. Functional representation
3. Computational representation

Conceptual representation involves a graphic idealization of the prototype by description of the geometric properties that are to be modeled and by identification of boundary conditions and interrelationships between various parts of the prototype. Usually, this process entails dividing the prototype into discrete "elements" of a size compatible with the objectives that the model must serve, defining these elements according to some simple geometric rules, and designating the mode by which they are connected, either physically or functionally, as integral parts of the whole. A part of this conceptual structuring is the designation of those boundary conditions to be considered in the simulation.

Functional representation entails formulation of the physical features, processes, and boundary conditions into sets of algebraic equations. It involves precise definition of each variable and its relationship to all other parameters that characterize the model or its input-output relationships.

Computational representation is the process whereby the functional model is translated into the mathematical forms and computational procedures required for solution of the problem over the desired time and space continuum. It is concerned with development of a specific solution technique that can be accommodated by the computer and with codification of the technique in computer language.

In the remainder of this section the Conceptual Representation of QUAL2E will be described together with its general functional representation for mass transport, hydraulic characteristics, and longitudinal dispersion.

Chapter 3 will discuss specific constituent reactions and interactions. Chapter 4 will develop the functional representation of stream temperature as simulated in QUAL2E.

2.2 CONCEPTUAL REPRESENTATION

Figure II-1 shows a stream reach (n) that has been divided into a number of subreaches or computational elements, each of length Δx . For each of these computational elements, the hydrologic balance can be written in terms of flows into the upstream face of the element (Q_{i-1}), external sources or withdrawals (Q_{x_i}), and the outflow (Q_i) through the downstream face of the element. Similarly, a materials balance for any constituent C can be written for the element. In the materials balance, we consider both transport ($Q \cdot C$) and dispersion ($A \frac{DL}{\Delta x} \frac{\partial C}{\partial x}$) as the movers of mass along the stream axis. Mass can be added to or removed from the system via external sources and withdrawals ($Q_{x_i} C_{x_i}$) and added or removed via internal sources or sinks (S_i) such as benthic sources and biological transformation. Each computational element is considered to be completely mixed.

Thus, the stream can be conceptualized as a string of completely mixed reactors--computational elements--that are linked sequentially to one another via the mechanisms of transport and dispersion. Sequential groups of these reactors can be defined as reaches in which the computational elements have the same hydrogeometric properties--stream slope, channel cross section, roughness, etc.--and biological rate constants--BOD decay rate, benthic source rates, algae settling rates, etc.--so that the stream shown at the left of Figure II-2 can be conceptually represented by the grouping of reaches and computational elements shown on the right of Figure II-2.

2.3 FUNCTIONAL REPRESENTATION

2.3.1 Mass Transport Equation

The basic equation solved by QUAL2E is the one dimensional advection-dispersion mass transport equation, which is numerically integrated over space and time for each water quality constituent. This equation includes the effects of advection, dispersion, dilution, constituent reactions and interactions, and sources and sinks. For any constituent, C, this equation can be written as:

$$\frac{\partial M}{\partial t} = \frac{\partial(A_x D_L \frac{\partial C}{\partial x})}{\partial x} dx - \frac{\partial(A_x \bar{u} C)}{\partial x} dx + (A_x dx) \frac{dC}{dt} + s \quad \text{II-1}$$

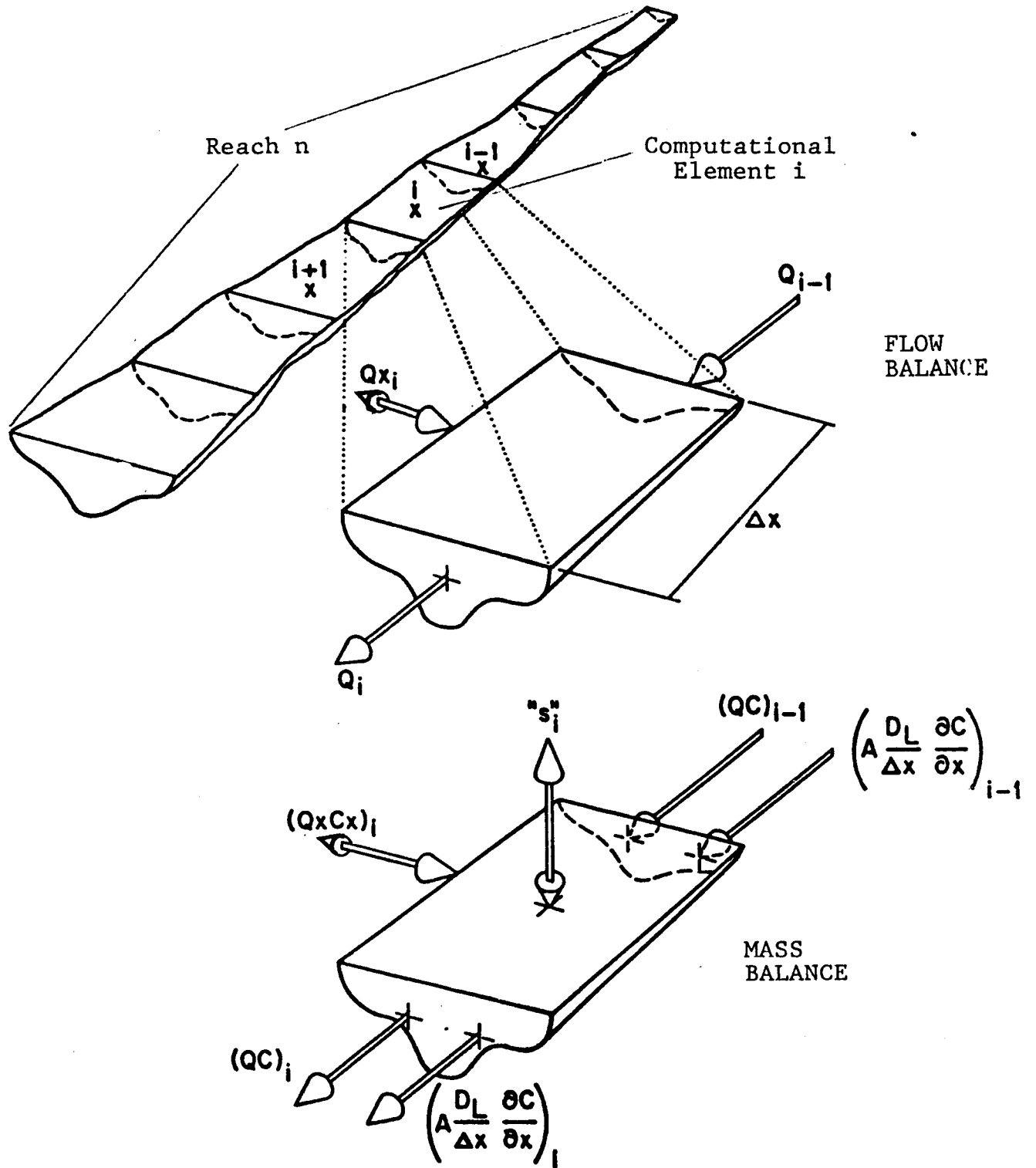


Figure II-1. Discretized Stream System

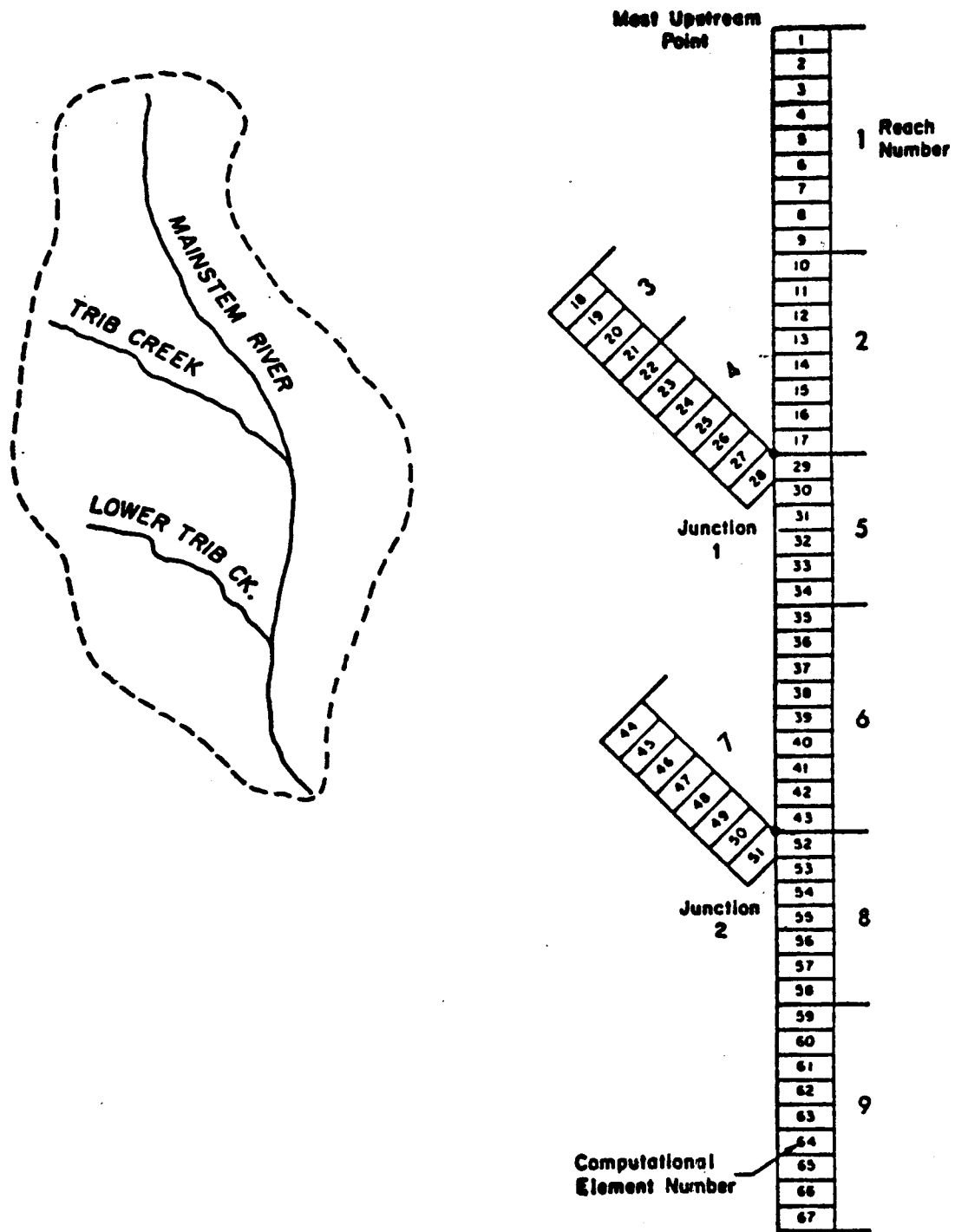


Figure II-2. Stream Network of Computational Elements and Reaches

where

- M = mass (M)
- x = distance (L)
- t = time (T)
- C = concentration (M L⁻³)
- A_x = cross-sectional area (L²)
- D_L = dispersion coefficient (L² T⁻¹)
- \bar{u} = mean velocity (L T⁻¹)
- s = external source or sinks (M T⁻¹)

Because M = VC, we can write

$$\frac{\partial M}{\partial t} = \frac{\partial(VC)}{\partial t} = V \frac{\partial C}{\partial t} + C \frac{\partial V}{\partial t} \quad \text{II-2a}$$

where

$$V = A_x dx = \text{incremental volume (L}^3\text{)}$$

If we assume that the flow in the stream is steady, i.e., $\partial Q/\partial t = 0$, then the term $\partial V/\partial t = 0$ and equation II-2a becomes

$$\frac{\partial M}{\partial t} = V \frac{\partial C}{\partial t} \quad \text{II-2b}$$

Combining equations II-1 and II-2b and rearranging,

$$\frac{\partial C}{\partial t} = \frac{\partial(A_x D_L \frac{\partial C}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} C)}{A_x \partial x} - \frac{dC}{dt} + \frac{s}{V} \quad \text{II-3}$$

The terms on the right-hand side of the equation represent, respectively, dispersion, advection, constituent changes, external sources/sinks, and dilution. The $\frac{dC}{dt}$ term refers only to constituent changes such as growth and decay, and should not be confused with the term $\frac{\partial C}{\partial t}$, the local concentration gradient. The latter term includes the effect of constituent changes as well as dispersion, advection, sources/sinks, and dilutions.

Under steady-state conditions, the local derivative becomes equal to zero; in other words:

$$\frac{\partial C}{\partial t} = 0 \quad \text{II-4}$$

Changes that occur to individual constituents or particles independent of advection, dispersion, and waste inputs are defined by the term

$$\frac{dC}{dt} = \text{individual constituents changes} \quad \text{II-5}$$

These changes include the physical, chemical, and biological reactions and interactions that occur in the stream. Examples of these changes are reaeration, algal respiration and photosynthesis, and coliform die-off.

2.4 HYDRAULIC CHARACTERISTICS

QUAL2E assumes that the stream hydraulic regime is steady-state; i.e., $\partial Q/\partial t = 0$, therefore, the hydrologic balance for a computational element can be written simply as (see Figure II-1):

$$\left(\frac{\partial Q}{\partial x}\right)_i = (Q_x)_i \quad \text{II-6}$$

where $(Q_x)_i$ is the sum of the external inflows and/or withdrawals to that element. i

2.4.1 Discharge Coefficients

Once equation II-6 has been solved for Q , the other hydraulic characteristics of the stream segments can be determined by equations of the form:

$$\bar{u} = aQ^b \quad \text{II-7}$$

$$A_x = Q/\bar{u} \quad \text{II-8}$$

and

$$d = \alpha Q^\beta \quad \text{II-9}$$

where a , b , α and β are empirical constants, and d is the stream depth. These constants usually can be determined from stage-discharge rating curves.

2.4.2 Trapezoidal Cross Sections

Alternatively, if the cross-sectional properties of the stream segment are available as a function of the depth d , u can be obtained as a function of discharge by the trial and error solution of Mannings equation:

$$Q = \frac{1.486}{n} A_x R_x^{2/3} S_e^{1/2} \quad \text{II-10}$$

where

A_x = cross-section area of the channel or canal, ft^2

R_x = mean effective hydraulic radius, ft

n = Manning roughness factor (usual range 0.010 to 0.10)

S_e = slope of the energy grade line (dimensionless)

Q = discharge, ft^3/sec

The value for \bar{u} is then determined from equation II-8.

2.4.3 Longitudinal Dispersion

Dispersion is basically a convective transport mechanism. The term "dispersion" is generally used for transport associated with spatially averaged velocity variation, as opposed to "diffusion," which is reserved for transport that is associated primarily with time-averaged velocity fluctuations.

Taylor (1956) derived a predictive equation for the longitudinal dispersion coefficient, D_L , in long straight pipes, as

$$D_L = 10 r_0 u^*, \quad \text{ft}^2/\text{sec} \quad \text{II-11}$$

where r_0 is the pipe radius and u^* is the average shear velocity defined as

$$u^* = \sqrt{\tau_0/\rho}, \quad \text{ft}/\text{sec} \quad \text{II-12}$$

where

τ_0 = boundary shear stress, lb/ft^2 , and

ρ = mass fluid density, $\text{lb}\cdot\text{sec}^2/\text{ft}^4$

Some investigators have attempted to apply Taylor's expression to streamflow. Such applications are only approximate, however, because of the difference between the geometry or velocity distributions in streamflow and those in a pipe.

Elder (1959) assumed that only the vertical velocity gradient was important in streamflow and developed an expression analogous to Taylor's expression:

$$D_L = Kdu^* \quad \text{II-13}$$

where d is the mean depth in feet of the stream. Elder used a value of 5.93 for K in this equation.

Other investigators have derived similar expressions for D_L and found it to be extremely sensitive to lateral velocity profiles. Elder's expression, however, seems adequate in one-dimensional situations where the channel is not too wide. For very wide channels, Fisher (1964) has shown that half-width rather than depth is the dominant scale and therefore is important to the definition of the longitudinal dispersion coefficient. Equations II-11 and II-13 can be written in terms of the Manning Equation and other variables characteristic of stream channels.

As an example, for steady-state open-channel flow.

$$u^* = C \sqrt{RS_e} \quad \text{II-14}$$

where

C = Chezy's coefficient

R = the hydraulic radius

S_e = the slope of the energy grade line

Chezy's coefficient is given by:

$$C = \frac{R^{1/6}}{n} \quad \text{II-15}$$

where n is the Manning roughness coefficient tabulated for different types of channels in Table II-1.

S_e , the slope of the energy gradient, is given by

$$S_e = \left(\frac{\bar{u} n}{1.486 R^{2/3}} \right)^2 \quad \text{II-16}$$

where \bar{u} is the mean velocity. Substituting equations II-14, II-15 and II-16 into equation II-13 and letting $R = d$ for a wide channel yields the expression

$$D_L = 3.82 K n \bar{u} d^{5/6} \quad \text{II-17}$$

TABLE II-1
VALUES OF MANNING'S "n" ROUGHNESS COEFFICIENT
After Henderson (1966)

Artificial Channels	n
Glass, plastic, machined metal	0.010
Dressed timber, joints flush	0.011
Sawn timber, joints uneven	0.014
Cement plaster	0.011
Concrete, steel troweled	0.012
Concrete, timber forms, unfinished	0.014
Untreated gunite	0.015-0.017
Brickwork or dressed masonry	0.014
Rubble set in cement	0.017
Earth, smooth, no weeds	0.020
Earth, some stones, and weeds	0.025
Natural River Channels	n
Clean and straight	0.025-0.030
Winding with pools and shoals	0.033-0.040
Very weedy, winding and overgrown	0.075-0.150
Clean straight alluvial channels	0.031 $d^{1/6}$

(d = D-75 size in ft.
= diameter that 75
percent of parti-
cles are smaller
than)

where

D_L = longitudinal dispersion coefficient, ft^2/sec

K = dispersion constant (dimensionless)

n = Manning's roughness coefficient (dimensionless)

\bar{u} = mean velocity, ft/sec

d = mean depth, ft

Typical values for dispersion coefficients, D_L , and values of the dispersion constant, K , cited by Fisher et al. (1979), are given in Table II-2. Note that the dispersion constant, K , shown in this table is one to three orders of magnitude greater than that used by Elder.

2.5 Flow Augmentation

When the DO concentration in a stream drops below some required target level, such as the state water quality standard for DO, it may be desirable to raise this DO concentration by augmenting the flow of the stream. According to the originators of the flow augmentation routine in QUAL2E, Frank D. Masch and Associates and the Texas Water Development Board (1971), the amount of flow necessary to bring the DO concentrations up to required standards cannot be calculated by an exact functional relationship. A good approximation of the relationship is used in QUAL2E and has the following quadratic form:

$$DO_R = DO_T - DO_{\min} \quad \text{II-18}$$

and

$$Q_R = Q_C \left[\frac{DO_R}{DO_T} + 0.15 \left(\frac{DO_R}{DO_T} \right)^2 \right] \quad \text{II-19}$$

where,

DO_R = dissolved oxygen concentration required to meet target conditions, mg/L

DO_T = required target level of DO, mg/L

DO_{\min} = minimum DO concentration (critical level) in the oxygen sag curve, mg/L

Q_R = amount of flow augmentation required, ft^3/sec

Q_C = flow at the critical point in the oxygen sag curve, ft^3/sec

TABLE II-2

EXPERIMENTAL MEASUREMENTS OF LONGITUDINAL DISPERSION IN OPEN CHANNELS

(After Table 5.3, Fisher et al., 1979)

Channel	Depth d (ft)	Width W (ft)	Mean Velocity \bar{u} (ft/sec)	Shear Velocity u^* (ft/sec)	Dispersion Coefficient D_L (ft ² /sec)	Dispersion Constant K
Chicago Ship Channel	26.5	160	0.89	0.063	32	20
Sacramento River	13.1	--	1.74	0.17	161	74
River Derwent	0.82	--	1.25	0.46	50	131
South Platte River	1.5	--	2.17	0.23	174	510
Yuma Mesa A Canal	11.3	--	2.23	1.13	8.2	8.6
Trapezoidal Laboratory Channel with roughened sides	0.115	1.31	0.82	0.066	1.3	174
	0.154	1.41	1.48	0.118	2.7	150
	0.115	1.31	1.48	0.115	4.5	338
	0.115	1.12	1.44	0.114	0.8	205
	0.069	1.08	1.48	0.108	4.3	392
	0.069	0.62	1.51	0.127	2.4	270
Green-Duwamish River	3.61	66	--	0.16	70-92	120-160
Missouri River	8.86	660	5.09	0.24	16,000	7500
Copper Creek (below gage)	1.61	52	0.89	0.26	215	500
	2.79	59	1.97	0.33	226	250
	1.61	52	0.85	0.26	102	245
Clinch River	2.79	154	1.05	0.22	151	235
	6.89	197	3.08	0.34	581	245
	6.89	174	2.62	0.35	506	210
Copper Creek (above gage)	1.31	62	0.52	0.38	97	220
Powell River	2.79	112	0.49	0.18	102	200
Clinch River	1.90	118	0.69	0.16	87	280
Coachella Canal	5.12	79	2.33	0.14	103	140
Bayon Anacoco	3.08	85	1.12	0.22	355	524
	2.98	121	1.31	0.22	420	640
Nooksack River	2.49	210	2.20	0.89	377	170
Wind/Bighorn Rivers	3.61	194	2.89	0.39	452	318
	7.09	226	5.09	0.56	1722	436
John Day River	1.90	82	3.31	0.46	151	172
	8.10	112	2.69	0.59	700	146

TABLE II-2

EXPERIMENTAL MEASUREMENTS OF LONGITUDINAL DISPERSION IN OPEN CHANNELS

(After Table 5.3, Fisher et al., 1979) (Continued)

Channel	Depth d (ft)	Width W (ft)	Mean Velocity \bar{u} (ft/sec)	Shear Velocity u^* (ft/sec)	Dispersion Coefficient D_L (ft ² /sec)	Dispersion Constant K
Comite River	1.41	52	1.21	0.16	151	650
Sabine River	6.69	341	1.90	0.16	3390	3100
	15.6	417	2.10	0.26	7200	1800
Yadkin River	7.71	230	1.41	0.33	1200	470
	12.6	236	2.49	0.43	2800	520

The model augments the stream flow by first comparing, after steady-state conditions have been reached, the simulated DO concentration with the prespecified target level of DO in each reach. If the calculated DO is below the target level, the program finds those upstream sources that the user has specified for dilution purposes, and adds water equally from all these sources. The DO calculations are then repeated. This process continues until the DO target level is satisfied. (NOTE: The flow augmentation subroutine can be used for DO only.)

3. CONSTITUENT REACTIONS AND INTERRELATIONSHIPS

3.1 GENERAL CONSIDERATIONS

One of the most important considerations in determining the waste-assimilative capacity of a stream is its ability to maintain an adequate dissolved oxygen concentration. Dissolved oxygen concentrations in streams are controlled by atmospheric reaeration, photosynthesis, plant and animal respiration, benthic oxygen demand, biochemical oxygen demand, nitrification, salinity, and temperature, among other factors.

The most accurate oxygen balance would consider all significant factors. The QUAL2E model includes the major interactions of the nutrient cycles, algae production, benthic oxygen demand, carbonaceous oxygen uptake, atmospheric aeration and their effect on the behavior of dissolved oxygen. Figure III-1 illustrates the conceptualization of these interactions. The arrows on the figure indicate the direction of normal system progression in a moderately polluted environment; the directions may be reversed in some circumstances for some constituents. For example, under conditions of oxygen supersaturation, which might occur as a result of algal photosynthesis, oxygen might be driven from solution, opposite to the indicated direction of the flow path.

Coliforms and the arbitrary nonconservative constituent are modeled as nonconservative decaying constituents and do not interact with other constituents. The conservative constituents, of course, neither decay nor interact in any way with other constituents.

The mathematical relationships that describe the individual reactions and interactions are presented in the following paragraphs.

3.2 CHLOROPHYLL a (PHYTOPLANKTONIC ALGAE)

Chlorophyll a is considered to be directly proportional to the concentration of phytoplanktonic algal biomass. For the purposes of this model algal biomass is converted to chlorophyll a by the simple relationship:

$$\text{Chl}_a = \alpha_0 A$$

III-1

where

Chl_a = chlorophyll a concentration, ug-Chla/L

A = algal biomass concentration, mg-A/L

α_0 = a conversion factor, ug Chla/mg A

The differential equation that governs the growth and production of algae (chlorophyll a) is formulated according to the following relationship.

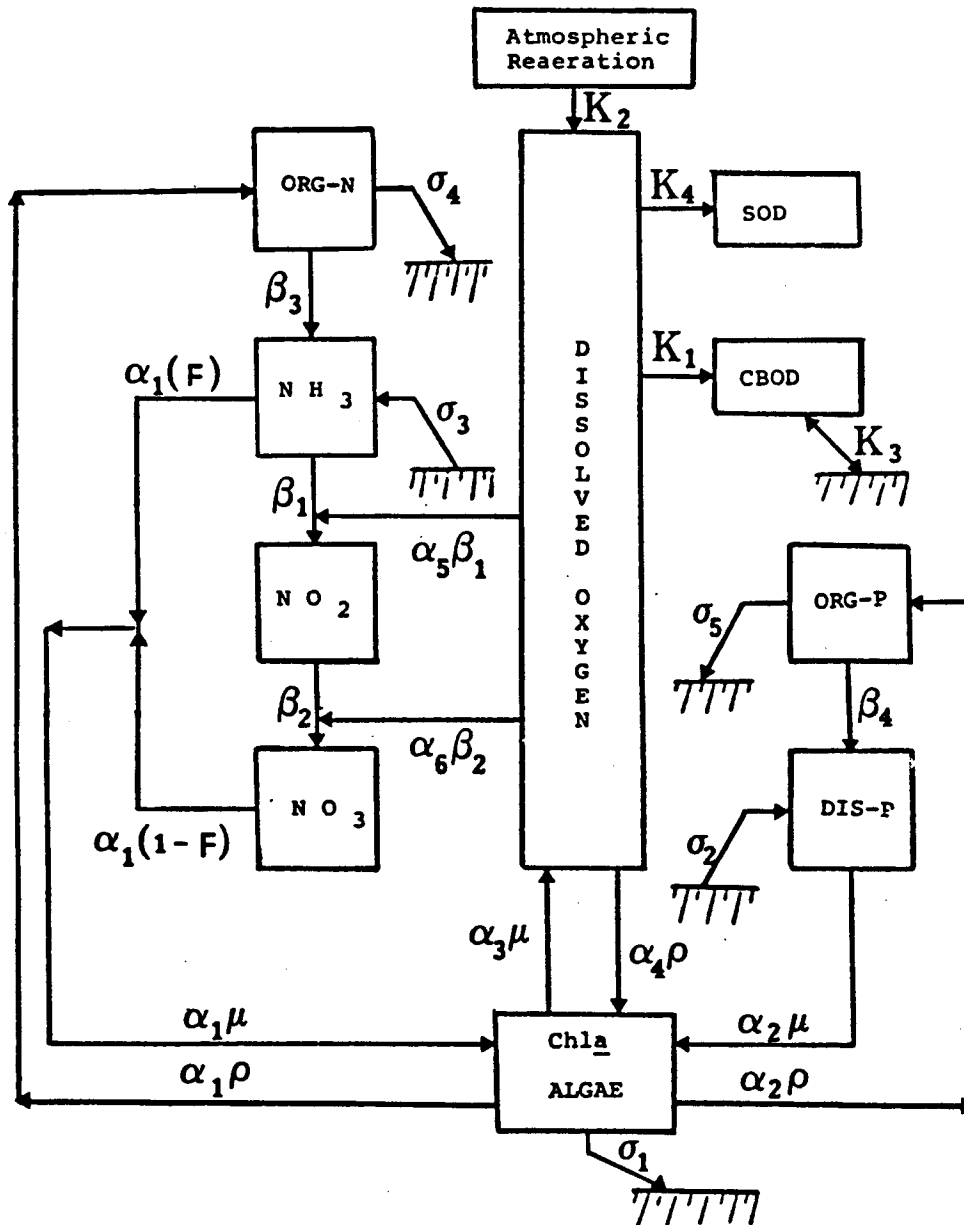


Figure III-1. Major Constituent Interactions in QUAL2E

$$\frac{dA}{dt} = \mu A - \rho A - \frac{\sigma_1}{d} A \quad \text{III-2}$$

where

- A = algal biomass concentration, mg-A/L
- t = time, day
- μ = the local specific growth rate of algae as defined below, which is temperature dependent, day⁻¹
- ρ = the local respiration rate of algae, which is temperature dependent, day⁻¹
- σ_1 = the local settling rate for algae, which is temperature dependent, ft/day
- d = average depth, ft

3.2.1 Algal Respiration Rate

In QUAL2E, the single respiration rate parameter, ρ , is used to approximate three processes: (a) the endogenous respiration of algae, (b) the conversion of algal phosphorus to organic phosphorus, and (c) the conversion of algal nitrogen to organic nitrogen. No attempt is made to use separate rate coefficients for these three processes, as is done in the State of Vermont, revised Meta Systems version of QUAL-II (JRB Associates, 1983; and Walker, 1981).

3.2.2 Algal Specific Growth Rate

The local specific growth rate of algae, μ , is known to be coupled to the availability of required nutrients (nitrogen and phosphorus) and light. A variety of mathematical expressions for expressing multiple nutrient-light limitations on algal growth rate have been reported (De Groot, 1983; Scavia and Park, 1976; and Swartzman and Bentley, 1979). QUAL2E has the capability of modeling the interaction among these limiting factors in three different ways.

Growth Rate Option 1. Multiplicative. The kinetic expressions used to represent the effects of nitrogen, phosphorus, and light are multiplied together to determine their net effect on the local algal growth rate. This option has as its biological basis the multiplicative effects of enzymatic processes involved in photosynthesis:

$$\mu = \mu_{\max} (FL) (FM) (FP) \quad \text{III-3a}$$

where

μ_{\max} = maximum specific algal growth rate, day⁻¹

FL = algal growth limitation factor for light

FN = algal growth limitation factor for nitrogen

FP = algal growth limitation factor for phosphorus

This formulation is used in the SEMCOG version of QUAL-II.

Growth Rate Option 2. Limiting Nutrient. This option represents the local algal growth rate as limited by light and either nitrogen or phosphorus, but not both. Thus, the nutrient/light effects are multiplicative, but the nutrient/nutrient effects are alternate. This formulation mimics Liebig's law of the minimum:

$$\mu = \mu_{\max} (FL) \text{ Min } (FN, FP) \quad \text{III-3b}$$

Thus, the algal growth rate is controlled by the nutrient (N or P) with the smaller growth limitation factor. This option is used in the State of Vermont version of QUAL-II.

Growth Rate Option 3. Harmonic Mean. This option, a compromise between options 1 and 2, is a modification of an intuitive form suggested by Scavia and Park (1976) and is mathematically analogous to the total resistance of two resistors in parallel. In this option, an effective nutrient limitation factor is computed as the average of the inverse reciprocals of the individual nitrogen and phosphorus growth limitation factors, i.e.,

$$\mu = \mu_{\max} (FL) \left[\frac{2}{1/FN + 1/FP} \right] \quad \text{III-3c}$$

Thus, the algal growth rate is controlled by a multiplicative relation between light and nutrients, but the nutrient/nutrient interactions are represented by a harmonic mean. This option has been used by Water Resources Engineers in the application of a QUAL-II-like model, WREDUN, to Lake Dunlap (Brandes and Stein, no date; see also Bowie et al., 1985).

Walker (1983) has cautioned against using the harmonic mean option in systems where one nutrient is in excess (say nitrogen, so that FN→1.0) and the other is extremely limiting (say phosphorus, so that FP→0.0). In this case the value of the nutrient attenuation factor approaches 2 FP, rather than FP, as expected.

3.2.3 Algal-Light Relationships

3.2.3.1 Light Functions

A variety of mathematical relationships between photosynthesis and light have been reported in the literature (Jassby and Platt, 1976; Field and Effler, 1982). Although they differ in mathematical form, the relationships exhibit similar characteristics. All show an increasing rate of photosynthesis with increasing light intensity up to a maximum or saturation value. At high light intensities, some of the expressions exhibit photoinhibition, whereas others show photosynthetic activity remaining at the maximum rate.

QUAL2E recognizes three options for computing the algal growth limitation factor for light, FL in Equations III-3a,b,c. Light attenuation effects on the algal growth rate may be simulated using a Monod half-saturation method, Smith's function (Smith, 1936), or Steele's equation (Steele, 1962).

Light Function Option 1. Half Saturation. In this option, the algal growth limitation factor for light is defined by a Monod expression:

$$FL_z = \frac{I_z}{K_L + I_z} \quad \text{III-4a}$$

where

FL_z = algal growth attenuation factor for light at intensity I_z

I_z = light intensity at a given depth (z), Btu/ft²-hr

K_L = half saturation coefficient for light, Btu/ft²-hr

z = depth variable, ft

Light Function Option 2. Smith's Function. In this option, the algal growth limitation factor for light is formulated to include second order effects of light intensity:

$$FL_z = \frac{I_z}{(K_L^2 + I_z^2)^{1/2}} \quad \text{III-4b}$$

where

K_L = light intensity corresponding to 71% of the maximum growth rate, Btu/ft²-hr

with the other terms as defined in Equation III-4a.

Light Function Option 3. Steel's Equation. This option incorporates an exponential function to model the effect of photoinhibition on the algal growth rate:

$$FL_z = \left(\frac{I_z}{K_L}\right) \exp\left(1 - \frac{I_z}{K_L}\right) \quad \text{III-4c}$$

where

K_L = saturation light intensity at which the algal growth rate is a maximum, Btu/ft²-hr

with the other terms as defined in Equation III-4a.

Note: The parameter K_L , which appears in all three light function equations is defined differently in each.

All of the light functions in Equations III-4a,b,c express the value of FL for an optically thin layer. In QUAL2E photosynthesis occurs throughout the depth of the water column. Light intensity varies with depth according to Beer's law:

$$I_z = I \exp(-\lambda z) \quad \text{III-5}$$

where

I_z = light intensity at a given depth (z), Btu/ft²-hr

I = surface light intensity, Btu/ft²-hr

λ = light extinction coefficient, ft⁻¹

z = depth variable, ft

When Equation III-5 is substituted into Equations III-4a,b,c and integrated over the depth of flow, the depth-averaged light attenuation factor is obtained. The resulting expressions for the three options are:

Option 1: Half Saturation

$$FL = (1/\lambda d) \ln \left[\frac{K_L + I}{K_L + I e^{-\lambda d}} \right] \quad \text{III-6a}$$

K_L = light intensity at which growth rate is 50% of the maximum growth rate.

Option 2: Smith's Function

$$FL = (1/\lambda d) \ln \left[\frac{I/K_L + (1 + (I/K_L)^2)^{1/2}}{(I/K_L)e^{-\lambda d} + (1 + (I/K_L)e^{-\lambda d})^2)^{1/2}} \right] \quad \text{III-6b}$$

K_L = light intensity at which growth rate is 71% of the maximum growth rate.

Option 3: Steel's Equation

$$FL = \frac{2.718}{\lambda d} [e^{-(e^{-\lambda d(I/K_L)})} - e^{-I/K_L}] \quad \text{III-6c}$$

K_L = light intensity at which growth rate is equal to the maximum growth rate.

where

FL = depth-averaged algal growth attenuation factor for light

K_L = light saturation coefficient, Btu/ft²-hr

λ = light extinction coefficient, ft⁻¹

d = depth of flow, ft

I = surface light intensity, Btu/ft²-hr

The relative merits of these light functions are discussed by various authors (Bannister, 1974; Platt et al., 1981; Swartzmann and Bentley, 1979; and Field and Effler, 1982). The half saturation method is the form used in the SEMCOG version of QUAL-II. Evidence shows that the use of Smith's function is preferable over the half saturation method if photoinhibition effects are unimportant (Jassby and Platt, 1976). The mathematical forms of Equations III-4a,b,c are compared graphically in Figure III-2. All three equations have a single parameter, K_L ; however, it is defined differently in each equation. In Figure III-2 the values of K_L are selected so that each curve passes through a common point, namely FL = 0.5 at I = 5 intensity units (i.e., a half saturation rate equal to 5 light intensity units).

3.2.3.2 Light Averaging Options

Steady state algal simulations require computation of an average value of FL, the growth attenuation factor for light, over the diurnal cycle.

There are four options in QUAL2E for computing this average. The options arise from combinations of situations regarding two factors:

- The source of the solar radiation data used in the computation, i.e., whether it is supplied externally by the user or calculated internally in the temperature heat balance.
- The nature of the averaging process, i.e., whether hourly values of FL are averaged, or a single daylight average value of solar radiation is used to estimate the mean value of FL.

The four daily light averaging options are defined below. In each case, the half saturation light function is used as an example; in practice any of the three light functions may be employed.

Option 1: FL is computed from one daylight average solar radiation value calculated in the steady state temperature heat balance:

$$FL = AFACT * f * FL_1 \quad \text{III-7a}$$

$$FL_1 = \frac{1}{\lambda d} \ln \left[\frac{K_L + \bar{T}_{alg}}{K_L + \bar{T}_{alg} e^{-\lambda d}} \right] \quad \text{III-7b}$$

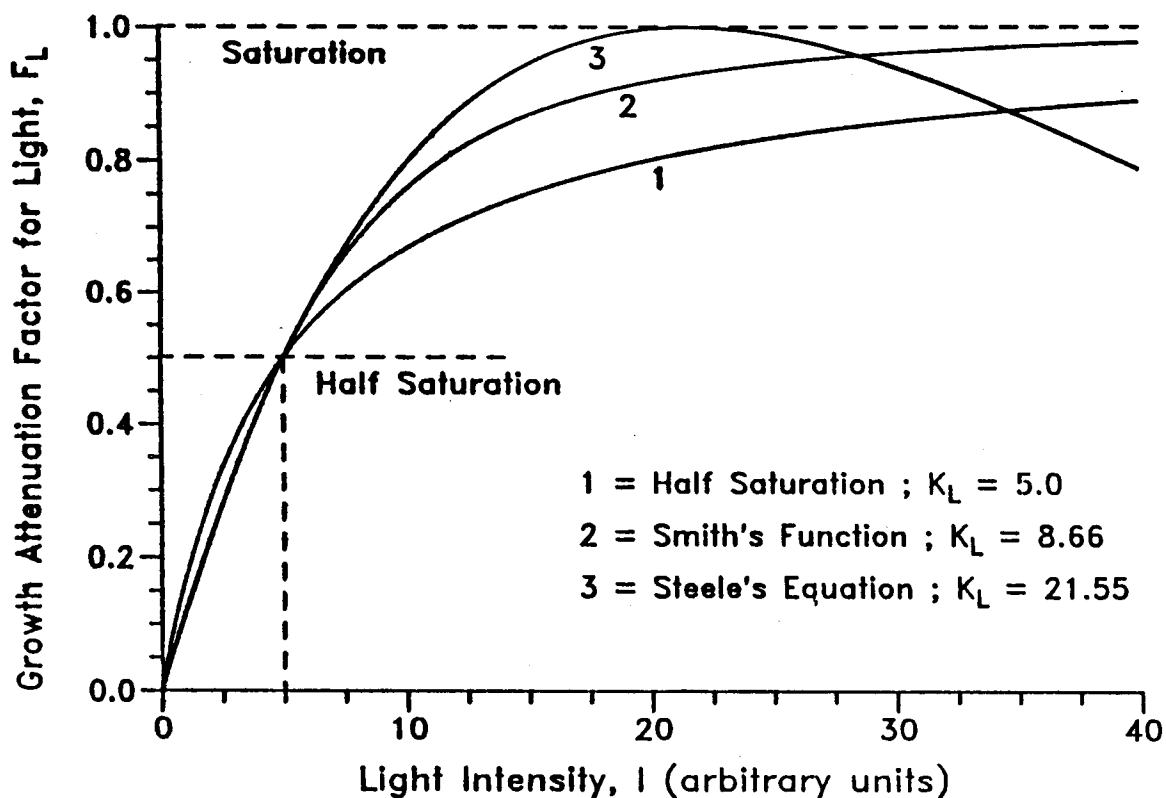


Figure III-2. QUAL2E Light Functions

$$\bar{I}_{alg} = TFACT * \bar{I}_{temp}$$

III-7c

where

FL = algae growth attenuation factor for light, adjusted for daylight hours and averaging method

AFACT = a light averaging factor, used to provide similarity between calculations using a single average value of solar radiation and computations using the average of hourly values of FL

f = fraction of daylight hours

FL₁ = growth attenuation factor for light, based on daylight average light intensity (\bar{I}_{alg})

λ = light extinction coefficient, ft⁻¹

d = mean depth of stream, ft

K_L = half saturation coefficient for light, Btu/ft²-hr

\bar{I}_{alg} = daylight average, photosynthetically active, light intensity, Btu/ft²-hr

TFACT = fraction of solar radiation computed in the temperature heat balance that is photosynthetically active

\bar{I}_{temp} = daylight average light intensity as computed in the temperature heat balance, Btu/ft²-hr

Option 2: FL is computed from one daylight average solar radiation value supplied externally by the user. The calculations required to obtain FL in option 2 are the same as those for option 1, except that the value of \bar{I}_{alg} is computed directly from user input of photosynthetically active solar radiation:

$$\bar{I}_{alg} = I_{tot}/N$$

III-8

where

I_{tot} = total daily photosynthetically active solar radiation, Btu/ft²

N = number of daylight hours per day, hr

Both I_{tot} and N are supplied by the user as input information. Equations III-8, III-7b, and III-7a are used to compute the value of FL. Because the user input value of I_{tot} is assumed to be the photosynthetically active radiation, the factor TFACT is not used in option 2.

Option 3: FL is obtained by averaging the hourly daylight values of FL that are computed from the hourly daylight values of solar radiation calculated in the steady state temperature heat balance:

$$FL = f * FL_2 \quad \text{III-9a}$$

$$FL_2 = \frac{1}{N} \sum_{i=1}^N \frac{1}{\lambda d} \left[\frac{K_L + I_{alg,i}}{K_L + I_{alg,i} e^{-\lambda d}} \right] \quad \text{III-9b}$$

$$I_{alg,i} = TFACT * I_{temp,i} \quad \text{III-9c}$$

where

- FL₂ = average of N hourly values of FL, based on hourly values of light intensity (I_{alg,i})
- I_{alg,i} = hourly value of photosynthetically active light intensity, Btu/ft²-hr
- I_{temp,i} = hourly value of light intensity as computed in the steady state temperature heat balance, Btu/ft²-hr

with other terms are defined in Equations III-7a,b,c, and III-8.

Because the average FL computed in option 3 (and 4) is an average of diurnally varying values of FL, the factor AFACT is not used in the calculations.

Option 4: FL is obtained by averaging the hourly daylight values of FL that are computed from the hourly daylight values of solar radiation calculated from a single value of total daily, photosynthetically active, solar radiation and an assumed cosine function. The calculations required to obtain FL are the same as those for option 3, except that the values of I_{alg,i} are computed from an internally specified cosine function:

$$I_{alg,i} = I_{tot}/N \left(1 - \frac{\cos 2 \pi i}{N + 1} \right), \quad i = 1, N \quad \text{III-10}$$

As in the case of option 2, both I_{tot} and N are supplied by the user. Equations III-10, III-9b, and III-9a are then used to compute the value of FL. Because the user specified value of I_{tot} is assumed to be photosynthetically active, the factor TFACT is not used with option 4.

Three empirical factors--diurnal cosine function, AFACT, and TFACT--are used in the formulations of the four light averaging options.

Two diurnal cosine functions were evaluated for use in QUAL2E: (1) a modified form of the one in the SEMCOG version of QUAL-II, and (2) the form used in QUAL-TX (Texas Water Development Board, 1984). The function in SEMCOG was modified to produce non-zero solar radiation values for each daylight hour, as given in Equation III-10. The form used in QUAL-TX is:

$$I_{alg,i} = \frac{I_{tot}}{2N} \left[\cos\left(\frac{\pi(i-1)}{N}\right) - \cos\left(\frac{\pi i}{N}\right) \right], \quad i=1,N \quad \text{III-11}$$

Equations III-10 and III-11 were evaluated by comparing simulated values of FL from modeling options 2 and 4 (i.e., in effect computing values of AFACT). Simulations were performed over a range of values of K_L , λ , d , I_{tot} , and N , as well as for each of the three light functions. The values of AFACT averaged 0.92 and 0.94 for the SEMCOG and Texas equations, respectively. There was no compelling reason to include both functions (with the user specifying the one to be used). The diurnal cosine function used in QUAL2E, therefore, is the modified SEMCOG version given in Equation III-10.

AFACT is the adjustment factor accounting for the nonlinear averaging inherent in computing a daily average value of FL. From the simulations just described, a reasonable value of AFACT is 0.92, with a range from 0.85 to 0.98. Bowie *et al.* (1985) report an implied value of 1.0 (Eq. 3.33), and Walker (1983) suggests using a value of 0.85.

TFACT is the photosynthetically active fraction of total solar radiation. When performing algae simulations, it is important that the value of light intensity and light saturation coefficient, K_L , be in units of photosynthetically active radiation, PAR (Bannister, 1974; Field and Effler, 1983; and Stefan *et al.*, 1983). Because the temperature heat balance computes total radiation over a wide spectrum, this value must be adjusted to PAR if it is to be used in the algae simulation. The ratio of energy in the visible band (PAR) to energy in the complete (standard) spectrum is approximately 0.43 to 0.45 (Bannister, 1974 and Stefan *et al.*, 1983). TFACT is a user input variable; thus a value to meet site specific conditions may be used.

Summary of Daily Averaging Options: The selection of a light averaging option depends largely on the extent to which the user wishes to account for the diurnal variation in light intensity. Options 1 and 2 use a single calculation of FL based on an "average" daily solar radiation value. Options 3 and 4 calculate hourly values of FL from hourly values of solar radiation and then average the hourly FL values to obtain the daily average value. Options 1 and 3 use the solar radiation from the temperature heat balance routines. (Thus both algae and temperature simulations draw on the same source for solar radiation.) Options 2 and 4 use the solar radiation value provided by the user for algae simulation. Thus, either option 2 or 4 must be selected when algae are simulated and temperature is not. The light

averaging factor (AFACT) is used to provide similarity in FL calculations between options 1 and 2 versus options 3 and 4. The solar radiation factor (TFACT) specifies the fraction of the solar radiation computed in the heat balance, which is photosynthetically active. It is used only with options 1 or 3.

In dynamic algae simulations, photosynthetically active radiation is computed hourly using Equation III-9c unless temperature is not simulated, in which case photosynthetically active solar radiation data must be supplied with the local climatology data.

3.2.3.3 Algal Self Shading

The light extinction coefficient, λ , in Equations III-6a,b,c is coupled to the algal density using the nonlinear equation

$$\lambda = \lambda_0 + \lambda_1 \alpha_0 A + \lambda_2 (\alpha_0 A)^{2/3} \quad \text{III-12}$$

where

λ_0 = non-algal portion of the light extinction coefficient, ft^{-1}

λ_1 = linear algal self shading coefficient, $\text{ft}^{-1} (\text{ug-Chl}_a/\text{L})^{-1}$

λ_2 = nonlinear algal self shading coefficient, $\text{ft}^{-1} (\text{ug-Chl}_a/\text{L})^{-2/3}$

α_0 = conversion factor, $\text{ug-Chl}_a / \text{mg A}$

A = algal biomass concentration, mg-A/L

Appropriate selection of the values of λ_1 and λ_2 allows modeling of a variety of algal self-shading, light-extinction relationships:

- No algal self shading (QUAL-II SEMCOG)

$$\lambda_1 = \lambda_2 = 0$$

- Linear algal self shading (JRB Associates, 1983)

$$\lambda_1 \neq 0, \quad \lambda_2 = 0$$

- Nonlinear algal self shading (Riley Eq., in Bowie et al., 1985)

$$\lambda_1 = 0.00268, \text{ft}^{-1} (\text{ug-Chl}_a/\text{L})^{-1}$$

$$\lambda_2 = 0.0165, \text{ft}^{-1} (\text{ug-Chl}_a/\text{L})^{-2/3}$$

or

$$\lambda_1 = 0.0088, m^{-1} (ug-Chla/L)^{-1}$$

$$\lambda_2 = 0.054, m^{-1} (ug-Chla/L)^{-2/3}$$

3.2.4 Algal Nutrient Relationships

The algal growth limitation factors for nitrogen (FN) and for phosphorus (FP) are defined by the Monod expressions:

$$FN = \frac{N_e}{N_e + K_N} \quad \text{III-13}$$

and

$$FP = \frac{P_2}{P_2 + K_p} \quad \text{III-14}$$

where

N_e = the effective local concentration of available inorganic nitrogen, mg-N/L

K_N = the Michaelis-Menton half-saturation constant for nitrogen, mg-N/L

P_2 = the local concentration of dissolved phosphorus, mg-P/L

K_p = the Michaelis-Menton half-saturation constant for phosphorus, mg-P/L

Algae are assumed to use ammonia and/or nitrate as a source of inorganic nitrogen. The effective concentration of available nitrogen is given by:

$$N_e = N_1 + N_3 \quad \text{III-15}$$

where

N_1 = concentration of ammonia nitrogen, mg-N/L

N_3 = concentration of nitrate nitrogen, mg-N/L

The empirical half-saturation constants for nitrogen, K_N , and phosphorus, K_p , are used to adjust the algal growth rate to account for those