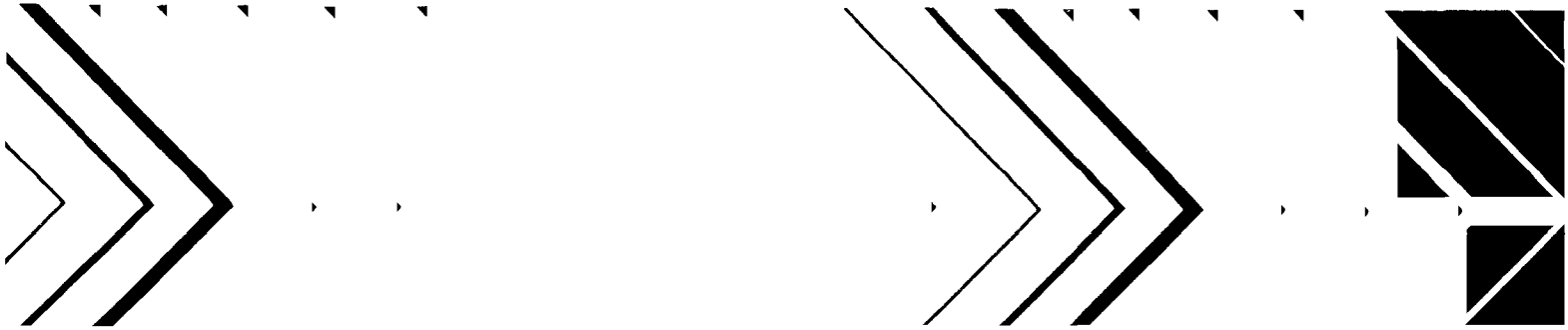

Research and Development



Computer Program Documentation for the Enhanced Stream Water Quality Model QUAL2E



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COMPUTER PROGRAM DOCUMENTATION FOR THE ENHANCED
STREAM WATER QUALITY MODEL QUAL2E

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 QUAL-II is widely used for waste load allocations, discharge permit determinations, and other conventional pollutant evaluations in the United States. Since its introduction in 1970, several different versions of the model have evolved. This manual presents the most recent modifications in the form of an enhanced state-of-the-art model called QUAL2E, which was developed by the National Council for Air and Stream Improvement (NCASI). Distribution and maintenance of the QUAL2E computer program, and training and assistance to model users, will be provided by EPA's Center for Water Quality Modeling at this Laboratory.

Rosemarie C. Russo, Ph.D.
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ABSTRACT

Presented in this manual are recent modifications and improvements to the widely used stream water quality model QUAL-II. Called QUAL2E, the enhanced model incorporates 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.

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, for example, can be used 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.

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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 taken directly from 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 reprint this material in the QUAL2E documentation 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 of Computer Sciences Corporation, Inc. and was made possible through the support of Mr. King Boynton of the US EPA's Office of Water and through an agreement with the US-Spain Joint Committee for Scientific and Technical Cooperation.

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.

1.1 QUAL2E DEVELOPMENT

1.1.1 History

QUAL2E, a new release of QUAL-II, was developed jointly by the National Council for Air and Stream Improvement, Inc. (NCASI) and the EPA Center for Water Quality Modeling (CWQM), Environmental Research Laboratory, Athens, GA. It includes many modifications made in the model since the revisions to the SEMCOG version of QUAL-II (NCASI, 1980). QUAL2E is intended to supersede all prior releases of QUAL-II.

QUAL-II is 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. This report describes the most recent modifications made to QUAL-II and fully documents the enhanced model, now named QUAL2E.

1.1.2 Enhancements to QUAL-II

QUAL2E, a modified version of QUAL-II/SEMCOG, incorporates improvements in eight areas:

1. Algal, nitrogen, phosphorus, dissolved oxygen interactions
 - Organic nitrogen state variable
 - Organic phosphorus state variable
 - Nitrification inhibition at low DO
 - Algal preference factor for NH_3
2. Algal growth rate
 - Growth rate dependent upon both NH_3 and NO_3 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)
 - New Standard Methods DO saturation function
 - Traditional SOD units ($\text{g/m}^2\text{-day}$ or $\text{g/ft}^2\text{-day}$)
 - 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 Information Sources

Major sources of information for this revised documentation were:

1. Roesner, L. A., Giguere, P. R. and Evenson, D. E. Computer Program Documentation for Stream Quality Modeling (QUAL-II). U.S. Environmental Protection Agency, 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.

This documentation of QUAL2E 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, which is intended to supplement the users manual (NCASI, 1985). The QUAL2E user manual contains a detailed description of data requirements, as well as the input coding forms and an example input/output data file. Both reports and a copy of the QUAL2E computer code are available from the Center for Water Quality Modeling, U.S. Environmental Protection Agency, Athens, GA 30613.

1.1.4 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 frame work for modeling temperature. It is extracted verbatim from Roesner et al., 1981. Chapter 5 describes the computational representation of the model and the numerical solution algorithm. A list of references used in this report is found in Chapter 6.

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 50
- Computational elements: no more than 20 per reach or a total of 500
- Headwater elements: a maximum of 10
- Junction elements: a maximum of 9
- Input and withdrawal elements: a maximum of 50

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 49 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.

The structural framework of QUAL2E has been modified from prior versions. 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, which have limited space for memory.

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

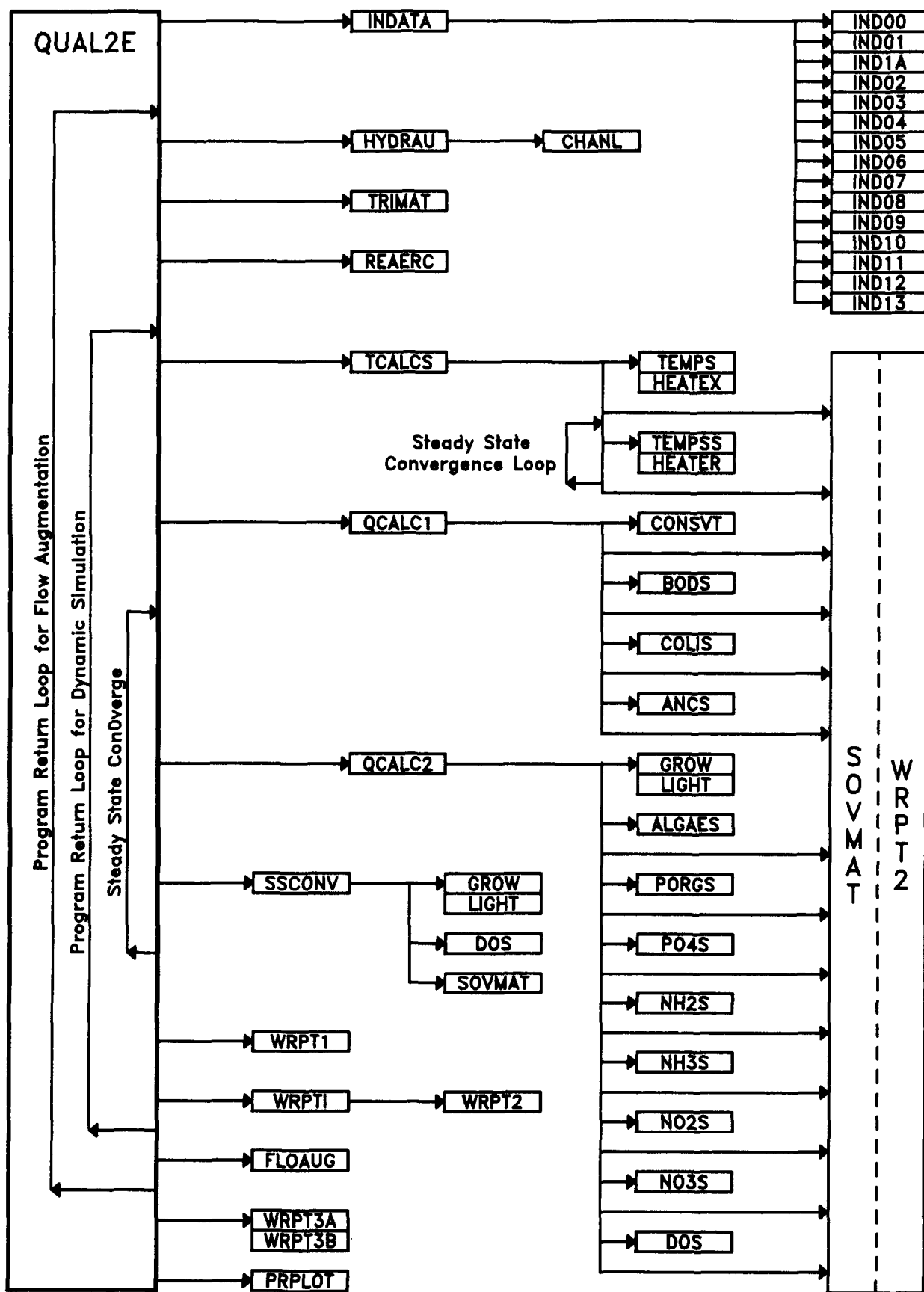


Figure I-1. General Structure of QUAL2E

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 5 or the output unit is not unit 6, then the variables "NI" and "NJ" in the subroutine INDATA 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 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 Representa-

tion 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_{xi}), 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 ($A \frac{D_L}{\Delta x} \frac{\partial C}{\partial x}$) as the movers

of mass along the stream axis. Mass can be added to or removed from the system via external sources and withdrawals ($Q_{xi}C_{xi}$) 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:

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

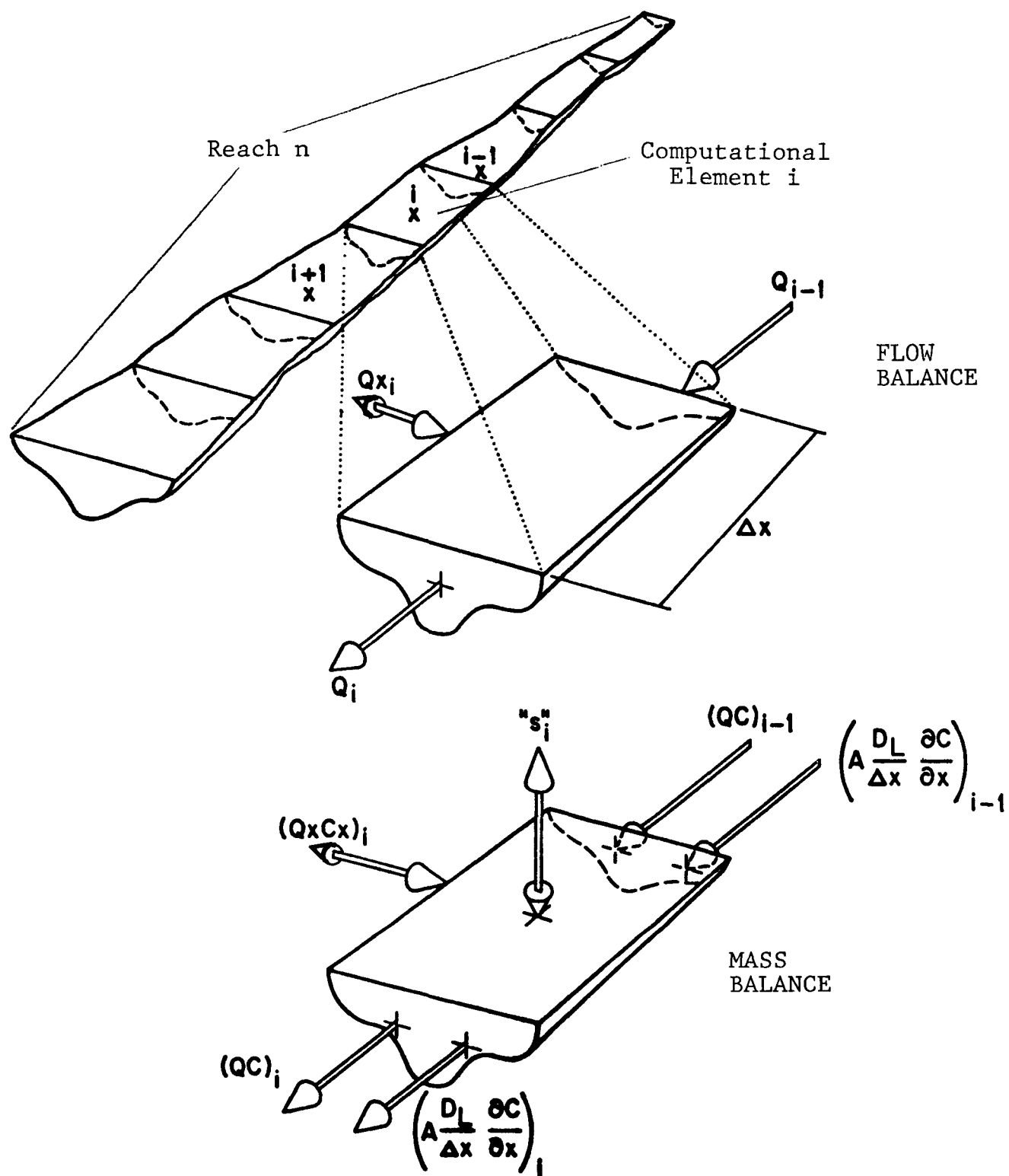


Figure II-1. Discretized Stream System

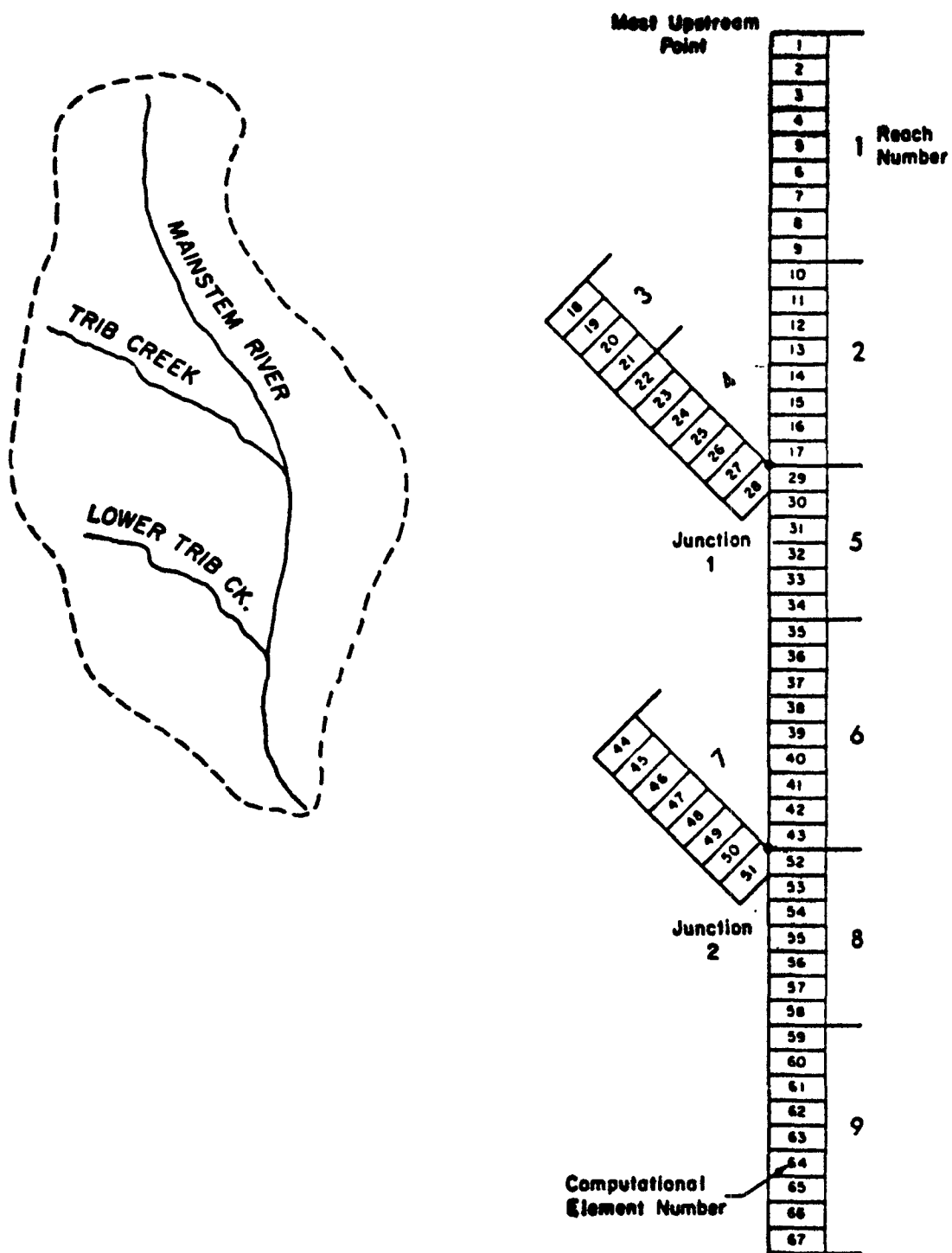


Figure II-2. Stream Network of Computational Elements and Reaches

where

M	=	mass (M)
x	=	distance (L)
t	=	time (T)
C	=	concentration (M L ⁻³)
A _x	=	cross-sectional area (L ²)
D _L	=	dispersion coefficient (L ² 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.

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 (unitless)

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) was able to derive a predictive equation for the longitudinal dispersion coefficient, D_L , in long straight pipes, as

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

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

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

where

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

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

Some investigators have attempted to apply Taylor's expression to stream-flow. 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:

$$D_L = K d u^* \quad \text{II-13}$$

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.

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

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	0.115	1.31	0.82	0.066	1.3	174
Channel with roughened	0.154	1.41	1.48	0.118	2.7	150
sides	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-Duwarmish River	3.61	66	--	0.16	70-92	120-160
Missouri River	8.86	66	5.09	0.24	16,000	75000
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
Cinch 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
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 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:

$$\text{Chl } \underline{a} = \alpha_0 A \quad \text{III-1}$$

where

Chl a = chlorophyll a concentration, ug-Chl a/L

A = algal biomass concentration, mg-A/L

α_0 = a conversion factor, ug Chl a/mg A

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

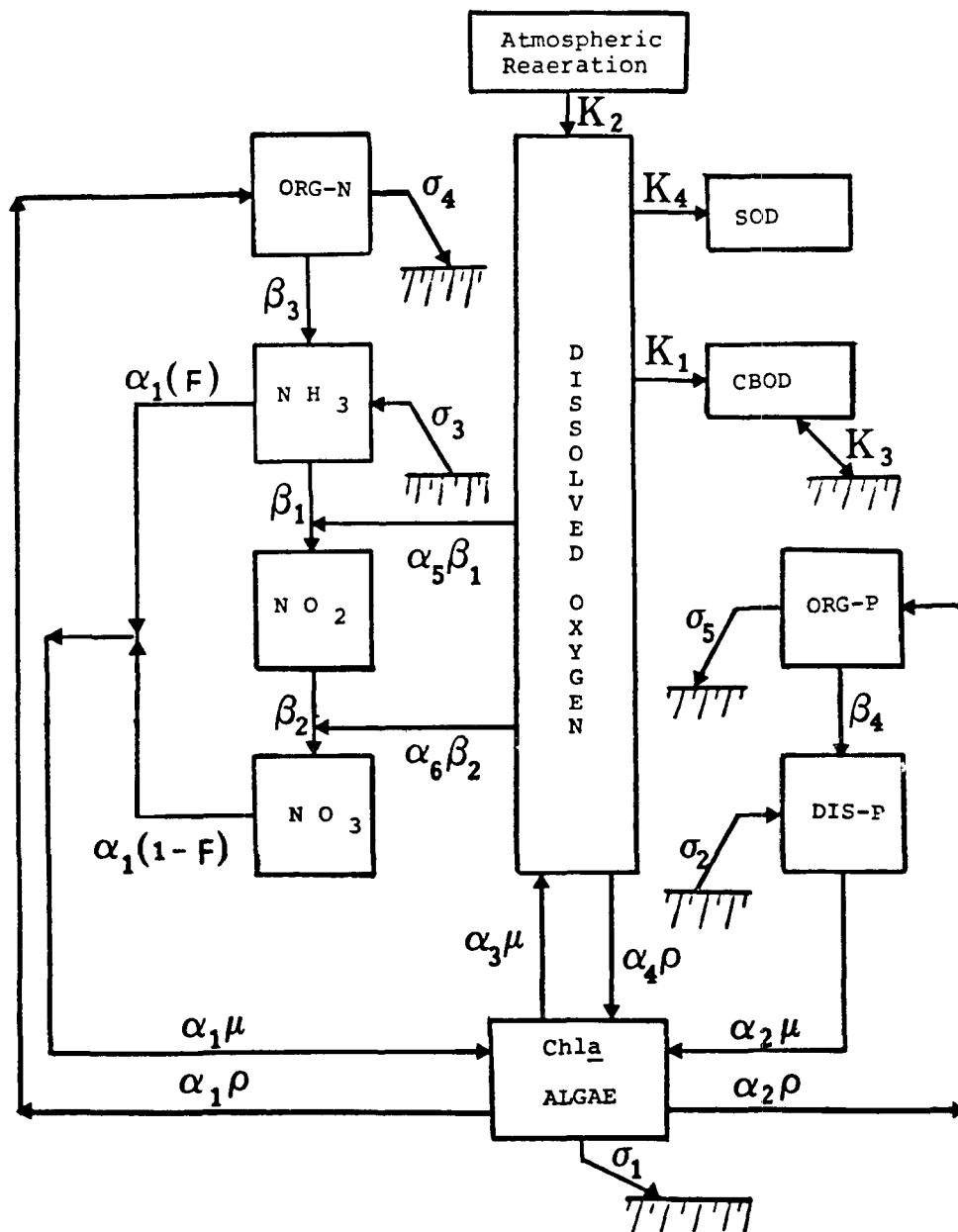


Figure III-1. Major Constituent Interactions in QUAL2E

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

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:

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

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. Inverse Additive. 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 series. 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 an inverse average. 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).

Walker (1983) has cautioned against using the inverse-additive option in systems where one nutrient is in excess (say nitrogen, so that $FN \rightarrow 1.0$) and the other is extremely limiting (say phosphorus, so that $FP \rightarrow 0.0$). 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:

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

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

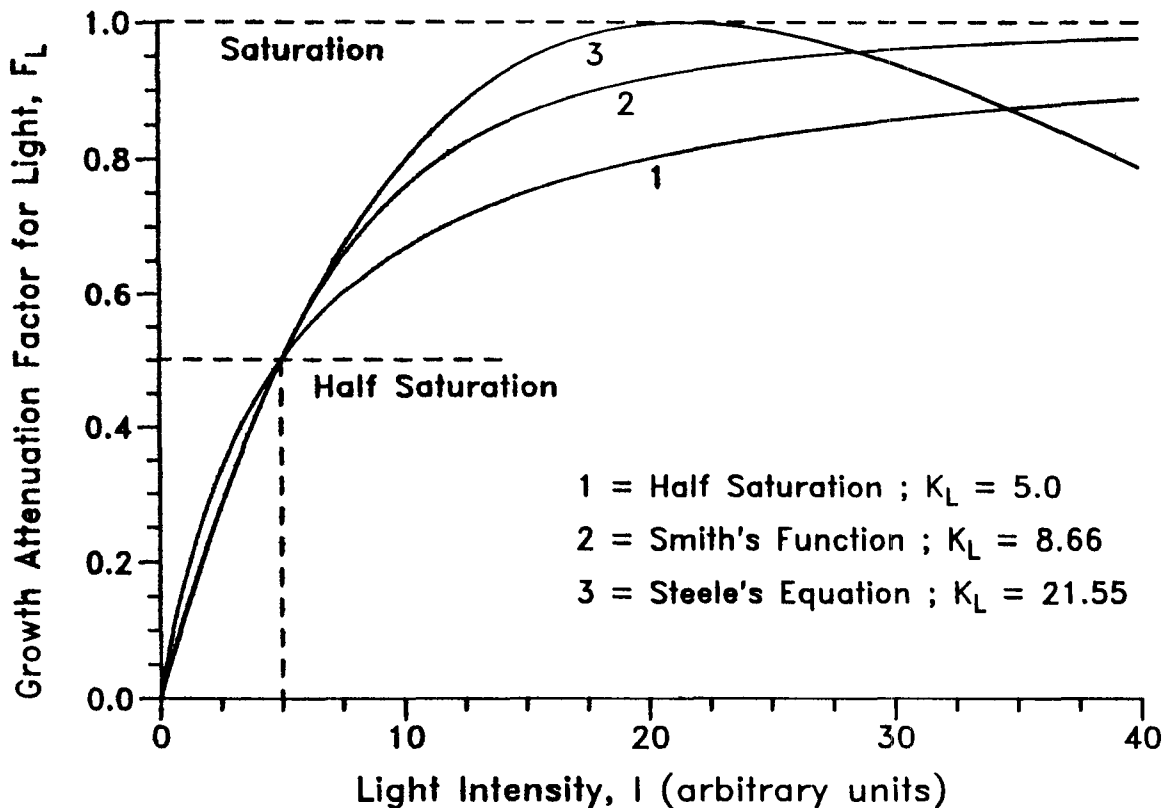


Figure III-2. QUAL2E Light Functions

$$\bar{I}_{alg} = TFACT * \bar{I}_{temp} \quad \text{III-7c}$$

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:

$$\bar{I}_{alg} = I_{tot}/N \quad \text{III-8}$$

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

FL_2 = 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 (the user specified 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. Zison *et al.* (1978) 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 (Meta Systems QUAL-II)

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

- Nonlinear algal self shading (Riley Eq., in Zison et al., 1978)

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

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

or

$$\lambda_1 = 0.0088, \text{ m}^{-1} (\text{ug-Chl}\underline{\text{a}}/\text{L})^{-1}$$

$$\lambda_2 = 0.054, \text{ m}^{-1} (\text{ug-Chl}\underline{\text{a}}/\text{L})^{-2/3}$$

3.2.4 Algal Nutrient Relationships

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

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

and

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

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

factors that can potentially limit algal growth. Each constant is actually the level at which that particular factor limits algal growth to half the maximal or "saturated" rate (Zison *et al.*, 1978). Table III-3 at the end of this chapter lists typical values of the half-saturation constants for nitrogen and phosphorus. If algal concentrations are simulated and either nitrogen, phosphorus, or both are not simulated, the program assumes that the parameter not simulated is not limiting.

3.2.5 Temperature Dependence in Algae Simulation

The algal growth rate and death rates are temperature dependent. They are corrected within the model, as are all other temperature dependent systems variables, according to the procedure explained in Section 3.10.

3.3 NITROGEN CYCLE

In natural aerobic waters, there is a stepwise transformation from organic nitrogen to ammonia, to nitrite, and finally to nitrate. The nitrogen cycle in QUAL2E contains all four of these components, as shown in Figure III-1. The incorporation of organic nitrogen as a state variable, an organic nitrogen settling term, and an algal nitrogen uptake preference factor are the primary enhancements to the nitrogen cycle in QUAL2E compared to the SEMCOG version of QUAL-II. The differential equations governing transformations of nitrogen from one form to another are shown below.

3.3.1 Organic Nitrogen

$$\frac{dN_4}{dt} = \alpha_1 \rho A - \beta_3 N_4 - \sigma_4 N_4 \quad \text{III-16}$$

where

N_4 = concentration of organic nitrogen, mg-N/L

β_3 = rate constant for hydrolysis of organic nitrogen to ammonia nitrogen, temperature dependent, day⁻¹

α_1 = fraction of algal biomass that is nitrogen, mg-N/mg-A

ρ = Algal respiration rate, day⁻¹

A = algal biomass concentration, mg-A/L

σ_4 = rate coefficient for organic nitrogen settling, temperature dependent, day⁻¹

3.3.2 Ammonia Nitrogen

$$\frac{dN_1}{dt} = \beta_3 N_4 - \beta_1 N_1 + \sigma_3/d - F_1 \alpha_1 \mu A \quad \text{III-17}$$

where

$$F_1 = P_N N_1 / (P_N N_1 + (1 - P_N) N_3) \quad \text{III-18}$$

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

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

N_4 = the concentration of organic nitrogen, mg-N/L

β_1 = rate constant for the biological oxidation of ammonia nitrogen, temperature dependent, day⁻¹

β_3 = organic nitrogen hydrolysis rate, day⁻¹

α_1 = fraction of algal biomass which is nitrogen, mg-N/mg-A

σ_3 = the benthos source rate for ammonia nitrogen, mg-N/ft²-day

d = mean depth of flow, ft

F_1 = fraction of algal nitrogen uptake from ammonia pool

μ = the local specific growth rate of algae, day⁻¹

A = algal biomass concentration, mg-A/L

P_N = preference factor for ammonia nitrogen (0 to 1.0)

The QUAL2E model includes an algal preference factor for ammonia, P_N (Zison et al., 1978; JRB Associates, 1983). The ammonia preference factor is equivalent to the fraction of algal nitrogen uptake from the ammonia pool when the concentrations of ammonia and nitrate nitrogen are equal.

3.3.3 Nitrite Nitrogen

$$\frac{dN_2}{dt} = \beta_1 N_1 - \beta_2 N_2 \quad \text{III-19}$$

where

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

N_2 = the concentration of nitrite nitrogen, mg-N/L

β_1 = rate constant for the oxidation of ammonia nitrogen,
temperature dependent, day⁻¹

β_2 = rate constant for the oxidation of nitrite nitrogen,
temperature dependent, day⁻¹

3.3.4 Nitrate Nitrogen

$$\frac{dN_3}{dt} = \beta_2 N_2 - (1 - F)\alpha_1 \mu A \quad \text{III-20}$$

where

F = fraction of algal nitrogen taken from ammonia pool, as
defined in Section 3.3.2

α_1 = fraction of algal biomass that is nitrogen, mg-N/mg-A

μ = local specific growth rate of algae, day⁻¹

3.3.5 Inhibition of Nitrification at Low Dissolved Oxygen

QUAL2E has the capability of inhibiting (retarding) the rate of nitrification at low values of dissolved oxygen. This inhibition effect has been reported by others (Department of Scientific and Industrial Research, 1964; Texas Water Development Board, 1984).

Nitrification rates are modified in QUAL2E by computing an inhibition correction factor (having a value between zero and one) and then applying this factor to the values of the nitrification rate coefficients, β_1 , and β_2 . The nitrification rate correction factor is computed according to a first order equation:

$$CORDO = 1.0 - \text{EXP}(-KNITRF * DO) \quad \text{III-21}$$

where

$CORDO$ = nitrification rate correction factor

EXP = exponential function

KNITRF = first order nitrification inhibition coefficient, mg/L⁻¹

D0 = dissolved oxygen concentration, mg/L

The correction factor is applied to the ammonia and nitrite oxidation rates by:

$$\text{Ammonia: } (\beta_1)_{\text{inhib.}} = \text{CORDO} * (\beta_1)_{\text{input}} \quad \text{III-22}$$

$$\text{Nitrite: } (\beta_2)_{\text{inhib.}} = \text{CORDO} * (\beta_2)_{\text{input}} \quad \text{III-23}$$

A value of 0.6 for KNITRF closely matches the inhibition formulation in QUAL-TX, the Texas Water Development Board version of QUAL-II, whereas, a value of 0.7 closely simulates the data for the Thames Estuary.

3.4 PHOSPHORUS CYCLE

The phosphorus cycle operates like the nitrogen cycle in many respects. Organic forms of phosphorus are generated by the death of algae, which then converts to the dissolved inorganic state, where it is available to algae for primary production. Phosphorus discharged from sewage treatment plants is generally in the dissolved inorganic form and is readily taken up by algae (Zison et al., 1978). QUAL2E revises the SEMCOG version of QUAL-II, which included only dissolved phosphorus, to simulate the interactions between organic and dissolved phosphorus. Below are the differential equations governing transformations of phosphorus from one form to another.

3.4.1 Organic Phosphorus

$$\frac{dP_1}{dt} = \alpha_2 \rho A - \beta_4 P_1 - \sigma_5 P_1 \quad \text{III-24}$$

where

P_1 = the concentration of organic phosphorus, mg-P/L

α_2 = phosphorus content of algae, mg P/mg-A

ρ = algal respiration rate, day⁻¹

A = algal biomass concentration, mg-A/L

β_4 = organic phosphorus decay rate, temperature dependent, day⁻¹

σ_5 = organic phosphorus settling rate, temperature dependent, day⁻¹

3.4.2 Dissolved Phosphorus

$$\frac{dP_2}{dt} = \beta_4 P_1 + \sigma_2/d - \alpha_2 \mu A \quad \text{III-25}$$

where

P_2 = concentration of inorganic or dissolved phosphorus, mg-P/L

σ_2 = benthos source rate for dissolved phosphorus, temperature dependent, mg-P/ft²-day

d = mean stream depth, ft

μ = algal growth rate, day⁻¹

A = algal biomass concentration, mg-A/L

3.5 CARBONACEOUS BOD

The QUAL2E model assumes a first order reaction to describe deoxygenation of ultimate carbonaceous BOD in the stream. The BOD function as expressed in the model also takes into account additional BOD removal due to sedimentation, scour and flocculation, which do not exert an oxygen demand (Thomas, 1948):

$$\frac{dL}{dt} = -K_1 L - K_3 L \quad \text{III-26}$$

where

L = the concentration of ultimate carbonaceous BOD, mg/L

K_1 = deoxygenation rate coefficient, temperature dependent, day⁻¹

K_3 = the rate of loss of carbonaceous BOD due to settling, temperature dependent, day⁻¹

QUAL2E simulates ultimate BOD in the general case; however, the user may choose to use 5-day BOD values for input and output. In this case, the model will make the necessary conversions from 5-day to ultimate BOD. The conversion equation is:

$$BOD_5 = BOD_u (1.0 - \text{EXP}(5 * KBOD)) \quad \text{III-27}$$

where

BOD_5 = 5-day BOD, mg/L

BOD_u = ultimate BOD, mg/L

$KBOD$ = BOD conversion rate coefficient, day⁻¹

The SEMCOG version of QUAL-II uses a value of 0.23 day⁻¹ for $KBOD$. With QUAL2E, the user may specify the appropriate value for this conversion. Note: when modeling 5-day BOD, the conversion coefficient is applied to all input BOD_5 forcing functions (headwaters, incremental flows, point loads, and the downstream boundary condition).

3.6 DISSOLVED OXYGEN

The oxygen balance in a stream system depends on the capacity of the stream to reaerate itself. This capacity is a function of the advection and diffusion processes occurring within the system and the internal sources and sinks of oxygen. The major sources of oxygen, in addition to atmospheric reaeration, are the oxygen produced by photosynthesis and the oxygen contained in the incoming flow. The sinks of dissolved oxygen include biochemical oxidation of carbonaceous and nitrogenous organic matter, benthic oxygen demand and the oxygen utilized by respiration (Zison et al., 1978).

The differential equation used in QUAL2E to describe the rate of change of oxygen is shown below. Each term represents a major source or sink of oxygen.

$$\frac{dO}{dt} = K_2(O^* - O) + (\alpha_3 \mu - \alpha_4 \rho) A - K_1 L - K_4/d - \alpha_5 \beta_1 N_1 - \alpha_6 \beta_2 N_2 \quad \text{III-28}$$

where

O = the concentration of dissolved oxygen, mg/L

O^* = the saturation concentration of dissolved oxygen at the local temperature and pressure, mg/L

$\alpha_3 \mu$ = the rate of oxygen production per unit of algal photosynthesis, mg-O/mg-A

$\alpha_4 \rho$ = the rate of oxygen uptake per unit of algae respired, mg-O/mg-A

α_5 = the rate of oxygen uptake per unit of ammonia nitrogen oxidation, mg-O/mg-N

- α_6 = the rate of oxygen uptake per unit of nitrite nitrogen oxidation, mg-O/mg-N
- μ = algal growth rate, temperature dependent, day⁻¹
- ρ = algal respiration rate, temperature dependent, day⁻¹
- A = algal biomass concentration, mg-A/L
- L = concentration of ultimate carbonaceous BOD, mg/L
- d = mean stream depth, ft
- K_1 = carbonaceous BOD deoxygenation rate, temperature dependent, day⁻¹
- K_2 = the reaeration rate in accordance with the Fickian diffusion analogy, temperature dependent, day⁻¹
- K_4 = sediment oxygen demand rate, temperature dependent, g/ft²-day
- β_1 = ammonia oxidation rate coefficient, temperature dependent, day⁻¹
- β_2 = nitrite oxidation rate coefficient, temperature dependent, day⁻¹
- N_1 = ammonia nitrogen concentration, mg-N/L
- N_2 = nitrite nitrogen concentration, mg-N/L

3.6.1 Dissolved Oxygen Saturation Concentration

The solubility of dissolved oxygen in water decreases with increasing temperature, increasing dissolved solids concentration, and decreasing atmospheric pressure (Zison et al., 1978). QUAL2E uses a predictive equation for the saturation (equilibrium) concentration of dissolved oxygen (APHA, 1985).

$$\ln O^* = -139.34410 + (1.575701 \times 10^5/T) - (6.642308 \times 10^7/T^2) + (1.243800 \times 10^{10}/T^3) - (8.621949 \times 10^{11}/T^4) \quad \text{III-29}$$

where:

O^* = equilibrium oxygen concentration at 1.000 atm, mg/L

T = temperature (°K) = (°C+273.150) and °C is within the range 0.0 to 40.0°C

For non-standard conditions of pressure, the equilibrium concentration of dissolved oxygen is corrected by the equation III-30:

$$O_p = O^*P \left[\frac{(1-P_{wv}/P) (1-\phi P)}{(1-P_{wv}) (1-\phi)} \right] \quad \text{III-30}$$

where

O_p = equilibrium oxygen concentration at non-standard pressure, mg/L

O^* = equilibrium oxygen concentration at 1.000 atm, mg/L

P = pressure (atm) and is within 0.000 to 2.000 atm

P_{wv} = partial pressure of water vapor (atm), which may be computed from:

$$\ln P_{wv} = 11.8571 - (3840.70/T) - 216961/T^2 \quad \text{III-31}$$

and

$$\phi = 0.000975 - (1.426 \times 10^{-5}t) + (6.436 \times 10^{-8}t^2) \quad \text{III-32}$$

where

t = temperature, °C

The equations in Standard Methods (1985) for computing dissolved oxygen saturation concentrations also include corrections for salinity and chloride. Because neither salinity nor chloride is explicitly modeled, QUAL2E does not correct O^* for chloride or salinity. Furthermore, the pressure correction to O^* (Equation III-30) is made only when temperature is modeled, because barometric pressure data are a primary requirement of the heat balance equations.

The dissolved oxygen saturation concentrations computed from the Texas and SEMCOG versions of QUAL-II are compared to those from the Standard Methods formulations of QUAL2E in Table III-1.

3.6.2 Atmospheric Reaeration Coefficient Estimation

The reaeration coefficient (K_2) is most often expressed as a function of stream depth and velocity. QUAL2E provides eight options for estimating or reading in K_2 values, which are discussed in the sections below. A comparative study of reaeration prediction equation performance has been reported by St. John et al. (1984).

TABLE III-1
COMPARISON OF DISSOLVED OXYGEN SATURATION CONCENTRATIONS
(Barometric Pressure = 1 atm, Chloride = 0.0 mg/L,
Equilibrium with Air Saturated with Water Vapor)

Temperature, °C	QUAL-II SEMOG	QUAL-TX Texas	QUAL2E Std. Meth.
0.	14.632	14.584	14.621
1.	14.227	14.187	14.217
2.	13.837	13.806	13.830
3.	13.461	13.441	13.461
4.	13.100	13.091	13.108
5.	12.752	12.755	12.771
6.	12.418	12.433	12.448
7.	12.096	12.124	12.139
8.	11.787	11.828	11.843
9.	11.489	11.544	11.560
10.	11.203	11.271	11.288
11.	10.927	11.009	11.027
12.	10.661	10.758	10.777
13.	10.406	10.517	10.537
14.	10.159	10.285	10.306
15.	9.922	10.062	10.084
16.	9.692	9.848	9.870
17.	9.471	9.642	9.665
18.	9.257	9.444	9.467
19.	9.050	9.253	9.276
20.	8.849	9.069	9.093
21.	8.655	8.891	8.915
22.	8.465	8.720	8.744
23.	8.281	8.555	8.578
24.	8.101	8.396	8.418
25.	7.925	8.241	8.264
26.	7.753	8.092	8.114
27.	7.584	7.948	7.969
28.	7.417	7.807	7.828
29.	7.252	7.672	7.691
30.	7.089	7.540	7.559
31.	6.927	7.412	7.430
32.	6.765	7.288	7.305
33.	6.604	7.167	7.183
34.	6.442	7.049	7.065
35.	6.280	6.935	6.949
36.	6.116	6.823	6.837
37.	5.950	6.715	6.727
38.	5.782	6.609	6.620
39.	5.612	6.506	6.515
40.	5.438	6.406	6.413

K₂ Option 1

Option 1 allows the user to read in K₂ values that have been previously selected by the modeler. This option is useful in modeling unusual situations such as ice cover (see Section 3.6.3).

K₂ Option 2

Using data collected in field measurements of stream reaeration, Churchill, Elmore, and Buckingham (1962) developed the following expression for K₂ at 20°C.

$$K_2^{20} = 5.026 \bar{u}^{0.969} d^{-1.673} \times 2.31 \quad \text{III-33}$$

where

\bar{u} = average velocity in the stream, ft/sec.

d = average depth of the stream, ft

K₂ = reaeration coefficient, day⁻¹

K₂ Option 3

O'Connor and Dobbins (1958) proposed equations based on the turbulence characteristics of a stream. For streams displaying low velocities and isotropic conditions, Equation III-34 was developed:

$$K_2^{20} = \frac{(D_m \bar{u})^{0.5}}{d^{1.50}} \quad \text{III-34}$$

For streams with high velocities and nonisotropic conditions, the relationship is:

$$K_2^{20} = \frac{480 D_m^{0.5} S_0^{0.25}}{d^{1.25}} \times 2.31 \quad \text{III-35}$$

where

S₀ = slope of the streambed, ft/ft

d = mean stream depth, ft

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

K₂ = reaeration coefficient, day⁻¹

and D_m is the molecular diffusion coefficient (ft^2/day), which is given by:

$$D_m = 1.91 \times 10^3 (1.037)^{T-20} \quad \text{III-36}$$

Equation III-34 has been found to be generally applicable for most cases and is the equation used in QUAL2E for Option 3. Equation III-35 can be used to calculate K_2 outside the model and input it directly under Option 1.

K_2 Option 4

Based on the monitoring of six streams in England, Owens et al. (1964) developed an equation for shallow, fast moving streams. Equation III-37 can be used with streams that exhibit depths of 0.4 to 11.0 feet and velocities of 0.1 to 5.0 ft/sec:

$$K_2^{20} = 9.4 \bar{u}^{0.67} / d^{1.85} \times 2.31 \quad \text{III-37}$$

where

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

d = mean depth, ft

K_2 Option 5 .

Thackston and Krenkel (1966) proposed the following equation based on their investigation of several rivers in the Tennessee Valley Authority system.

$$K_2^{20} = 10.8 (1 + F^{0.5}) \frac{u^*}{d} \times 2.31 \quad \text{III-38}$$

where F is the Froude number, which is given by:

$$F = \frac{u^*}{\sqrt{g d}} \quad \text{III-39}$$

and u^* is the shear velocity, ft/sec.:

$$u^* = \sqrt{d S_e g} = \frac{\bar{u} n \sqrt{g}}{1.49 d^{1.167}} \quad \text{III-40}$$

where

d = mean depth, ft

g = acceleration of gravity, ft/sec²

S_e = slope of the energy gradient

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

n = Manning's coefficient

K₂ Option 6

Langbien and Durum (1967) developed a formula for K_2 at 20°C:

$$K_2^{20} = 3.3 \bar{u}/d^{1.33} \times 2.31 \quad \text{III-41}$$

where

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

d = mean depth, ft

K₂ Option 7

This option computes the reaeration coefficient from a power function of flow. This empirical relationship is similar to the velocity and depth correlations with flow used in the hydraulics section of QUAL2E, i.e.,

$$K_2 = aQ^b \quad \text{III-42}$$

where

a = coefficient of flow for K_2

Q = flow, ft³/sec

b = exponent on flow for K_2

K₂ Option 8

The method of Tsivoglou and Wallace (1972) assumes that the reaeration coefficient for a reach is proportional to the change in elevation of the water surface in the reach and inversely proportional to the flow time through the reach. The equation is:

$$K_2^{20} = c \frac{\Delta h}{t_f} \quad \text{III-43}$$

where

c = escape coefficient, ft^{-1}

Δh = change in water surface elevation in reach, ft

t_f = flow time within reach, days

Assuming uniform flow, the change in water surface elevation is

$$\Delta h = S_e \Delta x \quad \text{III-44}$$

where

S_e = slope of the energy gradient, ft/ft

Δx = reach length, ft

and the time of passage through a reach is

$$t_f = \frac{\Delta x}{\bar{u}} \quad \text{III-45}$$

where

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

Substituting the above in equation III-43 gives

$$K_2^{20} = (3600 \times 24) c S_e \bar{u} \quad \text{III-46}$$

Equation III-46 is the form of Option 8 used in QUAL2E. The constants 3600 and 24 convert velocity to units of feet per day. The slope may be input directly for computing K_2 with this option, or it can be calculated by:

$$S_e = \frac{\bar{u}^2 n^2}{(1.49)^2 d^{4/3}} \quad \text{III-47}$$

where

d = mean depth, ft

n = Manning's coefficient

The escape coefficient is usually treated as a variable and determined empirically. TenEch (1978) recommends the following guideline in determining c values, analogous to that recommended for uncalibrated stream segments by Tsivoglou and Neal (1976):

$c = 0.054 \text{ ft}^{-1}$ (at 20°C) for $15 \leq Q \leq 3000 \text{ ft}^3/\text{sec}$

$c = 0.110 \text{ ft}^{-1}$ (at 20°C) for $1 \leq Q \leq 15 \text{ ft}^3/\text{sec}$

3.6.3 Ice Cover

Ice cover on streams during winter low flow conditions may significantly affect reaeration. Reaeration rates are decreased because ice cover reduces the surface area of the air-water interface through which reaeration occurs (TenEch, 1978). Approaches recommended by TenEch (1978) for estimating the extent of ice cover include:

- o Statistical analyses of past records
- o Steady state heat budget analysis (including the U.S. Army Corps of Engineers differential equations)
- o Extensive field observations

To adjust the reaeration rate for winter ice cover conditions in the QUAL2E model, the calculated reaeration rate must be multiplied by an "ice cover factor" and input under Option 1. TenEch recommends factors ranging from 0.05 for complete ice cover to 1.0 for no ice cover. Depending on the extent of cover, reaeration values can be greatly reduced.

3.6.4 K_2 Default Values

There are no default K_2 values in QUAL2E. In some versions of QUAL-II, a default value of K_2 is computed, accounting for the influences of wind-induced turbulence and diffusion under low-velocity conditions. In those models, when the calculated values of K_2 are less than two divided by the depth of the reach ($2/d$), K_2 is set equal to $2/d$. This feature has not always proved useful, particularly when simulating the very low reaeration rates; thus it is not included in QUAL2E.

3.6.5 Dam Reaeration

QUAL2E has the capability of modeling oxygen input to the system from reaeration over dams. The following equation described by Zison et al. (1978) and attributable to Gameson is used to estimate oxygen input from dam reaeration.

$$D_a - D_b = \left[1 - \frac{1}{1 + 0.11ab(1 + 0.046T)H} \right] D_a \quad \text{III-48}$$

where

D_a = oxygen deficit above dam, mg/L

D_b = oxygen deficit below dam, mg/L

T = temperature, °C

H = height through which water falls, ft

a = empirical parameter

= 1.25 in clear to slightly polluted water

= 1.0 in polluted water

b = empirical parameter

= 1.0 for weir with free fall

= 1.3 for step weir or cascades

The factors H , a and b are input for each dam. The model includes a provision for bypassing some or all of the flow around the dams (e.g., through generators). The fraction of the total flow that spills over the dam is supplied as an input variable.

3.7 COLIFORMS

Coliforms are used as an indicator of pathogen contamination in surface waters. Expressions for estimating coliform concentrations are usually first order decay functions, which only take into account coliform die-off (Zison et al., 1978). The QUAL2E model uses such an expression:

$$\frac{dE}{dt} = -K_5 E \quad \text{III-49}$$

where

E = concentration of coliforms, colonies/100 ml

K₅ = coliform die-off rate, temperature dependent, day⁻¹

3.8 ARBITRARY NONCONSERVATIVE CONSTITUENT

QUAL2E has the provision for modeling an arbitrary nonconservative constituent (ANC). In addition to a first order decay mechanism, there are source and sink terms in the mass balance. The differential equation describing the interactions for an arbitrary nonconservative constituent is:

$$\frac{dR}{dt} = -K_6 R - \sigma_6 R + \sigma_7/d \quad \text{III-50}$$

where

R = concentration of the nonconservative constituent, mg-ANC/L

K₆ = decay rate for the constituent, temperature dependent, day⁻¹

σ₆ = rate coefficient for constituent settling, temperature dependent, day⁻¹

σ₇ = benthic source for constituent, temperature dependent, mg-ANC/ft²-day

d = mean stream depth, ft

3.9 TEMPERATURE

Temperature is modeled by performing a heat balance on each computational element in the system. The heat balance accounts for temperature inputs and losses from the forcing functions as well as the heat exchanged between the water surface and the atmosphere. The air-water heat balance terms include long and short wave radiation, convection, and evaporation using:

$$H_n = H_{sn} + H_{an} - H_b - H_c - H_e \quad \text{III-51}$$

where

H_n = net heat flux passing the air water surface, Btu/ft²-day

H_{sn} = net short wave solar radiation after losses from absorption and scattering in the atmosphere and by reflection at the interface, Btu/ft²-day

H_{an} = net long wave atmosphere radiation after reflection, Btu/ft²-day

H_b = outgoing long wave back radiation, Btu/ft²-day

H_c = convective heat flux, Btu/ft²-day

H_e = heat loss by evaporation, excluding sensible heat loss, Btu/ft²-day

In order for QUAL2E to perform the heat balance computations, the user must supply a variety of data, including the longitude and latitude of the basin, the time of year, evaporation coefficients, and a dust attenuation coefficient. Local climatological information in the form of time of day, wet and dry bulb air temperatures, atmospheric pressure, cloud cover and wind velocity also must be provided. These data are applied uniformly over the entire river basin.

In the dynamic mode, local climatological data must be supplied at regular (typically 3 hour) intervals. In this manner the source/sink term for the heat balance is updated in time to simulate the diurnal response of the steady hydraulic system to changing temperature conditions.

In the steady state mode, average local climatological data must be supplied by the user. The program uses linear approximations for the longwave back radiation and evaporation terms for solution of the steady state heat balance. The reader is referred to Chapter 4 of this report for a detailed treatment of the temperature simulation.

3.10 TEMPERATURE DEPENDENCE OF RATE COEFFICIENTS

The temperature values computed in QUAL2E are used to correct the rate coefficients in the source/sink terms for the other water quality variables. These coefficients are input at 20°C and are then corrected to temperature using a Streeter-Phelps type formulation:

$$X_T = X_{20} \theta^{(T-20^\circ)} \quad \text{III-52}$$

where

X_T = the value of the coefficient at the local temperature (T)

X_{20} = the value of the coefficient at the standard temperature (20°C)

TABLE III-2
DEFAULT TEMPERATURE CORRECTION, θ , VALUES FOR QUAL2E

Rate Coefficient	Symbol	Default Values	
		SEMCOG	QUAL2E
BOD Decay	K_1	1.047	1.047
BOD Settling	K_3	-	1.024
Reaeration	K_2	1.0159	1.024
SOD Uptake	K_4	-	1.060
Organic N Decay	β_3	-	1.047
Organic N Settling	σ_4	-	1.024
Ammonia Decay	β_1	1.047	1.083
Ammonia Source	σ_3	-	1.074
Nitrite Decay	β_2	1.047	1.047
Organic P Decay	β_4	-	1.047
Organic P Settling	σ_5	-	1.024
Dissolved P Source	σ_2	-	1.074
Algal Growth	μ	1.047	1.047
Algal Respiration	ρ	1.047	1.047
Algal Settling	σ_1	-	1.024
Coliform Decay	K_5	1.047	1.047
ANC	K_6	1.047	1.000
ANC	σ_6	-	1.024
ANC	σ_7	-	1.000

Note: - = not temperature dependent in QUAL-II SEMCOG.

ANC = Arbitrary Nonconservative Constituent

θ = an empirical constant for each reaction coefficient

The values of the temperature correction factors, θ , may be specified by the user. In the absence of user specified values, the default values shown in Table III-2 are employed. For comparison purposes, the θ values used in the SEMCOG version of QUAL-II are also listed in Table III-2.

If temperature is not simulated, the temperature value specified for the initial condition is assumed to be the temperature for the simulation.

3.11 REACTION RATES AND PHYSICAL CONSTANTS

The chemical and biological reactions that are simulated by QUAL2E are represented by a complex set of equations that contain many system parameters; some are constant, some are spatially variable, and some are temperature dependent. Table III-3 lists these system parameters and gives the usual range of values, units, and types of variation. Kramer (1970), Chen and Orlob (1972), and Zison *et al.* (1978) give detailed discussions of the basic sources of data, ranges and reliabilities of each of these parameters. Final selection of the values for many of these system parameters or measurement of sensitive ones should be made during model calibration and verification.

TABLE III-3
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
α_0	Ratio of chlorophyll-a to algal biomass	$\frac{\text{ug-Chl a}}{\text{mg A}}$	10-100	No	No
α_1	Fraction of algal biomass that is Nitrogen	$\frac{\text{mg-N}}{\text{mg A}}$	0.07-0.09	No	No
α_2	Fraction of algal biomass that is Phosphorus	$\frac{\text{mg-P}}{\text{mg A}}$	0.01-0.02	No	No
α_3	O ₂ production per unit of algal growth	$\frac{\text{mg-O}}{\text{mg A}}$	1.4-1.8	No	No
α_4	O ₂ uptake per unit of algae respired	$\frac{\text{mg-O}}{\text{mg A}}$	1.6-2.3	No	No
α_5	O ₂ uptake per unit of NH ₃ oxidation	$\frac{\text{mg-O}}{\text{mg N}}$	3.0-4.0	No	No

TABLE III-3 (cont'd)
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
α_6	O ₂ uptake per unit of NO ₂ oxidation	$\frac{\text{mg-O}}{\text{mg N}}$	1.0-1.14	No	No
μ_{max}	Maximum algal growth rate	day ⁻¹	1.0-3.0	No	No
ρ	Algal respiration rate	day ⁻¹	0.05-0.5	No	No
K_L	Michaelis-Menton half-saturation constant for light (Option 1)	Btu/ft ² -min	0.02-0.10	No	No
K_N	Michaelis-Menton half-saturation constant for nitrogen	mg-N/L	0.01-0.20	No	No
K_P	Michaelis-Menton half-saturation constant for phosphorus	mg-P/L	0.01-0.05	No	No
λ_0	Non-algal light extinction coefficient	ft ⁻¹	Variable	No	No
λ_1	Linear algal self-shading coefficient	$\frac{1/\text{ft}}{\text{ug Chl-a/L}}$	0.002-0.02	No	No
λ_2	Nonlinear algal self-shading coefficient	$\frac{1/\text{ft}}{(\text{ug Chl-a/L})^{2/3}}$	0.0165 (Riley)	No	No
P_N	Algal preference factor for ammonia	-	0.0-1.0	No	No
σ_1	Algal settling rate	ft/day	0.5-6.0	Yes	Yes
σ_2	Benthos source rate for dissolved phosphorus	$\frac{\text{mg-P}}{\text{ft}^2\text{-day}}$	Variable	Yes	Yes
σ_3	Benthos source rate for ammonia nitrogen	$\frac{\text{mg-O}}{\text{ft}^2\text{-day}}$	Variable	Yes	Yes
σ_4	Organic nitrogen settling rate	day ⁻¹	0.001-0.10	Yes	Yes
σ_5	Organic phosphorus settling rate	day ⁻¹	0.001-0.10	Yes	Yes

TABLE III-3 (cont'd)
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
σ_6	Arbitrary non-conservative settling rate	day ⁻¹	Variable	Yes	Yes
σ_7	Benthic source rate for arbitrary non-conservative settling rate	$\frac{\text{mg-ANC}}{\text{ft}^2\text{-day}}$	Variable	Yes	Yes
K_1	Carbonaceous deoxygenation rate constant	day ⁻¹	0.02-3.4	Yes	Yes
K_2	Reaeration rate constant	day ⁻¹	0.0-100	Yes	Yes
K_3	Rate of loss of BOD due to settling	day ⁻¹	-0.36-0.36	Yes	Yes
K_4	Benthic oxygen uptake	$\frac{\text{m-O}}{\text{ft}^2\text{-day}}$	Variable	Yes	Yes
K_5	Coliform die-off rate	day ⁻¹	0.05-4.0	Yes	Yes
K_6	Arbitrary non-conservative decay coefficient	day ⁻¹	Variable	Yes	Yes
β_1	Rate constant for the biological oxidation of NH ₃ to NO ₂	day ⁻¹	0.10-1.00	Yes	Yes
β_2	Rate constant for the biological oxidation of NO ₂ to NO ₃	day ⁻¹	0.20-2.0	Yes	Yes
β_3	Rate constant for the hydrolysis of organic-N to ammonia	day ⁻¹	0.02-0.4	Yes	Yes
β_4	Rate constant for the decay of organic-P to dissolved-P	day ⁻¹	0.01-0.7	Yes	Yes

4. FUNCTIONAL REPRESENTATION OF TEMPERATURE

4.1 BASIC TEMPERATURE EQUATION

The basic mass transport equation for QUAL2E was given in Section II as (see equation II-3):

$$\frac{\partial C}{\partial t} = \frac{\partial(A_X D_L \frac{\partial C}{\partial x})}{A_X \partial x} - \frac{\partial(A_X \bar{u} C)}{A_X \partial x} + \frac{dC}{dt} + \frac{s}{V} \quad \text{IV-1}$$

In temperature modeling, C is taken as the concentration of heat (HL⁻³) and can be equated to temperature through the relationship

$$C = \rho c (T - T_0) \quad \text{IV-2}$$

where

- ρ = the density of water (M L⁻³)
- c = the heat capacity of water (HM⁻¹ D⁻¹)
- T = the water temperature
- T_0 = an arbitrary base temperature
- M = mass
- H = heat energy flux
- D = degrees

The parameters ρ and c can be considered constant for practical purposes. Also, the internal heat generation $\frac{dC}{dt}$, which results from viscous dissipation of energy and boundary friction, is generally small enough to be

considered negligible. Thus setting $\frac{dC}{dt} = 0$ in equation IV-1 and substituting equation IV-2 for C gives us (after some simplification):

$$\frac{\partial T}{\partial t} = \frac{\partial(A_x D_L \frac{\partial T}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} T)}{A_x \partial x} + \frac{1}{\rho c} \frac{s}{V} \quad \text{IV-3}$$

The source term s/V (with units of $HL^{-3}T^{-1}$) accounts for all heat transferred across the system boundaries, i.e., heat transferred across the air-water interface and heat conducted across mud-water interface. Heat transfer across the mud-water interface is generally insignificant; hence, s/V takes on the identify of the net rate of heat input per unit volume of stream through the air-water interface.

It is most convenient to represent the interfacial heat transfer rate as a flux (H_N) having units of $HL^{-2}T^{-1}$. For a stream element of length dx and mean surface width W , H_N is related to s/V as follows.

The total rate of heat input across the air-water interface is $H_N dx W$. This heat is distributed uniformly throughout the underlying volume of $\bar{A}_x dx$, where \bar{A}_x is the mean cross-sectional area of the element. Thus the rate of heat gain per unit volume of water, s/V , is computed as:

$$\frac{s}{V} = \frac{s}{A_x dx} = \frac{H_N (W dx)}{\bar{A}_x dx} = \frac{H_N}{d} \quad \text{IV-4}$$

where $d = \bar{A}_x/W$ is the hydraulic depth of the stream. Substituting equation IV-4 into equation IV-3 gives the generalized form of the temperature equation:

$$\frac{\partial T}{\partial t} = \frac{\partial(A_x D_L \frac{\partial T}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} T)}{A_x \partial x} + \frac{H_N}{\rho c d} \quad \text{IV-5}$$

4.2 DEFINITION OF H_N

Heat is transferred across the air-water interface of a surface water body by three difference processes: radiation exchange, evaporation, and conduction. The individual heat terms associated with these processes are shown in Figure IV-1 and are defined in Table IV-1 with the typical ranges of their magnitudes in northern latitudes also listed.

The expression that results from the summation of these various energy fluxes is:

$$H_N = H_{sn} + H_{an} - (H_b \pm H_c + H_e) \quad \text{IV-6}$$

where

H_N = net energy flux passing the air-water interface, Btu/ft²-day

H_{sn} = net short-wave solar radiation flux passing through the interface after losses due to absorption and scattering in the atmosphere and by reflection at the interface, Btu/ft²-day

H_{an} = net long-wave atmospheric radiation flux passing through the interface after reflection, Btu/ft²-day

H_b = outgoing long-wave back radiation flux, Btu/ft²-day

H_c = convective energy flux passing back and forth between the interface and the atmosphere, Btu/ft²-day

H_e = energy loss by evaporation, Btu/ft²-day

These mechanisms by which heat is exchanged between the water surface and the atmosphere are fairly well understood and are adequately documented in the literature by Edinger and Geyer (1965). The functional representation

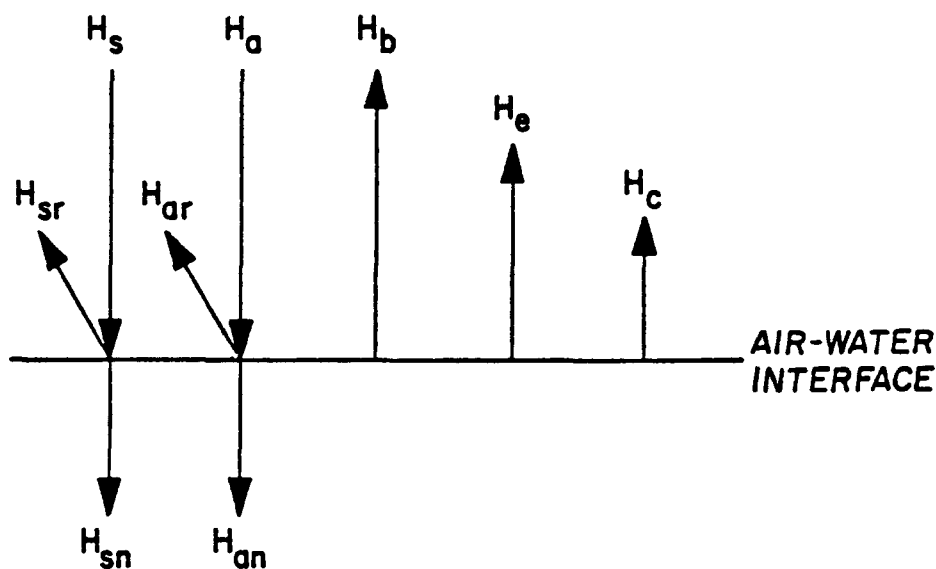


Figure IV-1. Heat Transfer Terms Associated with Interfacial Heat Transfer

TABLE IV-1
DEFINITION OF HEAT TRANSFER TERMS
ILLUSTRATED IN FIGURE IV-1

Heat Term		Units	Magnitude (BTU/ft ² -day ¹)
H_s	= total incoming solar or short-wave radiation	HL- ² T- ¹	400-2800
H_{sr}	= reflected short-wave radiation	HL- ² T- ¹	40-200
H_a	= total incoming atmospheric radiation	HL- ² T- ¹	2400-3200
H_{ar}	= reflected atmospheric radiation	HL- ² T- ¹	70-120
H_b	= back radiation from the water surface	HL- ² T- ¹	2400-3600
H_e	= heat loss by evaporation	HL- ² T- ¹	150-3000
H_c	= heat loss by conduction to atmosphere	HL- ² T- ¹	-320 to +400

of these terms has been defined by Water Resources Engineers, Inc. (1967). The formulations reported here were extracted from that more detailed work by Frank D. Masch and Associates and the Texas Water Development Board (1971).

4.3 NET SHORT-WAVE SOLAR RADIATION

The net incoming solar radiation is short-wave radiation which passes directly from the sun to the earth's surface. Its magnitude depends on: the altitude of the sun, which varies daily as well as seasonally for a fixed location on the earth; the dampening effect of scattering and absorption in the atmosphere due to cloud cover, and the reflection from the water surface.

The net amount of solar radiation which reaches the surface of the reach may be represented functionally on an hourly basis by:

$$H_{sn} = \underbrace{H_0}_{(i)} \underbrace{a_t}_{(ii)} \underbrace{(1 - R_s)}_{(iii)} \underbrace{(1 - 0.65C_L^2)}_{(iv)} \quad \text{IV-7}$$

where

- H_{sn} = net short-wave solar radiation flux, Btu/ft²-hr
- H_0 = amount of radiation flux reaching the earth's atmosphere, Btu/ft²-hr
- a_t = atmospheric transmission term
- R_s = Albedo or reflection coefficient
- C_L = cloudiness as a fraction of sky covered

It is appropriate for purposes of this discussion to identify and treat separately the four components in equation IV-7 as (i) extra-terrestrial solar radiation, (ii) radiation scattering and absorption, (iii) reflectivity, and (iv) cloudiness.

4.3.1 Extraterrestrial Radiation

The short-wave solar radiation flux that strikes the earth's outer atmosphere over a given period of time is given by Water Resources Engineers, Inc. (1967) as:

$$H_0 = \frac{H_{sc}}{r^2} \left\{ \sin \frac{\pi\phi}{180} \sin \delta (t_e - t_b) + \frac{12}{\pi} \cos \frac{\pi\phi}{180} \cos \delta \left[\sin \left(\frac{\pi t_e}{12} \right) - \sin \left(\frac{\pi t_b}{12} \right) \right] \right\} r \quad \text{IV-8}$$

where

- H_{sc} = solar constant = 438.0 Btu/ft²-hr
- r = normalized radius of the earth's orbit
- ϕ = latitude of the site, degrees

- δ = declination of the sun, degrees
- t_b, t_e = hour angles corresponding to the beginning and end, respectively, of any time interval between sunrise and sunset
- Γ = a correction factor for diurnal exposure to radiation flux

Listed below are several parameters in equation IV-8 requiring further definition as described by Water Resources Engineers, Inc. (1967).

a. Relative Earth-Sun Distance--

$$r = 1.0 + 0.17 \cos \left[\frac{2\pi}{365} (186 - D_y) \right] \quad \text{IV-9}$$

where D_y is the number of the day of the year (beginning January 1)

b. Declination--

$$\delta = \frac{23.45}{180} \pi \cos \left[\frac{2\pi}{365} (173 - D_y) \right] \quad \text{IV-10}$$

c. Hour Angles--

$$t_b = ST_b - \Delta t_s + ET - 12 \quad \text{IV-11}$$

and

$$t_e = ST_e - \Delta t_s + ET - 12 \quad \text{IV-12}$$

where ST_b , ST_e are the standard times at the beginning and end of the time interval selected

ET = an expression for time from a solar ephemeris that represents the difference in hours between "true solar time" and that computed on the basis of a yearly average. It is given for each day of the year, D_y , by

$$\begin{aligned}
 ET &= 0.000121 - 0.12319 \sin \left[\frac{2\pi}{365} (Dy-1) - 0.0714 \right] \\
 &= 0.16549 \sin \left[\frac{4\pi}{365} (Dy-1) + 0.3088 \right] \quad \text{IV-13}
 \end{aligned}$$

Δt_s = difference between standard and local civil time in hours as determined from:

$$\Delta t_s = \frac{\epsilon}{15} (L_{sm} - L_{lm}) \quad \text{IV-14}$$

where

ϵ = -1 for west longitude

ϵ = +1 for east longitude

L_{sm} = longitude of standard meridian, degrees

L_{lm} = longitude of local meridian, degrees

d. Diurnal Exposure--

$$\Gamma = 1 \text{ when } ST_r \leq ST_b \text{ or } ST_e \leq ST_s \quad \text{IV-15}$$

$$\Gamma = 0 \text{ when } ST_s \leq ST_b \text{ or } ST_e \leq ST_r \quad \text{IV-16}$$

where ST_r and ST_s are the standard times of sunrise and sunset, respectively, as determined from:

$$ST_r = 12 - \frac{12}{\pi} \arccos \left[\tan \left(\frac{\pi \phi}{180} \right) \tan \delta \right] + \Delta t_s \quad \text{IV-17}$$

and

$$ST_s = 24 - ST_r + 2\Delta t_s \quad \text{IV-18}$$

4.3.2 Radiation Scattering and Absorption

The atmospheric transmission term, a_t , is given by Water Resources Engineers, Inc. (1967) as:

$$a_t = \frac{a'' + 0.5 (1 - a' - d)}{1 - 0.5 R_s (1 - a' + d)} \quad \text{IV-19}$$

in which a'' is the mean atmospheric transmission coefficient after scattering and absorption, given by:

$$a'' = \exp \left\{ - [0.465 + 0.0408 P_{wc}] \right. \\ \left. [0.179 + 0.421 \exp (-0.721 \theta_{am})] \theta_{am} \right\} \quad \text{IV-20}$$

where θ_{am} is the optical air mass given by the expression:

$$\theta_{am} = \frac{\exp (-Z/2531)}{\sin \alpha + 0.15 \left(\frac{180\alpha}{\pi} + 3.885 \right) - 1.253} \quad \text{IV-21}$$

in which

Z = elevation of the site in feet

α = sun's altitude in radians, given by:

$$\alpha = \arcsin \left[\sin \frac{\pi \phi}{180} \sin \delta + \cos \frac{\pi \phi}{180} \right. \\ \left. \cos \delta \cos \frac{\pi t}{12} \right] \quad \text{IV-22}$$

in which t is the hour angle, described by an equation similar to equation IV-11 and IV-12.

P_{wc} in equation IV-20 is the mean daily precipitable water content in the atmosphere, given by the expression:

$$P_{wc} = 0.00614 \exp (0.0489 T_d) \quad \text{IV-23}$$

where T_d is the dewpoint in °F, which can be obtained from the expression:

$$T_d = \ln [(e_a + 0.0837)/0.1001]/0.03 \quad \text{IV-24}$$

where e_a is the water vapor pressure of the air.

The mean atmospheric coefficient, a' , can also be represented by an equation of the form of equation IV-20 as:

$$a' = \exp \{ - [0.465 + 0.0408 P_{wc}] [0.129 + 0.171 \exp (-0.880 \theta_{am})] \theta_{am} \} \quad \text{IV-25}$$

Dust attenuation of the solar radiation flux, which is represented in equation IV-19 by the quantity d , varies with optical air mass, season of the year, and geographic location. Water Resources Engineers, Inc. (1967) gives a range of 0-0.13 for several locations.

4.3.3 Cloudiness

The dampening effect on the solar radiation flux is given by Water Resources Engineers, Inc. (1967) as

$$C_s = 1.0 - 0.65 C_L^2 \quad \text{IV-26}$$

where C_L is the decimal fraction of the sky covered. Water Resources Engineers, Inc. (1967) reports that equation IV-26 gives satisfactory results except for heavy overcast conditions, i.e., when C_L approaches 1.0.

4.3.4 Reflectivity

The reflection coefficient, R_s , can be approximately computed as a function of the solar altitude, α , by Anderson's (1954) empirical formula:

$$R_s = A\alpha^B \quad \text{IV-27}$$

where α is in degrees, and A and B are functions of cloudiness, C_L . Values for A and B given by Anderson (1954) are shown in Table IV-2.

TABLE IV-2
EMPIRICAL COEFFICIENTS FOR DETERMINING R_s
After Anderson (1954)

Cloudiness C_L	0 Clear		0.1 - 0.5 Scattered		0.6 - 0.9 Broken		1.0 Overcast	
Coefficients	A	B	A	B	A	B	A	B
	1.18	-0.77	2.20	-0.97	0.95	-0.75	0.35	-0.45

4.4 LONG-WAVE ATMOSPHERIC RADIATION

The long-wave radiation emitted by the atmosphere varies directly with the moisture content of the atmosphere. Although it is primarily dependent on air temperature and humidity, it can also be affected by ozone, carbon dioxide, and possibly other materials in the atmosphere. Anderson (1954) indicated that the amount of atmospheric radiation is also significantly affected by cloud height. The amount of long-wave atmospheric radiation that is reflected is approximately a constant fraction of the incoming radiation, found by Anderson (1954) to be approximately 0.03.

The net atmospheric radiation flux can be expressed as:

$$H_{an} = [2.89 \times 10^{-6}] \sigma (T_a + 460)^6 (1.0 + 0.17C_L^2)(1-R_L) \quad \text{IV-28}$$

where

H_{an} = net long-wave atmospheric radiation flux, Btu/ft²-hr

σ = Stefan-Boltzman constant, 1.73×10^{-9} Btu/ft²/hr/
°Rankine⁴

T_a = air temperature at a level 6 feet above the water
surface, °F

R_L = reflectivity of the water surface for atmospheric
radiation = 0.03

C_L = cloudiness, fraction of cloud cover

4.5 WATER SURFACE BACK RADIATION

The third source of radiation transfer through the air-water interface is long-wave back radiation from the water surface, H_b , which represents a loss of heat from the water. It can be seen from Table IV-1 that back radiation accounts for a substantial portion of the heat loss from a body of water. This loss is expressed by the Stefan-Boltzman Fourth Power Radiation Law for a blackbody as:

$$H_b = 0.97 \sigma (T_s + 460)^4 \quad \text{IV-29}$$

where

H_b = water surface back radiation flux, Btu/ft²-hr

T_s = water surface temperature, °F

Equation IV-29 can be linearized over a given temperature range as

$$H_b = \alpha_2 + \beta_2 T_s \quad \text{IV-30}$$

where

$$\alpha_2, \beta_2 = \text{constants defined over the range 35 to 135 } ^\circ\text{F}$$

In the steady-state temperature solution, this linearized version of the back radiation equation is used to allow the temperature dependent terms to be separated out of the equation. Sets of α_2, β_2 are specified for 21 5°F temperature intervals between 35°F and 135°F . For dynamic simulations the heat flux term calculations are based on the temperature at the beginning of the time step.

4.6 EVAPORATION

A water body also loses heat to the atmosphere by evaporation. Each pound of water that leaves as water vapor carries its latent heat of vaporization (approximately 1050 BTU at 60°F) plus its sensible heat. This significant heat loss due to evaporation can be expressed as:

$$H_e = \gamma H_L E + H_v \quad \text{IV-31}$$

where

$$\gamma = \text{specific weight of the water being evaporated, lb/ft}^3$$

$$H_L = \text{latent heat of vaporization, Btu/lb, given by}$$

$$H_L = 1084 - 0.5 T_s$$

$$E = \text{evaporation rate, ft/hr}$$

$$H_v = \text{sensible heat loss Btu/ft}^2\text{-hr}$$

The evaporation rate, E , is most often expressed as

$$E = (a + bW) (e_s - e_a) \quad \text{IV-32}$$

where

$$a, b = \text{constants}$$

W = wind speed, in mph, measured 6 feet above the water surface

e_s = saturation vapor pressure of the air, in. of Hg, at the temperature of the water surface, as given by

$$e_s = 0.1001 \exp (0.03 T_s) - 0.0837$$

and

e_a = water vapor pressure, in. of Hg, at a height of 6 feet above the water surface, given as

$$e_a = e_{wb} - 0.000367 P_a (T_a - T_{wb}) \left(1.0 + \frac{T_{wb} - 32}{1571} \right) \quad \text{IV-34}$$

where

e_{wb} = saturation vapor pressure, in. of Hg, at the wet bulb temperature from the expression

$$e_{wb} = 0.1001 \exp (0.03 T_{wb}) - 0.0837 \quad \text{IV-35}$$

P_a = local barometric pressure, in. of Hg

T_{wb} = wet bulb air temperature, °F

T_a = dry bulb air temperature, °F

The literature contains a wide range of values for the evaporation constants a and b . Roesner (1969) reports that a good average value of a would be 6.8×10^{-4} ft/hr-in. of Hg, while b would best be represented by 2.7×10^{-4} ft/hr-in. of Hg.-mph.

To linearize the variation of evaporation rate with surface water temperature T_s , equation IV-34 is approximated over 5°F intervals as:

$$e_s = \alpha_1 + \beta_1 T_s \quad \text{IV-36}$$

Sets of α_1 , β_1 are specified for twenty-one 5°F intervals between 35°F and 135°F. The linearized evaporation expression is used in the steady-state temperature solution.

The sensible evaporative heat loss can be expressed simply as:

$$H_V = c \gamma E (T_S - T_0) \quad \text{IV-37}$$

where

c = heat capacity of water = 1 Btu/lb-°F

T_0 = reference temperature, °F

Sensible heat loss is very small compared to the other heat loss components in the energy budget and thus is not included in the QUAL2E temperature computation.

4.7 CONDUCTION

Heat that is transferred between the water and the atmosphere due to a temperature difference between the two phases is normally called conduction. Using the fact that transfer by conduction is a function of the same variables as evaporation, it is possible to arrive at a proportionality between heat conduction and heat loss by evaporation. This proportionality, known as Bowen's ratio, is expressed as:

$$B = \frac{H_C}{H_E} = C_B \left[\frac{T_S - T_a}{e_s - e_a} \right] \frac{P_a}{29.92} \quad \text{IV-38}$$

where C_B is a coefficient $\cong 0.01$.

By using Bowen's ratio, the rate of heat loss to the atmosphere by heat conduction, H_C , can be defined as:

$$H_C = \gamma H_L (a+bW) \left(0.01 \frac{P_a}{29.92} \right) (T_S - T_a) \quad \text{IV-39}$$

For practical purposes, the ratio ($P_a/29.92$) can be taken as unity.

5. COMPUTATIONAL REPRESENTATION

5.1 PROTOTYPE REPRESENTATION

To expand upon the basic conceptual representation presented in Sections 1 and 2, QUAL2E permits any branching, one-dimensional stream system to be simulated. The first step involved in approximating the prototype 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 so that all computational elements in all reaches are the same 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 mainstem that is 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 (downstream boundary); there should be only one element type 5. Element types 6 and 7 represent elements which have 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 flow data are constant for all computational elements within a reach.

5.2 FORCING FUNCTIONS

Forcing functions are the user specified inputs that drive the system being modeled. These inputs are specified in terms of flow, water quality characteristics, and local climatology. QUAL2E accommodates four types of hydraulic and mass load forcing functions in addition to local climatological factors--headwater inputs, point sources or withdrawals, incremental inflow/outflow along a reach, and the (optional) downstream boundary concentration.

1. Headwater Inputs - Headwater inputs are typically the upstream boundary conditions at the beginning of the system. They are the conditions required to generate the solution of the mass balance equations for the first computational element in each headwater reach. Headwaters are also the source of water for flow augmentation.

2. Point Sources and/or Withdrawals - These loads are used to represent point source discharges into the system (i.e., sewage and industrial waste, or storm water runoff) and losses from the system resulting from diversions. In QUAL2E point source discharges may represent either raw or treated waste loads. If raw waste loads are used, the effect of treatment can be simulated by applying a specific fractional removal for carbonaceous BOD to each point source load.

3. Incremental Inflow - QUAL2E has the capability to handle flow uniformly added or removed along a reach. The total flow increment along a reach is apportioned equally to all computational elements in the reach. This feature can be used to simulate the effects of non-point source inputs to the system, or the effect of loss of stream flow to the groundwater.

4. Downstream Boundary Concentration (optional) - QUAL2E has the capability of incorporating known downstream boundary concentrations of the water quality constituents into the solution algorithm. This feature is useful in modeling systems with large dispersion in the lower reaches (e.g., estuaries). When downstream boundary concentrations are supplied, the solution generated by QUAL2E will be constrained by this boundary condition. If the concentrations are not provided, the constituent concentrations in the most downstream element will be computed in the normal fashion using the zero gradient assumption (see Section 5.4.3).

Local climatological data are required for the dynamic simulation of algae and temperature. The temperature simulation uses a heat balance across the air-water interface and thus requires values of wet and dry bulb air temperatures, atmospheric pressure, wind velocity, and cloud

cover. The algal simulation requires values of net solar radiation. These climatological data must be input at regular time intervals over the course of the simulation. For modeling steady-state temperature and algae, average daily local climatological data are required. All climate data are applied uniformly over the entire river basin.

5.3 MODEL LIMITATIONS

QUAL2E has been developed to be a relatively general program; however, certain dimensional limitations have been imposed upon it during program development. These limitations are as follows:

Reaches: a maximum of 50

Computational elements: no more than 20 per reach or 500 in total

Headwater elements: a maximum of 10

Junction elements: a maximum of 9

Input and withdrawal elements: a maximum of 50 in total

(Note: These limitations may be modified, if necessary, by the user by altering the PARAMETER statement specifications in the common blocks of the program.)

QUAL2E can be used to simulate any combination of the following parameters or groups of parameters.

1. Conservative minerals (up to three at a time)
2. Temperature
3. BOD
4. Chlorophyll a
5. Phosphorus cycle (organic and dissolved)
6. Nitrogen cycle (organic, ammonia, nitrite, and nitrate)
7. Dissolved oxygen
8. Coliforms
9. An arbitrary nonconservative constituent

All parameters can be simulated under either steady-state or dynamic conditions. If either the phosphorus cycle or the nitrogen cycle are not being simulated, the model presumes they will not limit algal growth.

5.4 NUMERICAL SOLUTION TECHNIQUE

At each time step and for each constituent, Equation II-3 can be written I times, once for each of the I computational elements in the network. Because it is not possible to obtain analytical solutions to these equations under most prototype situations, a finite difference method is used--more specifically, the classical implicit backward difference method (Arden and Astill, 1970; Smith, 1966; and Stone and Brian, 1963).

The general basis of a finite difference scheme is to find the value of a variable (e.g., constituent concentration) as a function of space at a time step $n+1$ when its spatial distribution at the n th time step is known. Time step zero corresponds to the initial condition. Backward difference or implicit schemes are characterized by the fact that all spatial derivatives ($\partial/\partial x$) are approximated in difference form at time step $n+1$.

5.4.1 Formulation of the Finite Difference Scheme

The finite difference scheme is formulated by considering the constituent concentration, C , at four points in the mnemonic scheme as shown in Figure V-1.

Three points are required at time $n+1$ to approximate the spatial derivatives. The temporal derivative is approximated at distance step i .

Equation II-3 can be written in finite difference form in two steps. First, the advection and diffusion terms are differentiated once with respect to x , giving:

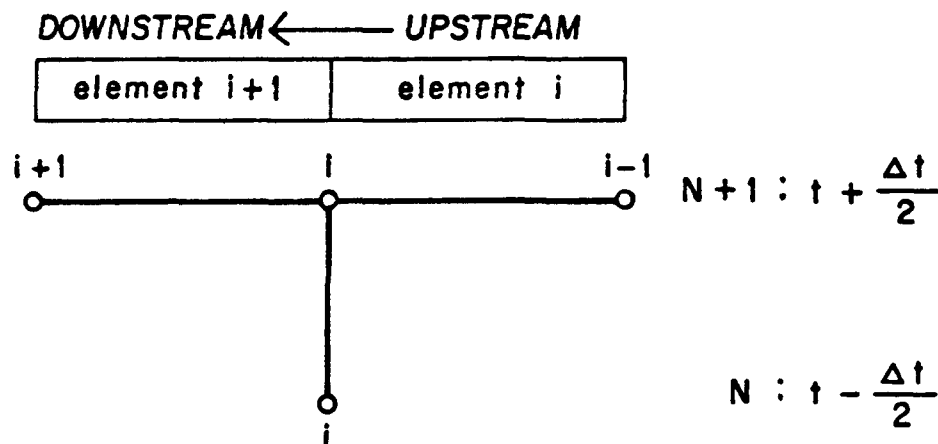


Figure V-1. Classical Implicit Nodal Scheme

$$\frac{\partial C_i}{\partial t} = \frac{(AD_L)_{i+1} \frac{\partial C}{\partial x} - (AD_L)_i \frac{\partial C}{\partial x}}{V_i} - \frac{(A \bar{u} C)_i - (A \bar{u} C)_{i-1}}{V_i} + \frac{dC_i}{dt} + \frac{s_i}{V_i} \quad V-1$$

where

$$V_i = A_i \Delta x_i$$

Secondly, expressing the spatial derivative of the diffusion terms in finite difference and thence the time derivative of C in finite difference, there results:

$$\begin{aligned} \frac{C_i^{n+1} - C_i^n}{\Delta t} = & \left(\frac{[(AD_L)_{i+1}] C_{i+1}^{n+1} - [(AD_L)_i] C_i^{n+1}}{V_i \Delta x_i} \right. \\ & \left. - \frac{[(AD_L)_{i-1}] C_i^{n+1} - [(AD_L)_{i-1}] C_{i-1}^{n+1}}{V_i \Delta x_i} \right) \\ & - \left(\frac{Q_i C_i^{n+1} - Q_{i-1} C_{i-1}^{n+1}}{V_i} \right) + r_i C_i^{n+1} + p_i + \frac{s_i}{V_i} \quad V-2 \end{aligned}$$

In equation V-2, the term dC/dt is expressed as:

$$\frac{dC_i}{dt} = r_i C_i^{n+1} + p_i$$

where

r_i = rate constant

p_i = internal constituent sources and sinks (e.g., nutrient loss from algal growth, benthos sources, etc.)

Note that the dC/dt for every constituent modeled by QUAL2E can be expressed in this form.

If equation V-2 is rearranged in terms of the coefficients of C_i^{n+1} , C_i^{n+1} , and C_{i-1}^{n+1} , we obtain the equation:

$$a_i C_{i-1}^{n+1} + b_i C_i^{n+1} + c_i C_{i-1}^{n+1} = Z_i \quad V-3$$

where

$$a_i = - \left[(AD_L)_{i-1} \frac{\Delta t}{V_i \Delta x_i} + \frac{Q_{i-1} \Delta t}{V_i} \right]$$

$$b_i = 1.0 + \left[(AD_L)_i + (AD_L)_{i-1} \right] \frac{\Delta t}{V_i \Delta x_i} + Q_i \frac{\Delta t}{V_i} - r_i \Delta t$$

$$c_i = - \left[(AD_L)_i \frac{\Delta t}{V_i \Delta x_i} \right]$$

$$Z_i = C_i^n + \frac{s_i \Delta t}{V_i} + p_i \Delta t$$

The values of a_i , b_i , c_i , and Z_i are all known at time n , and the C_i^{n+1} terms are the unknowns at time step $n+1$.

In the case of a junction element with a tributary upstream element, the basic equation becomes:

$$a_i C_{i-1}^{n+1} + b_i C_i^{n+1} + c_i C_{i-1}^{n+1} + d_j C_j^{n+1} = Z_i \quad V-4$$

where

$$d_j = - \left[(AD)_j \frac{\Delta t}{V_i \Delta x_i} + \frac{Q_j \Delta t}{V_i} \right]$$

j = the element upstream of junction element i

C_j^{n+1} = concentration of constituent in element j at time $n+1$

It can be seen that the d_j term is analogous to the a_i term. Both terms account for mass inputs from upstream due to dispersion and advection.

Under steady-state conditions, $\frac{\partial C_i}{\partial t} = 0$ in equation V-1. Working through the finite difference approximations and rearranging terms as before, the steady-state version of equation V-3 is derived:

$$a_i C_{i-1}^{n+1} + b_i C_i^{n+1} + c_i C_{i+1}^{n+1} = Z_i \quad V-5$$

where

$$a_i = -\left[\frac{(AD_L)_{i-1}}{V_i \Delta x_i} + \frac{Q_{i-1}}{V_i} \right]$$

$$b_i = \left[\frac{(AD_L)_i}{V_i \Delta x_i} + \frac{(AD_L)_{i-1}}{V_i \Delta x_i} + \frac{Q_i}{V_i} - r_i \right]$$

$$c_i = \left[\frac{(AD_L)_i}{V_i \Delta x_i} \right]$$

$$Z_i = \frac{S_i}{V_i} + P_i$$

Note that equation V-5 is the same as equation V-3, with three changes:

- o $\Delta t = 1.0$
- o the constant 1.0 in $b_i = 0.0$
- o the initial concentration C_i^n in $Z_i = 0.0$

5.4.2 Method of Solution

Equations V-3 and V-5 each represent a set of simultaneous linear equations whose solution provides the values of C_i^{n+1} for all i 's. Expressed in matrix form, this set of equations appears as:

$$\begin{bmatrix}
 b_1 & c_1 & & & & \\
 a_2 & b_2 & c_2 & & & \\
 & a_3 & b_3 & c_3 & & \\
 & & & \ddots & \ddots & \ddots \\
 & & & & a_i & b_i & c_i \\
 & & & & & \ddots & \ddots & \ddots \\
 & & & & & & a_{I-1} & b_{I-1} & c_{I-1} \\
 & & & & & & & a_I & b_I
 \end{bmatrix}
 \times
 \begin{bmatrix}
 c_1^{n+1} \\
 c_2^{n+1} \\
 c_3^{n+1} \\
 \vdots \\
 c_i^{n+1} \\
 \vdots \\
 \vdots \\
 c_{I-1}^{n+1} \\
 c_I^{n+1}
 \end{bmatrix}
 =
 \begin{bmatrix}
 Z_1 \\
 Z_2 \\
 Z_3 \\
 \vdots \\
 Z_i \\
 \vdots \\
 \vdots \\
 Z_{I-1} \\
 Z_I
 \end{bmatrix}
 \quad \text{V-6}$$

The left matrix is a tri-diagonal matrix. An efficient method that readily lends itself to a computer solution of such a set of equations is:

Divide through the first equation in V-6 by b_1 to obtain:

$$c_1^{n+1} + W_1 c_2^{n+1} = G_1 \quad \text{V-7}$$

where

$$W_1 = c_1/b_1 \text{ and } G_1 = Z_1/b_1.$$

Combine the expression for b_i (see V-3) and the second equation in V-6 to eliminate a_2 and the result is:

$$c_2^{n+1} + W_2 c_3^{n+1} = G_2 \quad \text{V-8}$$

where

$$W_2 = \frac{c_2}{b_2 - a_2 W_1} \text{ and } G_2 = \frac{Z_2 - a_2 G_1}{b_2 - a_2 W_1}$$

Combine equation V-8 and the third equation in V-6 to eliminate a_3 and the result is:

$$C_3^{n+1} + W_3 C_4^{n+1} = G_3 \quad V-9$$

where

$$W_3 = \frac{C_3}{b_3 - a_3 W_2} \quad \text{and} \quad G_3 = \frac{Z_3 - a_3 G_2}{b_3 - a_3 W_2}$$

Proceed through the equations, eliminating a_i and storing the values of W_i and G_i given by:

$$W_i = \frac{C_i}{b_i - a_i W_{i-1}}, \quad i = 2, 3, \dots, I \quad V-10$$

and

$$G_i = \frac{Z_i - a_i G_{i-1}}{b_i - a_i W_{i-1}}, \quad i = 2, 3, \dots, I \quad V-11$$

The last equation is solved for C_I^{n+1} by

$$C_I^{n+1} = G_I \quad V-12$$

Solve for C_{i-1}^{n+1} , C_{i-2}^{n+1} , \dots , C_1^{n+1} by back substitution.

$$C_i^{n+1} = G_i - W_i C_{i-1}^{n+1}, \quad i = I-1, I-2, \dots, 1 \quad V-13$$

5.4.3 Boundary Conditions

In most situations of interest, transport is unidirectional in nature, i.e., there is no significant transport upstream. Therefore, the concentration at some point just upstream from the beginning or end of the stream reach of interest can be used as the boundary condition.

5.4.3.1 Upstream Boundary (Headwater Elements)

For headwater elements there is no upstream, $i-1$, element. Thus, the headwater driving force is substituted in Equation V-3 for the upstream concentration C_{i-1} . Because the headwater concentrations are fixed, they are incorporated on the right hand side of Equation V-3 in the known term Z_i , for headwater elements as follows.

$$Z_1 = C_1^n + \frac{s_1 \Delta t}{V_1} + p_1 \Delta t - a_1 C_0 \quad V-14$$

where C_0 is the upstream boundary condition (headwater concentration).

5.4.3.1 Downstream Boundary (Last Element in the System)

QUAL2E has two options for modeling the downstream boundary. One uses a zero gradient assumption; the other incorporates fixed downstream constituent concentrations into the solution algorithm.

Zero Gradient Assumption (Arden and Astill, 1970)--For the last computational element in the system, there is no downstream, $i+1$, element. At this boundary, a zero gradient assumption is made that replaces C_{i+1} with C_{i-1} . In this manner, the downstream boundary acts as a mirror to produce a zero gradient for the concentration of the constituent variable. The coefficient a_i , therefore, is modified to include the dispersion effect normally found in the coefficient c_i for the last element in the system. Thus, the equation for a_i in V-3 becomes:

$$a_I = -[(AD_L)_{I-1} + (AD_L)_I] \frac{\Delta t}{V_I \Delta x_I} + \frac{Q_{I-1} \Delta t}{V_I} \quad .V-15$$

and

$$c_I = 0 \quad V-16$$

where I = index of the downstream boundary element

Fixed Downstream Constituent Concentrations--For this boundary option, the user supplies known downstream boundary concentrations C_{LB} for each water quality constituent. Thus, the value of C_{i+1} in Equation V-3 becomes

$$C_{I+1} = C_{LB} \quad V-17$$

Because the boundary concentrations are known in this option, they are incorporated on the right hand side of Equation V-3 in the known term Z_i for the downstream boundary element then results as

$$Z_I = C_I^0 + \frac{S_I \Delta t}{V_I} + p_I \Delta t - c_I C_{LB} \quad V-18$$

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APPENDIX A
QUAL2E User Manual*

The following sections illustrate the coding of input data forms.

A. Title Data

All 16 cards are required in the order shown. The first two are title cards, and columns 22 through 80 may be used to describe the base, date of simulation, etc. Title cards 3 through 15 require either a "yes" or "no" in columns 10 through 12 and are right justified. Note that each of the nitrogen and phosphorus series must be simulated as a group.

For each conservative substance (up to three) and the arbitrary non-conservative, the constituent name must be entered in columns 49 through 52. Corresponding input data units are entered in columns 57 through 60 (e.g., mg/L).

QUAL2E simulates ultimate BOD in the general case. If the user wishes to use 5-day BOD for input and output, the program will internally make the conversions to ultimate BOD. This conversion is based upon first order kinetics and a decay rate that can be specified by the user (Type 1 Data, line 8). If no value is specified, the program uses a default value of 0.23 per day, base e. NCASI recommends that users work only with ultimate BOD unless they have detailed knowledge of the river water and point source BOD kinetics. To use the 5-day BOD input/output option, write "5-Day Biochemical Demand" in mg/L on the title 7 card beginning in column 22.

Card 16 must read ENDTITLE beginning in column 1.

*From: Modifications to the QUAL-2 Water Quality Model and User Manual for QUAL-2E Version 2.2. National Council of the Paper Industry for Air and Stream Improvement, Inc., New York, NY. NCASI Tech. Bulletin No. 457. April 1985. Used by permission.

B. Data Type 1 - Program Control

Type 1 Data define the program control options and the characteristics of the stream system configuration, as well as some of the geographical/meteorological conditions for modeling temperature. There are a maximum of 17 Data 1 cards. The first 13 are required, while the last four are necessary only if temperature is being simulated.

The QUAL2E program recognizes Type 1 Data by comparing the first four characters (columns 1-4) of each data card with a set of internally fixed codes. If a match between the code and characters occurs, then the data are accepted as supplied on the card by the user. If a match does not occur, then the program control options will revert to default values and the system variables for the unmatched codes will be assigned the value zero (0.0).

The first seven cards control program options. If any characteristics other than those shown below are inserted in the columns 1 through 4, the actions described will not occur.

LIST - Card 1, list the input data.

WRIT - Card 2, write the intermediate output report,
WRPT2 (see SUBROUTINE WRPT2 in the documentation
manual, NCASI Technical Bulletin No. 391).

FLOW - Card 3, use flow augmentation.

STEA - Card 4 shows this is a steady-state simulation. If it is not to be a steady-state, write DYNAMIC SIMULATION, or NO STEADY STATE, and it is automatically a dynamic simulation.

TRAP - Card 5, cross-sectional data will be specified for each reach. If discharge coefficients are to be used for velocity and depth computations, write DISCHARGE COEFFICIENTS, or NO TRAPEZOIDAL CHANNELS, beginning in column 1.

PRIN - Card 6, local climatological data specified globally for the basin simulation will appear in the final output listing.

PLOT - Card 7, dissolved oxygen and BOD will be plotted in final output listing.

The next two cards provide further program flags and coefficients. This information is supplied in two data fields per card; columns 26-35, and 71-80. Note that the character codes

in columns 1-4 must occur as shown in order for the data to be accepted by the program.

FIXE - Card 8, specifies: (a) whether the downstream boundary water quality constituent concentrations are fixed (user specified), and (b) the value of the rate coefficient for converting input 5-day BOD to ultimate BOD. A value of 1.0 (or larger) in columns 26-35 specifies that the downstream boundary water quality constituent concentrations will be supplied in Data Types 13 and 13A. A value less than 1.0 (usually 0.0 or blank) in these columns means that the downstream boundary concentrations are not user specified. In this case, the concentrations in the most downstream element (Type 5) will be computed in the normal fashion using the zero gradient assumption (1, 11). The second value on this card, columns 71-80, is the rate coefficient for converting 5-day to ultimate BOD. It is used only when 5-day BOD is being modeled (Title Card 7). If the columns are left blank, the model uses a default value of 0.23 per day, base e. Note that this conversion factor is applied to all input BOD₅ forcing functions (headwaters, incremental flows, point loads, and the downstream boundary condition).

INPU - Card 9, specifies whether the user will input and/or output in metric or English units. The value of 1.0 (or larger) in card columns 26-35 specifies metric input. The value of 1.0 (or larger) in card column 71-80 specifies metric units for output. Any value less than 1.0 (usually 0.0 or blank) will specify English units.

The next four cards describe the stream system. There are two data fields per card, columns 26-35 and 71-80. The program restrictions on the maximum number of headwaters, junctions, point loads, and reaches are defined by PARAMETER statements in the Fortran code. These statements may be modified by the user to accommodate a particular computer system or QUAL2E simulation application. The values of the maximum constraints are as follows:

Maximum number of headwaters	10
Maximum number of junctions	9
Maximum number of point loads	50
Maximum number of reaches	50
Maximum number of computational elements	500

NUMB - Card 10, defines the number of reaches into which the stream is segmented and the number of stream junctions (confluences) within the system.

- NUM_ - Card 11, shows the number of headwater sources and the number of inputs or withdrawals within the system. The inputs can be small streams, wasteloads, etc. Withdrawals can be municipal water supplies, canals, etc. NOTE: Withdrawals must have a minus sign ahead of the flow in Data Type 11 and must be specified as withdrawals in Data Type 4 by setting IFLAG = 7 for that element. Note, the code for Card 11 is 'NUM_' (read: NUM space) to distinguish it from the code for Card 10, NUMB.
- TIME - Card 12, contains the time step interval in hours and the length of the computational element in miles (kilometers). The time step interval is used only for a dynamic simulation, thus it may be omitted if the simulation is steady-state.
- MAXI - Card 13, provides information with different meanings depending on whether a dynamic or steady-state simulation is being performed. For a dynamic simulation, the maximum route time is specified in columns 26-35. This value represents the approximate time in hours required for a particle of water to travel from the most upstream point in the system to the most downstream point. The time increment in hours for intermediate summary reports of concentration profiles is specified in columns 71-80. For a steady-state simulation, the maximum number of iterations allowed for solution convergence is entered in columns 26-35. The value in columns 71-80 may be left blank because it is not required in the steady-state solution.

The next four cards provide geographical and meteorological information and are required only if temperature is being simulated. There are two data fields per card, columns 26-35 and 71-80. Note: the character codes in columns 1-4 must occur as shown in order for the data to be accepted by the program.

- LATI - Card 14, contains the basin latitude and longitude and represent mean values in degrees for the basin.
- STAN - Card 15, shows the standard meridian in degrees, and the day of the year the simulation is to begin.
- EVAP - Card 16, specifies the evaporation coefficients. Typical values are $AE = 6.8 \times 10^{-4}$ ft/hr-in Hg and $BE = 2.7 \times 10^{-4}$ ft/hr-in Hg-mph of wind for English units input, or $AE = 6.2 \times 10^{-6}$ m/hr-mbar and $BE = 5.5 \times 10^{-6}$ m/hr-mbar-m/sec of wind for metric units input.

ELEV - Card 17, contains the mean basin elevation in feet (meters) above mean sea level, and the dust attenuation coefficient (unitless) for solar radiation. The dust attenuation coefficient generally ranges between zero and 0.13. Users may want to consult with local meteorologists for more appropriate values.

Data Type 1 must end with an ENDATA1 card.

C. Data Type 1A - Global Algal, Nitrogen, Phosphorus, and Light Parameters

These parameters and constants apply to the entire simulation and represent the kinetics of the algal, nutrient, light interactions. It is important to note that proper use of all options in QUAL2E requires detailed knowledge of the algal growth kinetics appropriate for the water body being simulated.

These data cards are required only if algae, the nitrogen series (organic, ammonia, nitrite, and nitrate), or the phosphorus series (organic and dissolved) are to be simulated. Otherwise they may be omitted, except for the ENDATA1A card). Information is supplied in two data fields per card, columns 33-39 and 74-80. As with Type 1 Data, the QUAL2E program recognizes Type 1A Data by comparing the first four characters (columns 1-4) of each card with a set of internally fixed codes. If a match between the codes and the characters occurs, then the data are accepted as supplied on the card by the user. If a match does not occur, then the system variables for the unmatched codes will be assigned the value zero (0.0). Note: the spaces (under bars) are an integral (necessary) part of the four character code.

O_UP - Card 1, specifies the oxygen uptake per unit of ammonia oxidation, and oxygen uptake per unit of nitrite oxidation.

O_PR - Card 2, contains data on oxygen production per unit of algae growth, usually 1.6 mg O/mg A, with a range of 1.4 to 1.8. It also contains data on oxygen uptake per unit of algae, usually 2.0 mg O/mg A respired, with a range of 1.6 to 2.3.

N_CO - Card 3, concerns the nitrogen content and phosphorus content of algae in mg per mg of algae. The fraction of algae biomass which is nitrogen is about 0.08 to 0.09, and the fraction of algae biomass which is phosphorus is about 0.012 to 0.015.

- ALG_ - Card 4, specifies the growth and respiration rates of algae. The maximum specific growth rate has a range of 1.0 to 3.0 per day. The respiration value of 0.05 is for clean streams, while 0.2 is used where the N_E and P_2 concentrations are greater than twice the half saturation constants.
- N_HA - Card 5, contains the nitrogen and phosphorus half saturation coefficients. The range of values for nitrogen is from 0.2 to 0.4 mg/L and for phosphorus the value normally used is 0.04 mg/L.
- LIN_ - Card 6, contains the linear and nonlinear algal self shading light extinction coefficients. The coefficients λ_1 and λ_2 are defined below.

λ_1 = linear algae self-shading coefficient
(1/ft)/(ug chla/L), or (1/m)/(ug chla/L)

λ_2 = nonlinear algae self-shading coefficient
(1/ft)/ug chla/L)^{2/3}, or (1/m)/(ug chla/L)^{2/3}

These two self-shading coefficients are used with λ_0 , the non-algal light extinction coefficient (Type 6B Data) in the general light extinction equation shown below:

$$\lambda = \lambda_0 + \lambda_1 \alpha_0 A + \lambda_2 (\alpha_0 A)^{2/3}$$

where λ is the total light extinction coefficient and A is the algae biomass concentration in mg A/L and α_0 is the chlorophyll a to algae biomass ratio as ug chla/mg A. Appropriate selection of the values of λ_0 , λ_1 and λ_2 allows a variety of light extinction relationships to be simulated as follows:

* No self-shading (SEMCOG)

$$\lambda_1 = \lambda_2 = 0$$

* Linear algal self-shading (META)

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

* Nonlinear self-shading (Riley Eq., metric units)

$$\lambda_1 = 0.0088$$

$$\lambda_2 = 0.054$$

LIGH - Card 7, contains the solar light function option for computing the effects of light attenuation on the algal growth rate, and the light saturation coefficient. QUAL2E recognizes three different solar light function options. The light saturation coefficient is coupled to the selection of a light function, thus care must be exercised in specifying a consistent pair of values.

The depth integrated form of the three light functions and the corresponding definitions of the light saturation coefficient are given in Figure A-1 and outlined in the following table.

<u>Light Function Option</u> <u>(Columns 33 - 39)</u>	<u>Light Saturation Coefficient*</u> <u>(Columns 74 - 80)</u>
1 (Half Saturation)	Half Saturation Coefficient
2 (Smith's Function)	Light intensity corresponding to 71% of maximum growth rate
3 (Steele's Function)	Saturation Light Intensity
* Units of the Light Saturation Coefficient are as follows: English: BTU/ft ² -min and Metric: Langley's/min	

Light Function Option 1 utilizes a Michaelis-Menton half saturation formulation for modeling the algal growth limiting effects of light (FL). It is the method used in the SEMCOG version of QUAL-2. Option 2 is similar to Michaelis-Menton, but utilizes a second order rather than first order light effect. Both options 1 and 2 are monotonically increasing functions of light intensity. Option 3 includes a photo-inhibition effect at high light intensities and has been reported in (9,13).

DAIL - Card 8, contains the light averaging option (columns 33-39) and the light averaging factor (columns 74-80). These values are used only in a steady-state simulation. The light averaging option allows the user to specify the manner in which the light attenuation factor (FL in Figure A-1) is computed, from the available values of solar radiation. A summary of these options is given below.

<u>Option</u>	<u>Description</u>
1	FL is computed from one daily average solar radiation value calculated in the steady-state temperature subroutine (HEATER).
2	FL is computed from one daily average solar radiation read from Data Type 1A.
3	FL is obtained by averaging the 24 hourly values of FL, that are computed from the 24 hourly values of solar radiation calculated in the steady-state temperature subroutine (HEATER).
4	FL is obtained by averaging the 24 hourly values of FL, that are computed from the 24 hourly values of solar radiation computed from the total daily solar radiation (Data Type 1A) and an assumed cosine function.

Note: that if options 1 or 3 are selected, temperature must be simulated.

The light averaging factor (columns 74-80) is used to make a single calculation using daylight average solar radiation (Option 1 or 2) agree with average of calculations using hourly solar radiation values (Option 3 or 4). The factor has been reported to vary from 0.85 to 1.00.

The selection of a daily (diurnal) light averaging option depends largely on the detail to which the user wishes to account for the diurnal variation in light intensity. Options 1 and 2 utilize a single calculation of FL based on an average daylight 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 average daylight 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 in Data Type 1A for the algae simulation. Thus either option 2 or 4 must be selected when algae are simulated and temperature is not. The light averaging factor is used to provide similarity in FL calculations between options 1 and 2 versus options 3 and 4. The solar radiation factor (Data Type 1A, card 11) 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.

Light Functions (LFNOPT)

- Option 1: Half saturation (SEMCOG)

$$FL = \left(\frac{1}{\lambda d}\right) \ln \left[\frac{KL + I}{KL + I e^{-\lambda d}} \right]$$

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

- Option 2: Smith's Function (14)

$$FL = \left(\frac{1}{\lambda d}\right) \ln \left[\frac{I/KL + (1 + (I/KL)^2)^{1/2}}{I/KL e^{-\lambda d} + (1 + (I/KL e^{-\lambda d})^2)^{1/2}} \right]$$

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

- Option 3: Steele's Equation (9)

$$FL = \frac{2.718}{\lambda d} [e^{-(e^{-\lambda d}(I/KL))} - e^{-I/KL}]$$

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

Notation: FL = light attenuation factor
 λ = extinction coefficient *
d = depth
I = surface light intensity
KL = light saturation coefficient

* Algal Self-shading

- General Equation $\lambda = \lambda_0 + \lambda_1 \alpha_0 A + \lambda_2 (\alpha_0 A)^{2/3}$

where: λ = light extinction coefficient

λ_0 = non-algal extinction

λ_1 = linear algal self shading coefficient

λ_2 = non-linear algal self shading coefficient

A = algal biomass concentration (mg/L)

α_0 = chlorophyll a to algae biomass ratio (ug chla/mgA)

- Special Cases

- No Self-shading (SEMCOG)

$$\lambda_1 = \lambda_2 = 0$$

- Linear Self-shading (META)

$$\lambda_1 \neq \lambda_0 \quad \lambda_2 = 0$$

- Non-linear Self-shading (TetraTech)

$$\lambda_1 \neq \lambda_2 \neq 0$$

e.g. $\lambda = \lambda_0 + 0.0088 \alpha_0 A + 0.054 (\alpha_0 A)^{2/3}$ (Riley Eq., metric units)

FIGURE A-1. ALGAL GROWTH RATE

In dynamic algae simulations option 3 is used (default) unless temperature is not simulated in which case solar radiation data are read in with the local climatology data.

NUMB - Card 9, contains the number of daylight hours (columns 33-39), and the total daily radiation (BTU/ft², or Langleys) (columns 74-80). This information is used if light averaging options 2 or 4 are specified for the simulation.

ALGY - Card 10, contains the light-nutrient option for computing the algae growth rate (columns 33-39), and the algal preference factor for ammonia nitrogen (columns 74-80). The light-nutrient interactions for computing algae growth rate are as follows (see also Figure A-1):

Option	Description
1	Multiplicative: $(FL) * (FN) * (FP)$
2	Limiting Nutrient: $FL * [\text{minimum}(FN, FP)]$
3	Inverse Additive: $\frac{FL * 2}{1/FN + 1/FP}$

Option 1 is the form used in QUAL-2 SEMCOG, while option 2 is used in the META Systems Version of QUAL-2. Option 3 is described by Scavia and Park (13).

The algal preference factor for ammonia (columns 74-80) defines the relative preference of algae for ammonia and nitrate nitrogen (see also Figure A-2). The user defines this preference by specifying a decimal value between 0 and 1.0, for example:

Algal Preference
factor
for Ammonia

Interpretation

0.0	Algae will use only nitrate for growth.
0.5	Algae will have equal preference for ammonia and nitrate.
1.0	Algae will use only ammonia for growth.

Nutrient Attenuation Factors

- Nitrogen: $NE = NH_3 + NO_3$ (mg-N/L)
 $FN = NE / (KN + NE)$
where: FN = Nitrogen attenuation factor
KN = Nitrogen half saturation coefficient (mg-N/L)
- Phosphorus: $FP = P_2 / (KP + P_2)$
 P_2 = Dissolved Phosphorus (mg-P/L)
where: FP = Phosphorus attenuation factor
KP = Phosphorus half saturation coefficient (mg-P/L)

Algal Preference for Ammonia

$$F = \frac{(P_N)(NH_3)}{(P_N)(NH_3) + (1-P_N)NO_3}$$

- where: P_N = Algal preference for ammonia nitrogen (0-1.0)
 $P_N = 0.0$; algae will use only nitrate for growth
 $P_N = 0.5$; algae will have equal preference for ammonia and nitrate for growth
 $P_N = 1.0$; algae will use only ammonia for growth
 F = Fraction of algal nitrogen uptake from ammonia pool.

FIGURE A-2. ALGAL GROWTH RATE

ALG/ - Card 11, contains the factor for converting the solar radiation value from the heat balance to the solar radiation value appropriate for the algae simulation (columns 33-39) and the value of the first order nitrification inhibition coefficient (columns 74-80).

The solar radiation factor specifies the fraction of the solar radiation computed in the heat balance (subroutine HEATER) that is photosynthetically active (i.e., used by algal cells for growth). It is required only in steady-state simulations when light averaging options 1 or 3 (Data Type 1A, card 8) are selected. A decimal value between 0 and 1.0 specifies the value of this fraction. Typically the value of this fraction is about 0.45 (14).

The first order nitrification inhibition coefficient is the value of KNITRF in the following equation (see Figure A-3).

$$CORDO = 1.0 - \text{EXP} (-\text{KNITRF} * DO)$$

where:

DO = dissolved oxygen concentration (mg/L), and
CORDO = correction factor applied to ammonia and nitrite
oxidation rate coefficients.

Nitrification Rate Correction Factor (CORDO)

- $CORDO = 1.0 - \text{EXP}(-KNITRF * DO)$
- The value of KNITRF is supplied by the user, the default value in QUAL-2E is 10.0

Applied to Ammonia and Nitrite Oxidation Rates

Ammonia: $(\beta_1)_{\text{inhib.}} = (\beta_1)_{\text{input}} * (CORDO)$

Nitrite: $(\beta_2)_{\text{inhib.}} = (\beta_2)_{\text{input}} * (CORDO)$

Magnitude of Correction Factor

The following table contains values of CORDO as a function of DO (row) and KNITRF (column).

DO (mg/L)	KNITRF					
	0.5	0.7	1.0	2.0	5.0	10.0
0.1	.05	.07	.10	.18	.39	.63
0.2	.10	.13	.18	.33	.63	.86
0.3	.14	.19	.26	.45	.78	.95
0.4	.18	.24	.33	.55	.86	.98
0.5	.22	.30	.39	.63	.92	.99
0.7	.30	.39	.50	.75	.97	1.00
1.0	.39	.50	.63	.86	.99	1.00
1.5	.53	.65	.78	.95	1.00	1.00
2.0	.63	.75	.86	.98	1.00	1.00
3.0	.78	.88	.95	1.00	1.00	1.00
4.0	.86	.94	.98	1.00	1.00	1.00
5.0	.92	.97	.99	1.00	1.00	1.00
7.0	.97	.99	1.00	1.00	1.00	1.00
10.0	.99	1.00	1.00	1.00	1.00	1.00

* KNITRF = 0.6, closely matches the nitrification inhibition function in QUAL-2 Texas (4).

* KNITRF = 0.7, closely matches the nitrification inhibition data of the Thames Estuary (12).

FIGURE A-3. NITRIFICATION INHIBITION AT LOW DO

A value of 0.6 for KNITRF closely matches the inhibition formulation in QUAL-2 Texas, while a value of 0.7 closely matches the data for the Thames Estuary (12). The default value of KNITRF is 10.0, i.e., no inhibition of nitrification at low dissolved oxygen. A table of CORDO values as a function of KNITRF and DO is given in Figure A-3.

ENDA - The last card in Data Type 1A must be an ENDATA1A card, regardless of whether algae, nitrogen, or phosphorus are simulated.

D. Data Type 1B - Temperature Correction Factors

Several of the processes represented in QUAL2E are affected by temperature. The user may elect to input specific temperature correction factors. In the absence of such information, default values are used as noted in Figure A-4. The user need supply only those values that are to be changed.

Data Type 1B information is supplied as follows:

Alphanumeric code for each temperature coefficient as noted in <u>Figure A-4</u> :	Columns 10-17
User specific temperature coefficient	Columns 19-26

The last card in Data Type 1B must be an ENDATA1B card, regardless of whether any of the default values are modified.

E. Data Type 2 - Reach Identification and River Mile/Kilometer Data

The cards of this group identify the stream reach system by name and river mile/kilometer by listing the stream reaches from the most upstream point in the system to the most downstream point. When a junction is reached, the order is continued from the upstream point of the tributary. There is one card per reach. The following information is on each card:

Reach Order or Number	Columns 16-20
Reach Identification or Name	Columns 26-40
River Mile/Kilometer at Head of Reach	Columns 51-60
River Mile/Kilometer at End of Reach	Columns 71-80

INDEX	RATE COEFFICIENT	DEFAULT VALUES		CODE
		SEPCOG	QUAL-2E	
1	BOD Decay	1.047	1.047	BOD DECA
2	BOD Settling	-	1.024	BOD SETT
3	Reaeration	1.0159	1.024	OXY TRAN
4	SOD Uptake	-	1.060	SOD RATE
5	Organic N Decay	-	1.047	ORGN DEC
6	Organic N Settling	-	1.024	ORGN SET
7	Ammonia Decay	1.047	1.083	NH3 DECA
8	Ammonia Source	-	1.074	NH3 SRCE
9	Nitrite Decay	1.047	1.047	NO2 DECA
10	Organic P Decay	-	1.047	PORG DEC
11	Organic P Settling	-	1.024	PORG SET
12	Dissolved P Source	-	1.074	DISP SRC
13	Algae Growth	1.047	1.047	ALG GROW
14	Algae Respiration	1.047	1.047	ALG RESP
15	Algae Settling	-	1.024	ALG SETT
16	Coliform Decay	1.047	1.047	COLI DEC
17	Non-cons Decay	1.047	1.000	ANC DECA
18	Non-cons Settling	-	1.024	ANC SETT
19	Non-cons Source	-	1.000	ANC SRCE

FIGURE A-4. DEFAULT THETA VALUES FOR QUAL2E

A very useful feature of QUAL2E pertaining to modifications of reach identification once the system has been coded is that existing reaches may be subdivided (or new reaches added) without renumbering the reaches for the whole system. If, for example, it is desired to divide the river reach originally designated as REACH 3 into two reaches, the division is made by calling the upstream portion REACH 3 and the "new reach" downstream REACH 3.1. Up to nine such divisions can be made per reach (3.1-3.9); thus REACH 3 (or any other reach) can be divided into as many as 10 reaches numbered 3, 3.1-3.9. This option of dividing a reach is useful particularly when new field data indicate a previously unknown or a change in geomorphology, or when the addition of a new or proposed load alters the biochemistry in the downstream portion of the reach. If this option is invoked, the number of reaches specified in Data Type 1 must be changed to the new total number of reaches.

Note: It is important to realize that this option cannot be used to subdivide a reach into more (and thus smaller)

computational elements, in an attempt to provide greater detail to the simulation. All computational elements must have the same length (as specified in Type 1 Data).

This option also will allow the user to add a new reach to the system; for example, taking a tributary that was initially modeled as a point source and changing it to a modeled reach (or reaches) in the basin. This type of modification adds a junction to the system and thus the junction information in Data Types 1, 4, and 9 must be modified accordingly.

This group of cards must end with ENDATA2.

F. Data Type 3 - Flow Augmentation Data

These cards, except ENDATA 3, are required only if flow augmentation is to be used. The cards in this group contain data associated with determining flow augmentation requirements and available sources of flow augmentation. There must be as many cards in this group as in the reach identification group. The following information is on each card.

Reach Order or Number	Columns 26-30
Augmentation Sources (the number of headwater sources which are available for flow augmentation)	Columns 36-40
Target Level (minimum allowable dissolved oxygen concentration (mg/L) in this reach)	Columns 41-50
Order of Sources (order of available headwaters, starting at most upstream points)	Columns 51-80

This card group must end with ENDATA3, even if no flow augmentation is desired.

G. Data Type 4 - Computational Elements Flag Field Data

This group of cards identifies each type of computational element in each reach. These data allow the proper form of the routing equations to be used by the program. There are seven element types allowed, they are listed below.

<u>IFLAG</u>	<u>Type</u>
1	Headwater source element.
2	Standard element, incremental inflow/ outflow only.
3	Element on mainstream immediately upstream of a junction.
4	Junction element.
5	Most downstream element.
6	Input (point source) element.
7	Withdrawal element.

Each card in this group (one for each reach), contains the following information:

Reach Order or Number	Columns 16-20
Number of Elements in the Reach	Columns 26-30
Element Type (these are numbers of a set, identifying each element by type).	Columns 41-80

Remember that once a system has been coded, reaches can be divided or new ones added without necessitating the renumbering of the entire system (see Data Type 2 - Reach Identification and River Mile/Kilometer Data for application and constraints). When this option is invoked, the element types and number of elements per reach for the affected reaches must be adjusted in Data Type 4 to reflect the changes.

This card group must end with ENDATA4.

H. Data Type 5 - Hydraulics Data

Two options are available to describe the hydraulic characteristics of the system. The first option utilizes a functional representation while the second option utilizes a geometric representation. The option desired is specified in Data Type 1, card 5. The code "TRAPEZOIDAL" specifically denotes the geometric representation. Any other code, such as "NO TRAPEZOIDAL", or "DISCHARGE COEFFICIENTS", specifies the functional representation.

Note: With either option, the effect is global (for the entire system). This option is not reach variable.

If the first option is selected, velocity is calculated as $V = aQ^b$ and depth is found by $D = \alpha Q^\beta$. Each card represents one reach and contains the values of a, b, α , and β , as described below.

Reach Order or Number	Columns 16-20
Dispersion Constant	Columns 23-30
a, coefficient for velocity	Columns 31-40
b, exponent for velocity	Columns 41-50
α , coefficient for depth	Columns 51-60
β , exponent for depth	Columns 61-70
Mannings "n" for reach (if not specified, the program default value is 0.02)	Columns 71-80

The dispersion constant is the value of K in the general expression relating the longitudinal dispersion coefficient to the depth of flow and shear velocity (10).

$$D_L = Kdu^*$$

where:

D_L = longitudinal dispersion coefficient,
(ft²/day, m²/day)

K = dispersion constant, dimensionless

d = mean depth of flow, (ft,m)

u^* = shear velocity, (ft/sec, m/sec) = $(gdS)^{1/2}$

g = gravitational constant (ft/sec², m/sec²)

S = slope of the energy grade line (ft/ft, m/m)

Substitution of the Manning equation for S, leads to the following expression for the longitudinal dispersion coefficient, D_L .

$$D_L = 3.82 \text{ KnVd}^{5/6}$$

where:

n = Mannings roughness coefficient, and

V = Mean stream velocity (ft/sec, m/sec).

Typical values of K range from 6 to 6000. A value of 5.93 leads to the Elder equation for longitudinal dispersion, which is the one used in the SEMCOG version of QUAL-2.

The coefficients a, b, α , and β should be expressed to relate velocity, depth and discharge units as follows:

<u>System</u>	<u>Q</u>	<u>V</u>	<u>D</u>
Metric	m ³ /sec	m/sec	m
English	ft ³ /sec	ft/sec	ft

If the second option is selected, each reach is represented as a trapezoidal channel. This data form is also used to specify the trapezoidal cross-section (bottom width and side slope), the channel slope and the Manning's "n" corresponding to the reach. The program computes the velocity and depth from this data using Manning's Equation and the Newton-Raphson (iteration) method. One card must be prepared for each reach as follows:

Reach Order or Number	Columns 16-20
Dispersion Constant, K	Columns 23-30
Side Slope 1 (run/rise; ft/ft, m/m)	Columns 31-40
Side Slope 2 (run/rise; ft/ft, m/m)	Columns 41-50
Bottom Width of Channel, (feet, meters)	Columns 51-60
Channel Slope (ft/ft, m/m)	Columns 61-70
Mannings "n" (Default = 0.020)	Columns 71-80

This group of data must end with an ENDATA5 card.

I. Data Type 6 - BOD and DO Reaction Rate Constants Data

This group of cards includes reach information on the BOD decay rate coefficient and settling rate, sediment oxygen demand, as well as the method of computing the reaeration coefficient. Eight options for reaeration coefficient calculation are available. These are listed below.

<u>K2 OPT</u>	<u>Method (9)</u>
1	Read in values of K2.
2	Churchill.
3	O'Connor and Dobbins.
4	Owens and Gibbs.
5	Thackston and Krenkel.
6	Langbien and Durum.
7	Use equation $K2 = aQ^b$
8	Tsivoglou-Wallace.

One card is necessary for each reach, and contains the following information:

Reach Order or Number	Columns 16-20
BOD Decay Rate Coefficient (1/day)	Columns 21-28
BOD Removal Rate by Settling (1/day)	Columns 29-36
Sediment Oxygen Demand (gm/ft ² -day, gm/m ² -day)	Columns 37-44
Option for K2 (1-8, as above)	Columns 45-48
K2 (Option 1 only) Reaeration Coefficient, per day, base e, 20C	Columns 49-56
a, Coefficient for K2 (Option 7) or Coefficient for Tsivoglou (Option 8)	Columns 57-64
b, Exponent for K2 (Option 7) or Slope of the Energy Gradient, S _e , (Option 8)	Columns 65-72

The units of a and b vary depending on whether option 7 or 8 is used and on whether the input data are in English or Metric units, as follows:

<u>Units of a:</u>	<u>English</u>	<u>Metric</u>
Option 7 (Coefficient)	Consistent with flow in cfs	Consistent with flow in cms
Option 8 (Coefficient)	1/ft	1/m
<u>Units of b:</u>	<u>English</u>	<u>Metric</u>
Option 7 (Exponent)	Consistent with flow in cfs	Consistent with flow in cms
Option 8 (S_e)	Dimensionless	Dimensionless

For option 8 (Tsivoglou's option), the energy gradient, S_e need not be specified if a Manning "n" value was assigned under Hydraulic Data Type 5. S_e will be calculated from Manning's Equation using the wide channel approximation for hydraulic radius.

This group of cards must end with ENDATA6.

J. Data Type 6A - N and P Coefficients

This group of cards is required if algae, the nitrogen series (organic nitrogen, ammonia, nitrite, and nitrate), or the phosphorus series (organic and dissolved) are to be simulated. Otherwise, they may be omitted. Each card of this group, one for each reach, contains the following information:

Reach Order or Number	Columns 20-24
Rate Coefficient for Organic-N Hydrolysis (1/day)	Columns 25-31
Rate Coefficient for Organic-N Settling (1/day)	Columns 32-38
Rate Coefficient for Ammonia Oxidation (1/day)	Columns 39-45
Benthos Source Rate for Ammonia (mg/ft ² -day, mg/m ² -day)	Columns 46-52

Rate Coefficient for Nitrite Oxidation (1/day)	Columns 53-59
Rate Coefficient for Organic Phosphorus Decay (1/day)	Columns 60-66
Rate Coefficient for Organic Phosphorus Settling (1/day)	Columns 67-73
Benthos Source Rate for Dissolved Phosphorus (mg/ft ² -day, mg/m ² -day)	Columns 74-80

Note that the benthos source rates are expressed per unit of bottom area. Other versions of QUAL-2 use values per length of stream. To convert to the areal rate, divide the length value by the appropriate stream width.

This group of cards must end with ENDATA6A, even if algae, nitrogen, or phosphorus are not simulated.

K. Data Type 6B - Algae/Other Coefficients

This group of cards is required if algae, the nitrogen series, the phosphorus series, coliform, or the arbitrary non-conservative is to be simulated. Otherwise, they may be deleted. Each card of the group, one per reach, contains the following information:

Reach Order or Number	Columns 20-24
Chlorophyll <u>a</u> to Algae Ratio (ug chl _a /mg algae)	Columns 25-31
Algal Settling Rate (ft/day, m/day)	Columns 32-38
Non-Algal Light Extinction Coefficient (1/ft, 1/m)	Columns 39-45
Coliform Decay Coefficient (1/day)	Columns 46-52
Arbitrary Non-Conservative Decay Coefficient (1/day)	Columns 53-59
Arbitrary Non-Conservative Settling Coefficient (1/day)	Columns 60-66
Benthos Source Rate for Arbitrary Non-Conservative (mg/ft ² -day, mg/m ² -day)	Columns 67-73

This group of cards must end with ENDATA6B, even if algae, nitrogen, phosphorus, coliform, or the arbitrary non-conservative are not simulated.

L. Data Type 7 - Initial Conditions - 1

This card group, one card per reach, establishes the initial conditions of the system, with respect to temperature, dissolved oxygen concentration, BOD concentrations, and conservative minerals. Initial conditions for temperature must always be specified whether it is simulated or not. The reasons for this requirement are: (a) when temperature is not simulated, the initial condition values are used to set the value of the temperature dependent rate constants; (b) for dynamic simulations the initial condition for temperature, and every other quality constituent to be simulated, defines the state of the system at time zero; and (c) for steady state simulations of temperature, an initial estimate of the temperature between freezing and boiling is required to properly initiate the heat balance computations. Specifying 68°F or 20°C for all reaches is a sufficient initial condition for the steady state temperature simulation case. The information contained is as follows:

Reach Order or Number	Columns 20-24
Temperature (F or C)	Columns 25-31
Dissolved Oxygen (mg/L)	Columns 32-38
BOD (mg/L)	Columns 39-45
Conservative Mineral I*	Columns 46-52
Conservative Mineral II*	Columns 53-59
Conservative Mineral III*	Columns 60-66
Arbitrary Non-Conservative*	Columns 67-73
Coliform (No./100 ml)	Columns 74-80

* - Units are those specified on the Title Card.

This group of cards must end with ENDATA7.

M. Data Type 7A - Initial Conditions - 2

This group of cards is required if algae, the nitrogen series, or the phosphorus series are to be simulated. The information is coded as follows:

Reach Order or Number	Columns 20-24
Chlorophyll <u>a</u> (ug/L)	Columns 25-31
Organic Nitrogen as N (mg/L)	Columns 32-38
Ammonia as N (mg/L)	Columns 39-45
Nitrite as N (mg/L)	Columns 46-52
Nitrate as N (mg/L)	Columns 53-59
Organic Phosphorus as P (mg/L)	Columns 60-66
Dissolved Phosphorus as P (mg/L)	Columns 67-73

This group of cards must end with ENDATA7A, even if algae, nitrogen, or phosphorus are not simulated.

N. Data Type 8 - Incremental Inflow - 1

This group of cards, one per reach, accounts for the additional flows into the system not represented by point source inflows or headwaters. These inflows, which are assumed to be uniformly distributed over the reach, are basically groundwater inflows and/or distributed surface runoff that can be assumed to be approximately constant through time.

An important new feature to QUAL2E is that incremental outflow along a reach may be modeled. This option is useful when field data show a decreasing flow rate in the downstream direction indicating a surface flow contribution to groundwater.

Each card, one for each reach, contains the following information:

Reach Order or Number	Columns 20-24
Incremental Inflow (cfs, m ³ /sec) outflows are indicated with a minus "-" sign.	Columns 25-31
Temperature (F, C)	Columns 32-38

Dissolved Oxygen (mg/L)	Columns 39-44
BOD (mg/L)	Columns 45-50
Conservative Mineral I	Columns 51-56
Conservative Mineral II	Columns 57-62
Conservative Mineral III	Columns 63-68
Arbitrary Non-Conservative	Columns 69-74
Coliform (No./100 ml)	Columns 75-80

This group of cards must end with ENDATA8.

O. Data Type 8A - Incremental Inflow - 2

This group of cards is a continuation of Data Type 8, and is required only if algae, the nitrogen series or the phosphorus series are to be simulated. Each card, one per reach, contains the following information:

Reach Order or Number	Columns 20-24
Chlorophyll <u>a</u> Concentration (ug/L)	Columns 25-31
Organic Nitrogen as N (mg/L)	Columns 32-38
Ammonia as N (mg/L)	Columns 39-45
Nitrite as N (mg/L)	Columns 46-52
Nitrate as N (mg/L)	Columns 53-59
Organic Phosphorus as P (mg/L)	Columns 60-66
Dissolved Phosphorus as P (mg/L)	Columns 67-73

This group of cards must end with ENDATA8A, even if algae, nitrogen, or phosphorus are not simulated.

P. Data Type 9 - Stream Junction Data

This group of cards is required if there are junctions or confluences in the stream being simulated. Otherwise, they may be omitted. The junctions are ordered starting with the most upstream junction. For systems containing a junction(s) on a tributary, the junctions must be ordered in the manner

indicated in Figure A-5; that is, the junctions must be ordered so that the element numbers just downstream of the junction are specified in ascending order. In Figure A-5, the downstream element numbers for Junction 1, 2 and 3 are 29, 56, and 64, respectively. There is one card per junction, and the following information is on each card:

Junction Order or Number Columns 21-25

Junction Names or Identification Columns 35-50

Order Number of the Last Element in the reach immediately upstream of the junction (see Figure A-5). In the example, for Junction 1, the order number of the last element immediately upstream of the junction is number 17. For Junction 2, it is number 49. For Junction 3, it is number 43. Columns 56-60

Order Number of the First Element in the reach immediately downstream from the junction. It is these numbers that must be arranged in ascending order. Thus, for Figure A-5 these order numbers are as follows: Columns 66-70

<u>Junction</u>	<u>Downstream Element No.</u>
1	29
2	56
3	64

Order Number of the Last Element in the last reach of the tributary entering the junction. For Figure A-5 these order numbers for Junctions 1, 2, and 3 are 28, 55, and 63, respectively. Columns 76-80

This group of cards must end with ENDDATA9, even if there are no junctions in the system.

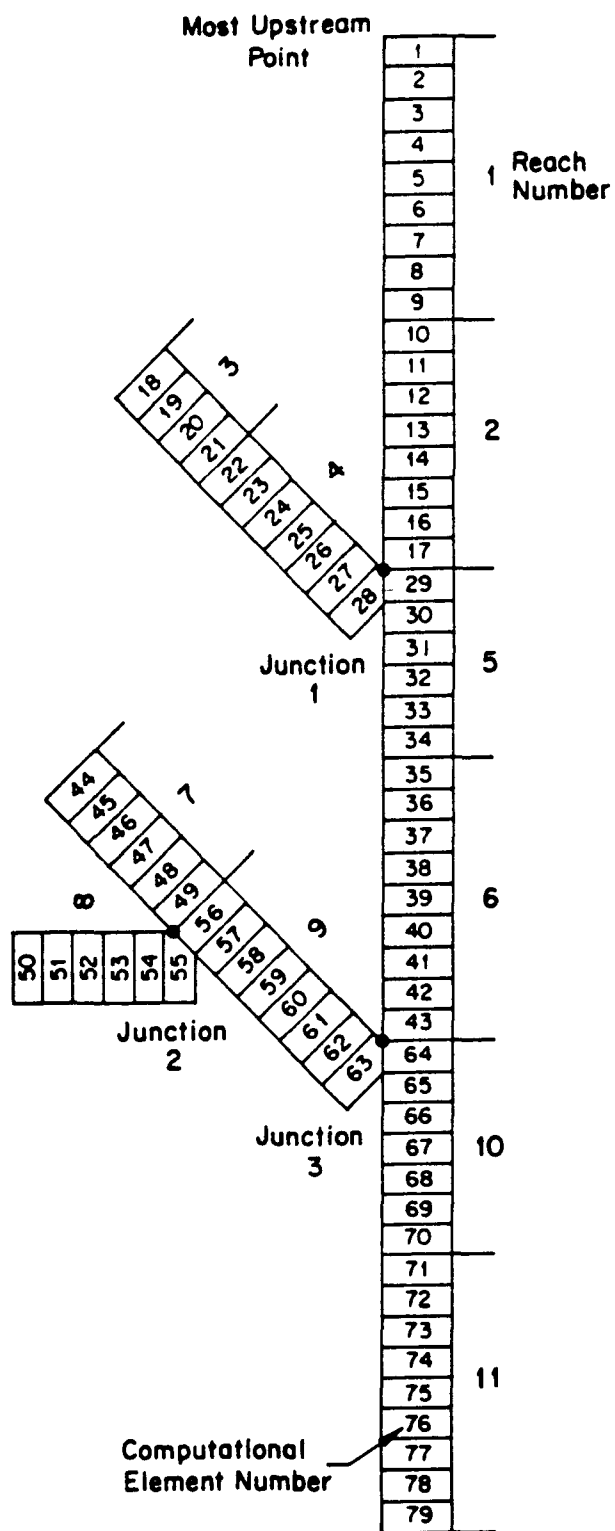


FIGURE A-5. STREAM NETWORK EXAMPLE TO ILLUSTRATE DATA INPUT

Q. Data Type 10 - Headwater Sources Data - 1

This group of cards, one per headwater, defines the flow, temperature, dissolved oxygen, BOD, conservative mineral, algae, nutrient, coliform, and arbitrary nonconservative concentrations of the headwater. The following information is on each card:

Headwater Order or number Starting at Most Upstream Point	Columns 15-19
Headwater Name or Identification	Columns 20-35
Flow (cfs, m ³ /sec)	Columns 36-44
Temperature (F, C)	Columns 45-50
Dissolved Oxygen Concentration (mg/L)	Columns 51-56
BOD Concentration (mg/L)	Columns 57-62
Conservative Mineral I	Columns 63-68
Conservative Mineral II	Columns 69-74
Conservative Mineral III	Columns 75-80

This group of cards must end with ENDATA10.

R. Data Type 10A - Headwater Sources Data - 2

This group of cards supplements the information in Data Type 10, and is required if algae, the nitrogen series, the phosphorus series, coliform, or arbitrary non-conservative are to be simulated. Each card, one per headwater, contains the following data:

Headwater Order or Number	Columns 16-20
Arbitrary Non-Conservative	Columns 21-26
Coliform, (No./100 ml)	Columns 27-32
Chlorophyll <u>a</u> (ug/L)	Columns 33-38
Organic Nitrogen as N (mg/L)	Columns 39-44
Ammonia as N (mg/L)	Columns 45-50
Nitrite as N (mg/L)	Columns 51-56

Nitrate as N (mg/L)	Columns 57-62
Organic Phosphorus as P (mg/L)	Columns 63-68
Dissolved Phosphorus as P (mg/L)	Columns 69-74

This group of cards must end with ENDATA10A, even if algae, nitrogen, phosphorus, coliform, or arbitrary non-conservative are not simulated.

S. Data Type 11 - Point Load - 1

This group of cards is used to define point source inputs and point withdrawals from the stream system. Point sources include both wasteloads and unsimulated tributary inflows. One card is required per inflow or withdrawal. Each card describes the percent of treatment (for wastewater treatment), inflow or withdrawal, temperature, and dissolved oxygen, BOD, and conservative mineral concentrations. They must be ordered starting at the most upstream point. The following information is on each card:

Point Load Order or Number	Columns 15-19
Point Load Identification or Name	Columns 20-31
Percent Treatment (use only if influent BOD values are used)	Columns 32-36
Point Load Inflow or Withdrawal (cfs, m ³ /sec) (a withdrawal must have a minus ("-") sign)	Columns 37-44
Temperature (F, C)	Columns 45-50
Dissolved Oxygen Concentration (mg/L)	Columns 51-56
BOD Concentration (mg/L)	Columns 57-62
Conservative Mineral I	Columns 63-68
Conservative Mineral II	Columns 69-74
Conservative Mineral III	Columns 75-80

This group of cards must end with ENDATA11.

T. Data Type 11A - Point Load - 2

This group of cards supplements Data Type 11 and contains the algal, nutrient, coliform and arbitrary non-conservative concentrations of the point source loads. This information is necessary only if algae, the nitrogen series, the phosphorus series, coliform, or the arbitrary non-conservative are to be simulated. Each card, one per waste load (withdrawal) contains the following information:

Point Load Order or Number	Columns 16-20
Arbitrary Non-Conservative	Columns 21-26
Coliform (No./100 ml)	Columns 27-32
Chlorophyll <u>a</u> (ug/L)	Columns 33-38
Organic Nitrate as N (mg/L)	Columns 39-44
Ammonia as N (mg/L)	Columns 45-50
Nitrite as N (mg/L)	Columns 51-56
Nitrate as N (mg/L)	Columns 57-62
Organic Phosphorus as P (mg/L)	Columns 63-68
Dissolved Phosphorus as P (mg/L)	Columns 69-74

This group of cards must end with ENDATA11A, even if algae, nitrogen, phosphorus, coliform, or arbitrary non-conservative are not simulated.

U. Data Type 12 - Dam Reaeration

This group of cards is required if oxygen input from reaeration over dams is to be modeled as a component of the dissolved oxygen simulation. Dam reaeration effects are estimated from the empirical equation attributed to Gameson (9). The following inputs are required:

Dam Order or Number	Columns 20-24
Reach Number of Dam	Columns 25-30
Element Number Below Dam	Columns 31-36

ADAM Coefficient:	Columns 37-42
ADAM = 1.25 for clear to slightly polluted waters	
ADAM = 1.00 for polluted water	
BDAM Coefficient:	Columns 43-48
BDAM = 1.00 for weir with free fall	
BDAM = 1.30 for step weirs or cascades	
Percent of Flow Over Dam (as a fraction 0.0-1.0)	Columns 49-54
Height of Dam (ft, m)	Columns 55-60

This group of cards must end with ENDATA12, even if oxygen input from dam reaeration is not to be modeled.

V. Data Type 13 - Downstream Boundary - 1

This data card supplies the constituent concentrations at the downstream boundary of the system. It is required only if specified in Data Type 1, card 8. This feature of QUAL2E is useful in modeling systems with large dispersion in the lower reaches (e.g., estuaries). When downstream boundary concentrations are supplied the solution generated by QUAL2E will be constrained by this boundary condition. If the concentrations are not provided, the constituent concentrations in the most downstream element will be computed in the normal fashion using the zero gradient assumption (1, 11).

Downstream boundary values for temperature, dissolved oxygen, BOD, conservative mineral, coliform, and arbitrary non-conservative are required as follows:

Temperature (F, C)	Columns 25-31
Dissolved Oxygen (mg/L)	Columns 32-38
BOD Concentration (mg/L)	Columns 39-45
Conservative Mineral I	Columns 46-52
Conservative Mineral II	Columns 53-59
Conservative Mineral III	Columns 60-66

Arbitrary Non-Conservative

Columns 67-73

Coliform (No./100 ml)

Columns 74-80

This data group must end with an ENDATA13 card, even if the fixed downstream boundary concentration option is not used in the simulation.

W. Data Type 13A - Downstream Boundary - 2

This group of data (one card) is a continuation of Data Type 13. It is required only if the fixed downstream boundary condition is used and if algae, the nitrogen series, the phosphorus series are to be simulated. This card contains the downstream boundary concentrations for algae, nitrogen, and phosphorus as follows:

Chlorophyll a (ug/L)

Columns 25-31

Organic Nitrogen as N (mg/L)

Columns 32-38

Ammonia as N (mg/L)

Columns 39-45

Nitrite as N (mg/L)

Columns 46-52

Nitrate as N (mg/L)

Columns 53-59

Organic Phosphorus as P (mg/L)

Columns 60-66

Dissolved Phosphorus as P (mg/L)

Columns 67-73

This data group must end with an ENDATA13A card, even if the fixed downstream boundary condition is not used, and if algae, nitrogen, or phosphorus are not simulated.

X. Climatological Data

Climatological data are required for the following cases:

1. Temperature simulations, both steady-state and dynamic,
2. Dynamic simulations where algae is being simulated, and temperature is not.

If neither temperature nor dynamic algae are being simulated, these cards may be omitted.

For steady-state temperature simulation, only one card is required which gives average values of the climatological data. For dynamic simulation, each card represents readings at three hour intervals, chronologically ordered. There must be a sufficient number of cards to cover the time period specified for the simulation (Data Type 1, card 13, maximum route time). The following information is on each card.

Month	Columns 18-19
Day	Columns 21-22
Year (last two digits)	Columns 24-25
Hour of Day	Columns 26-30
Net Solar Radiation* (BTU/ft ² -hr, Langleys/hour)	Columns 31-40
Cloudiness**, fraction in tenths of cloud cover	Columns 41-48
Dry Bulb Temperature** (F, C)	Columns 49-56
Wet Bulb Temperature** (F, C)	Columns 57-64
Barometric pressure (inches Hg, millibars)	Columns 65-72
Wind speed** (ft/sec, m/sec)	Columns 73-80

* Required only if dynamic algae is simulated and temperature is not.

** Required if temperature is simulated.

There is no end card for the climatological data.

Y. Plot Reach Data

This data type is required if the plotting option for DO/BOD is selected (Data Type 1, card 7, PLOT DO/BOD). The following information is required for QUAL2E to produce a line printer plot.

1. Card 1 - BEGIN RCH
Reach number at which plot
is to begin Columns 11-15
2. Card 2 - PLOT RCH
 - a. Reach numbers in their
input order (1, 2, 3..NREACH) Columns 11-15
Columns 16-20
21-26
etc.
76-80
 - b. If a reach is not to be
plotted, (i.e., a tributary)
replace the reach number
with a zero.
 - c. Use additional PLOT RCH cards
if there are more than 14
reaches in the system.
3. Additional plots can be obtained by repeating the
sequence of BEGIN RCH and PLOT RCH cards.

As an example of the plotting option, suppose that for the river system shown in Figure A-5, one wishes to obtain two DO/BOD plots: one for the main stream (Reaches 1, 2, 5, 6, 10, and 11) and one for the second tributary (Reaches 7 and 9). The plot data would appear in the following order.

```
BEGIN RCH 1
PLOT RCH 1 2 0 0 5 6 0 0 0 10 11
BEGIN RCH 7
PLOT RCH 0 0 0 0 0 0 7 0 9 0 0
```

No ENDATA card is required for the PLOT information.

Z. Summary

Constructing a consistent and correct input data set for a QUAL2E simulation must be done with care. This user's guide is designed to assist the user in this process. It has been NCASI's and EPA's experience that two of the most frequently made errors in constructing a QUAL2E input data set are:

- (a) Using a numerical value that is inconsistent with the units option selected, and
- (b) Not adhering to the 4 character input codes for Data Types 1 and 1A.

As an aid to the units problem, Table A-1 is included in this report. It provides a complete summary of all the input variables whose dimensions are dependent on whether English or metric units are selected. Finally, the user is encouraged to check and recheck the input codes in Data Types 1 and 1A for accuracy, especially the codes for cards 10 and 11 of Data Type 1 (i.e., "NUMB" and "NUM_").

REFERENCES - APPENDIX A

1. "A Review of the Mathematical Water Quality Model QUAL-2 and Guidance for its Use", NCASI Technical Bulletin No. 338, October 1980 (Revised No. 391, December, 1982).
2. "Computer Program Documentation for the Stream Quality Model QUAL-2", prepared for Southeast Michigan Council of Governments (SEMCOG), Detroit, Michigan (July, 1977).
3. "Users Manual for the Stream Quality Model QUAL-2", prepared for Southeast Michigan Council of Governments (SEMCOG), Detroit, Michigan (July, 1977).
4. "QUAL-TX User's Manual (Draft)", Texas Water Development Board, Austin, Texas (June, 1981).
5. "Calibration and Application of QUAL-2 to the Lower Win-ooski River: Preliminary Studies", prepared for state of Vermont by Meta Systems, Inc. (July, 1979).
6. Norton, W.R., et al, "Computer Program Documentation for the Stream Quality Model-QUAL-2", for EPA Contract 68-01-1869 (August, 1974).
7. Patterson, D., et al, "Water Pollution Investigation Lower Green Bay and Lower Fox River", Wisconsin DNR, (EPA 68-01-1572), (June, 1975).
8. "A Study of the Selection, Calibration, and Verification of Mathematical Water Quality Models", NCASI Technical Bulletin No. 367, (March 1982).
9. "Rates, Constants, and Kinetic Formulations in Surface Water Quality Modeling", USEPA, Athens, Georgia, NTIS PB-290938 (March, 1978).
10. Fisher, H.B., E.J. List, R.C.Y. Koh, J. Imberger, N.H. Brooks, Mixing in Inland and Coastal Waters, Academic Press, 1979.

TABLE A-1. LIST OF QUAL2E INPUT VARIABLES THAT ARE
ENGLISH/METRIC UNIT DEPENDENT

DATA TYPE	CARD OR LINE	VARIABLE DESCRIPTION	FORTRAN CODE NAME	UNITS	
				ENGLISH	METRIC
1	8	Input Units Specification	METRIC	0	1
	8	Output Units Specification	METOUT	0	1
1	11	Length of Computational Element	DELX	mile	kilometer
1	15	Evaporation Coefficient	AE	ft/hr-in Hq	m/hr-mbar
	15	Evaporation Coefficient	BE	ft/hr-in Hg-mph	m/hr-mbar-m/sec
1	16	Basin Elevation	ELEV	ft	meters
1A	6	Linear Algal Extinction Coeff.	EXALG1	1/ft-ug chla/L	1/m-ug chla/L
	6	Non-linear Algal Extinction Coefficient	EXALG2	1/ft-(ug chla/L ^{2/3})	1/m-(ug chla/L ^{2/3})
1A	7	Light Saturation Coefficient	CKL	BTU/ft ²	langley/min
1A	9	Total Daily Solar Radiation	SONET	BTU/ft ²	langleys
2	all	River Mile/km to Head of Reach	RMTHOR	mile	kilometer
	all	River Mile/km to End of Reach	RMTEOR	mile	kilometer
5	all	Coefficient Flow for Velocity	COEFQV	Consistent with flow, velocity and depth in cfs, fps, ft respectively	Consistent with flow, velocity, and depth in cms, mps, m respectively
(Discharge Coefficient)		Exponent Flow for Velocity	EXPOQV		
		Coefficient on Flow for Depth	COEFQH		
		Exponent on Flow for Depth	EXPOQH		
5	all	Bottom Width of Channel	WIDTH	ft	meters
(Trapezoidal)					
6	all	SOD Rate	CK4	gm/ft ² -day	gm/m ² -day
6	all	Option 7 for k ₂	COEQK2	Consistent with flow in cfs	Consistent with flow in cms
		Coefficient on flow for k ₂	EXPQK2		
		Exponent on flow for k ₂			
6	all	Option 8 for K ₂	COEQK2	1/ft	1/meter
		Coefficient for Tsivoglou Eq.	EXPQK2		
		Slope of Energy Gradient		ft/ft	meter/meter
6A	all	Benthic Source Rate for Ammonia-N	SNH3	mg/ft ² -day	mg/m ² -day
		Benthic Source Rate for Phosphorus	SPHOS	mg/ft ² -day	mg/m ² -day
6B	all	Algal Settling Rate	ALGSET	ft/day	m/day
		Non-algal Extinction Coefficient	EXCOEF	1/day	1/meter
		Arbitrary Nonconservative			
		Benthic Source Rate	SRANC	mg/ft ² -day	mg/m ² -day
7	all	Initial Condition-Temperature	TINIT	F	C
8	all	Incremental Inflow			
		Flow Rate	QI	cfs	cms
		Temperature	TI	F	C
10	all	Headwater Conditions			
		Flow Rate	HWFLOW	cfs	cms
		Temperature	HWTEMP	F	C
11	all	Point Source/Withdrawal			
		Flow Rate	WSFLOW	cfs	cms
		Temperature	WFTEMP	F	C
12	all	Height of Dam	HDAM	ft	meters
13	1	Downstream Boundary-Temperature	LBTEMP	F	C
LCD	all	Solar Radiation	SOLHR	BTU/ft ² -hr	langleys/hr
		Dry Bulb Temperature	DRYBLB	F	C
		Wet Bulb Temperature	WETBLB	F	C
		Barometric Pressure	ATMPR	in Hg	mbar
		Wind Speed	WIND	ft/sec	m/sec

11. Arden, B.W. and K.N. Astill, Numerical Algorithms: Origins and Applications, Addison-Wesley, 1970.
12. Department of Scientific and Industrial Research, Effects of Polluting Discharge on the Thames Estuary, Water Pollution Research Technical Paper No. 11, Her Majesty's Stationery Office, London, 1964.
13. Scavia, D. and R.A. Park, "Documentation at Selected Constructs and Parameter Values in the Aquatic Model CLEANER", Ecological Modelling, Vol. 2, pp. 33-58, 1976.
14. Bannister, T.T., "Production Equations in Terms of Chlorophyll Concentration, Quantum Yield, and Upper Limit to Production", Limnology and Oceanography, Vol. 19, No. 1, pp. 1-12 (Jan., 1974).

APPENDIX B. EXAMPLE INPUT/OUTPUT DATA SETS

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

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TITLE DATA

CARD TYPE										SIMULATE YES/NO										ALPHANUMERIC NAME																				PARAMETER NAME										UNITS																													
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
TITLE01																				TITLE OF RUN																																																											
TITLE02																				NAME OF BASIN																																																											
TITLE03																				CONSERVATIVE MINERAL																																																											
TITLE04																				CONSERVATIVE MINERAL																																																											
TITLE05																				CONSERVATIVE MINERAL																																																											
TITLE06																				TEMPERATURE																																																											
TITLE07																				BIOCHEMICAL OXYGEN DEMAND																																																											
TITLE08																				ALGAE AS CHL-A IN UG/L																																																											
TITLE09																				PHOSPHORUS CYCLE AS P IN MG/L																																																											
TITLE10																				(ORGANIC-P) DISSOLVED-P																																																											
TITLE11																				NITROGEN CYCLE AS N IN MG/L																																																											
TITLE12																				(ORGANIC-N) AMMONIA-N; NITRITE-N																																																											
TITLE13																				DISSOLVED OXYGEN IN MG/L																																																											
TITLE14																				FECAL COLIFORMS IN NO./100 ML																																																											
TITLE15																				ARBITRARY NON-CONSERVATIVE																																																											
ENDTITLE																																																																															

FORMAT (20 A4)

NOTE: The nitrogen cycle variables and the phosphorus cycle variables must each be stimulated as a group.

DATA TYPE I	PROGRAM CONTROL DATA
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
16	16
17	17
18	18
19	19
20	20
21	21
22	22
23	23
24	24
25	25
26	26
27	27
28	28
29	29
30	30
31	31
32	32
33	33
34	34
35	35
36	36
37	37
38	38
39	39
40	40
41	41
42	42
43	43
44	44
45	45
46	46
47	47
48	48
49	49
50	50
51	51
52	52
53	53
54	54
55	55
56	56
57	57
58	58
59	59
60	60
61	61
62	62
63	63
64	64
65	65
66	66
67	67
68	68
69	69
70	70
71	71
72	72
73	73
74	74
75	75
76	76
77	77
78	78
79	79
80	80
81	81
82	82
83	83
84	84
85	85
86	86
87	87
88	88
89	89
90	90
91	91
92	92
93	93
94	94
95	95
96	96
97	97
98	98
99	99
100	100

[illegible]

FORMAT (6A4, A1, F10.0, 10X, 6A4, A1, F10.0)

* These lines may be omitted if temperature is not simulated.

<u>PARAMETER</u>	<u>ENGLISH UNITS</u>	<u>METRIC UNITS</u>
Length of Computational Element	miles	kilometers
Evaporation Coef. AE	(ft/hr) / (in-Hg)	(m/hr) / millibar
Evaporation Coef. BE	(ft/hr) / (in-Hg-mi/hr)	(m/hr) / (mbar-m/sec)
Elevation of Basin	feet	meters

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FORMAT (8A4, F7.0, 2X, 8A4, F7.0)

*Data Type IA information, except the ENDATAIA may be omitted unless algae, nitrogen, or phosphorus are to be simulated.

Units Notation: H = depth, INT = light intensity

PARAMETER	ENGLISH UNITS	METRIC UNITS
Linear Algae Self Shade Coef.	l/ft - ugChlo/L	l/m - ugChlo/L
Nonlinear Algae Self Shade Coef.	l/ft - (ugChlo/L) ^{2/3}	l/m - (ugChlo/L)
Light Saturation Coefficient (PAR)	Btu/ft ² - min	Langley's/min
Total Daily Solar Radiation (PAR)	Btu/ft ²	Langley's

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FORMAT (2A4, IX, 2A4, IX, F8.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

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DATA TYPE 2 REACH IDENTIFICATION DATA

DATA TYPE															REACH IDENTIFICATION										RIVER MI/KM AT HEAD OF REACH										RIVER MI/KM AT END OF REACH																																												
ORDER															ALPHANUMERIC NAME																																																																
REACH															RCH =										FROM										TO																																												
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
STREAM REACH															RCH =										FROM										TO																																												
STREAME REACH															RCH =										FROM										TO																																												
END AT A 2															RCH =										FROM										TO																																												

FORMAT (3A4,3X,F5.0,5A4,3X,A4,3X,F10.0,4X,A2,4X,F10.0)

NOTE: Once data has been coded, reaches may be subdivided without having to renumber the whole system - see text for intructions.

FORM 6 of 24

FORM 6 of 24

```
FORMAT (5A4, 5X, F5.0, 5X, F5.0, F10.0, 6F5.0)
```

123

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM 7 of 24 DATA TYPE 4 COMPUTATIONAL ELEMENT FLAG FIELD DATA

DATA TYPE																ORDER OF REACH	NO. OF COMP. ELEM.	COMPUTATIONAL ELEMENT FLAGS																																																													
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
FLAG FIELD RCH =																																																																															
FLAG FIELD RCH =																																																																															
ENDATA4																																																																															
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80

FORMAT (2A4, A2.5X, F5.0, 5X, F5.0, 10X, 20F 2.0)

NOTE: If subdivision of reaches is necessary after initial system has been coded, it can be done without renumbering the entire system - see text under REACH IDENTIFICATION AND RIVER MI/KM DATA.

FORM 8 of 24

FORM 8 of 24

FORMAT (2A4, A2, 5X, F5.0, 2X, F8.0, 5F10.0)

NOTE: The discharge coefficients must be expressed to relate flow, velocity, and depth units as follows:

VARIABLE	ENGLISH UNITS	METRIC UNITS
Flow	ft ³ /sec	m ³ /sec
Velocity	ft/sec	m/sec
Depth	ft	m

FORM 10 of 24

DATA	TYPE	6A	N	AND	P	COEFFICIENTS
------	------	----	---	-----	---	--------------

DATA TYPE																			ORDER OF REACH		ORG-N HYDROLYSIS (1/DAY)		ORG-N SETT COEF (1/DAY)		NH-3 OXIDATION (1/DAY)		BENTHAL SOURCE NH-3		NO-2 OXIDATION (1/DAY)		ORG-P DECAY (1/DAY)		ORG-P SETT COEF (1/DAY)		BENTHAL SOURCE DIS-P	
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19																		
N	A	N	D	P	C	O	E	F	R	C	H	=																								
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17																				

VARIABLE *	ENGLISH UNITS	METRIC UNITS
------------	---------------	--------------

Benthic Source for NH ₃ -N	mg/ft ² -day	mg/m ² -day
Benthic Source for DIS-P	mg/ft ² -day	mg/m ² -day

DATA TYPE 6B ALGAE/OTHER COEFFICIENTS

[illegible]

FORMAT(3A4, A2, 5X, F5.0, 7F7.0)

* VARIABLE

ENGLISH UNITS

METRIC UNITS

Algal Settling Rate

Algal Settling Rate	Non-algal Light Extinction Coef.
0.0000	0.0000
0.0001	0.0000
0.0002	0.0000
0.0003	0.0000
0.0004	0.0000
0.0005	0.0000
0.0006	0.0000
0.0007	0.0000
0.0008	0.0000
0.0009	0.0000
0.0010	0.0000
0.0011	0.0000
0.0012	0.0000
0.0013	0.0000
0.0014	0.0000
0.0015	0.0000
0.0016	0.0000
0.0017	0.0000
0.0018	0.0000
0.0019	0.0000
0.0020	0.0000
0.0021	0.0000
0.0022	0.0000
0.0023	0.0000
0.0024	0.0000
0.0025	0.0000
0.0026	0.0000
0.0027	0.0000
0.0028	0.0000
0.0029	0.0000
0.0030	0.0000
0.0031	0.0000
0.0032	0.0000
0.0033	0.0000
0.0034	0.0000
0.0035	0.0000
0.0036	0.0000
0.0037	0.0000
0.0038	0.0000
0.0039	0.0000
0.0040	0.0000
0.0041	0.0000
0.0042	0.0000
0.0043	0.0000
0.0044	0.0000
0.0045	0.0000
0.0046	0.0000
0.0047	0.0000
0.0048	0.0000
0.0049	0.0000
0.0050	0.0000
0.0051	0.0000
0.0052	0.0000
0.0053	0.0000
0.0054	0.0000
0.0055	0.0000
0.0056	0.0000
0.0057	0.0000
0.0058	0.0000
0.0059	0.0000
0.0060	0.0000
0.0061	0.0000
0.0062	0.0000
0.0063	0.0000
0.0064	0.0000
0.0065	0.0000
0.0066	0.0000
0.0067	0.0000
0.0068	0.0000
0.0069	0.0000
0.0070	0.0000
0.0071	0.0000
0.0072	0.0000
0.0073	0.0000
0.0074	0.0000
0.0075	0.0000
0.0076	0.0000
0.0077	0.0000
0.0078	0.0000
0.0079	0.0000
0.0080	0.0000
0.0081	0.0000
0.0082	0.0000
0.0083	0.0000
0.0084	0.0000
0.0085	0.0000
0.0086	0.0000
0.0087	0.0000
0.0088	0.0000
0.0089	0.0000
0.0090	0.0000
0.0091	0.0000
0.0092	0.0000
0.0093	0.0000
0.0094	0.0000
0.0095	0.0000
0.0096	0.0000
0.0097	0.0000
0.0098	0.0000
0.0099	0.0000
0.0100	0.0000
0.0101	0.0000
0.0102	0.0000
0.0103	0.0000
0.0104	0.0000
0.0105	0.0000
0.0106	0.0000
0.0107	0.0000
0.0108	0.0000
0.0109	0.0000
0.0110	0.0000
0.0111	0.0000
0.0112	0.0000
0.0113	0.0000
0.0114	0.0000
0.0115	0.0000
0.0116	0.0000
0.0117	0.0000
0.0118	0.0000
0.0119	0.0000
0.0120	0.0000
0.0121	0.0000
0.0122	0.0000
0.0123	0.0000
0.0124	0.0000
0.0125	0.0000
0.0126	0.0000
0.0127	0.0000
0.0128	0.0000
0.0129	0.0000
0.0130	0

Benthal Source for Arbitrary Non Cons.

ft/day

m/day

 $1/\pi$ mg-Anc/tt²-day

FORM 12 of 24

DATA TYPE 7 INITIAL CONDITIONS-1

[illegible]

FORMAT(3A4, A2, 5X, F5. 0, 8F7.0)

FORM 13 of 24

DATA TYPE 7A INITIAL CONDITIONS-2

DATA TYPE																			ORDER OF REACH		CHL-A (μ G/L)	ORG-N (MG/L)	NH ₃ -N (MG/L)	NO ₂ -N (MG/L)	NO ₃ -N (MG/L)	ORG-P (MG/L)	DIS-P (MG/L)	(not used)																																																			
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
INITIAL COND - 2																			RCH =																																																												
INITIAL COND - 2																			RCH =																																																												
ENDATA7A																																																																															
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
INITIAL COND - 2																			RCH =																																																												
ENDATA7A																																																																															

FORMAT (3A4, A2, 5X, F5.0, 7F7.0)

DATA TYPE 8 INCREMENTAL FLOW 1

U

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM (15) of (24)

DATA TYPE 8A INCREMENTAL FLOW - 2

DATA TYPE										ORDER OF REACH	CHL-A (µG/L)	ORG-N (MG/L)	NH3-N (MG/L)	NO2-N (MG/L)	NO3-N (MG/L)	ORG-P (MG/L)	DIS-P (MG/L)	(not used)																																																													
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
INCR INFLOW - 2										RCH =																																																																					
INCR INFLOW - 2										RCH =																																																																					
ENDATA 8A																																																																															
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80

FORMAT (3A4, A2, 5X, F5.0, 7F7.0)

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

DATA TYPE 9 STREAM JUNCTION DATA

FORM 16 of 24

DATA TYPE		ORDER OF JUNCTION	JUNCTION IDENTIFICATION	ELEMENT TYPE																																																																											
				TYPE 3 NO. OF ELEMENT UPSTRM OF JUNC	TYPE 4 NO. OF ELEMENT DNSTRM OF JUNC	TYPE 2 NO OF ELEMENT ON TRIB.																																																																									
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
STREAM JUNCTION																																																																															
ENDATA9																																																																															
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80																																																																															

FORMAT (3A4, A3, 5X, F5.0, 5X, 5A4, 3(5X, F5.0)

DATA TYPE 10 HEADWATER-1

FORM 17 of 24

[illegible]

1	2	3	4	5	6	7	8	9	10
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FORMAT (2A4, A2, 4X, F5.0, 4A4, F9.0, 6F6.0)

* VARIABLE
Headwater Flow
Temperature

METRIC UNITS
m³/sec
C

FORM 18 of 24

DATA TYPE 10A HEADWATER-2

[illegible]

FORMAT (2A4, A2, 5X, F5.0, 9F6.0)

FORM 19 of 24

DATA TYPE										ORDER OF LOAD	ALPHANUMERIC NAME	% TREATMENT	INFLOW or WITHDRAWAL *	TEMP *	DISSOLVED OXYGEN (MG / L)	BOD (MG/L)	CONS 1	CONS 2	CONS 3																				
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36				
POINT ID - I										PTL =																													
POINT ID - I										PTL =																													
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FORMAT (2A4, A1, 5X, F5.0, 3A4, F5.0, F8.0, 6F6.0)

* VARIABLE	ENGLISH UNITS	METRIC UNITS
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Inflow or withdrawal

Temperature

FORM (20) of (24)

FORM (20) of (24)

[illegible]

EPA/NCASI STREAM QUALITY ROUTING MODEL - QUAL2E INPUT DATA CODING FORMS

FORM (21) of (24)

DATA TYPE 12 DAM REAERATION COEFFICIENTS

DATA TYPE																		DAM NO.	RCH. NO. OF DAM	ELE. NO. BELOW DAM	ADAM	BDAM	FRACTION FLOW OVER DAM FDAM	HEIGHT OF DAM HDAM (FT, M)																																																							
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
DAM DATA																		DAM =																																																													
DAM DATA																		DAM =																																																													
END DATA 1 2																		DAM =																																																													
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80

FORMAT (3A4, A2, 5X, F5.0, bF6.0)

EPA / NCASI STREAM QUALITY ROUTING MODEL – QUAL2E INPUT DATA CODING FORMS

FORM 23 of 24

LOCAL CLIMATOLOGICAL DATA

DATA TYPE												MONTH, DAY AND YEAR												HOUR OF DAY												NET SOLAR RADIATION												CLOUDINESS												DRY BULB TEMP												WET BULB TEMP												BAROMETRIC PRESSURE												WIND SPEED																																																																															
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80																																																																																																
LOCAL CLIMATOLOGY																																																																																																																																																																															
LOCAL CLIMATOLOGY																																																																																																																																																																															

* Must be chronologically ordered. FORMAT (30X, F10.0, 5F8.0)

Net solar radiation is not required if temperature is simulated, but is only required for dynamic algae simulation when temperature is not simulated.

VARIABLE	ENGLISH UNITS	METRIC UNITS
Net Solar Radiation (PAR)	BTU/ft ² -hr	Langley/hr
Wetbulb, Drybulb Temps	F	C
Barometric Pressure	in Hg	millibars
Wind Speed	ft/sec	m/sec

DO AND BOD REACH PLOT DATA

[illegible]

```
FORMAT (A4, 6X, I5); FORMAT (I0X, I4 I5)
```

BEGIN RCH = Id number of first reach in the plot.

PLOT RCH = Reach numbers in the proper order for plotting.

NOTE: Multiple plots are obtained by repeating the sequence of BEGIN RCH and PLOT RCH information (see User's Manual for example).