# THE WATER QUALITY ANALYSIS SIMULATION PROGRAM, WASP5

# PART B:

# THE WASP5 INPUT DATASET

*Version 5.00, September 20, 1993*

by

Robert B. Ambrose, Jr., P.E.
Tim A. Wool[1]
James L. Martin, Ph.D.,P.E.[1]

Environmental Research Laboratory
Athens, Georgia 30605

[1]AScI Corporation
Athens, Georgia 30605

**CONTENTS**

# CHAPTER 1

# INTRODUCTION

## 1.1 GENERAL CONSIDERATIONS

This section describes the input required to run the WASP5 water quality program. The user should be cautioned about potential changes to the dataset or manual that may accompany version updates of the software. The printed manual may become dated as enhancements are made or errors are identified and corrected. Please download the latest manual accompanying the current version of WASP5.

To arrange the input into a logical format, WASP5 data are divided into 10 groups, A through J:

A - Model Identification and Simulation Control

B - Exchange Coefficients

C - Volumes

D - Flows

E - Boundary Concentrations

F - Waste Loads

G - Environmental Parameters

H - Chemical Constants

I - Time Functions

J - Initial Conditions

The following is a brief explanation of each data group:

DATA GROUP A provides for descriptive model identification and contains simulation control options. The user must specify the number of segments and the number of systems. The user must also specify calculational time steps and print intervals here.

DATA GROUP B contains dispersive exchange information. Dispersion occurs between segments and along a characteristic length. Dispersion coefficients vary with time in a piecewise linear time function.

DATA GROUP C supplies initial segment volume information, and information on the segment type and underlying segment numbers. Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow. These values are used in reaeration and volatilization calculations only (not in the basic transport calculations.)

DATA GROUP D supplies flow and sediment transport information between segments. Flows may be contained in the WASP input dataset, or may be imported from an external hydrodynamic file. Flows in the WASP5 input dataset vary with time following a piecewise linear time function.

DATA GROUP E supplies concentrations for each system at the boundaries. All system concentrations must be supplied for each boundary. Boundary concentrations vary with time in a piecewise linear time function.

DATA GROUP F defines the waste loads and segments that receive the waste loads for both point and diffuse sources. Point source loads vary with time in a piecewise linear time fuction. Nonpoint source loads vary with time in a daily step function.

DATA GROUP G contains appropriate environmental characteristics of the water body. These parameters are spatially variable, varying with each model segment.

DATA GROUP H contains appropriate chemical characteristics or constants. Constants in WASP remain constant in both time and space.

DATA GROUP I contains appropriate environmental or kinetic time functions.

DATA GROUP J contains initial concentrations for each segment and each system, along with dissolved fractions and the density of solids systems.

The input dataset is a formatted ASCII file. The user must carefully place input data in the appropriate fields, and be sure to right justify integers.

## 1.2 THE EUTROPHICATION MODEL

EUTRO4 requires the same input format as the basic WASP5 model. This format is explained in detail in the chapters below. This section summarizes the variables needed specifically for

EUTRO4.

As described in detail in Chapter 5, the 8 systems for eutrophication modeling are ammonia nitrogen, nitrate nitrogen, inorganic phosphorus, phytoplankton carbon, carbonaceous BOD, dissolved oxygen, organic nitrogen, and organic phosphorus.

**Table 1** EUTRO4 Systems and Levels of Complexity

| System Number | Symbol | Name | Use in Complexity Level 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|---|---|
| 1 | NH3 | Ammonia nitrogen | | X | X | X | X | X |
| 2 | NO3 | Nitrate nitrogen | | | X | X | X | X |
| 3 | PO4 | Inorganic phosphorus | | | | X | X | X |
| 4 | CHL | Phytoplankton carbon | | | | X | X | X |
| 5 | CBOD | Carbonaceous BOD | X | X | X | X | X | X |
| 6 | DO | Dissolved oxygen | X | X | X | X | X | X |
| 7 | ON | Organic nitrogen | | | X | X | X | X |
| 8 | OP | Organic phosphorus | | | | X | X | X |

| Complexity Level | Explanation |
|---|---|
| 1 | "Streeter-Phelps" BOD-DO with SOD |
| 2 | "Modified Streeter-Phelps" with NBOD |
| 3 | Linear DO balance with nitrification |
| 4 | Simple eutrophication |
| 5 | Intermediate eutrophication |
| 6 | Intermediate eutrophication with benthos |

Table 1 summarizes these systems and their use in six discrete levels of complexity.

The user should note that these discrete levels of complexity are suggestive only. The user may choose to simulate

any combination of these variables using any combination of the parameter functions and values described below. In fact, during calibration, the user may choose to simulate only one variable, such as CBOD, while bypassing (and thus holding constant) all other variables.

## 1.3 THE TOXIC CHEMICAL MODEL

TOXI4 requires the same input format as the basic WASP5 model. This format is explained in detail in the chapters below. This section summarizes the variables needed specifically for TOXI4.

**Table 2** TOXI4 Systems and Levels of Complexity

| System Number | Symbol | Name | Levels of Complexity for: Solids 1, 2 | Solids 3 | Solids 4 | Kinetics 1-3 | Kinetics 4 |
|---|---|---|---|---|---|---|---|
| 1 | $C_1$ | **Chemical 1** | **X** | **X** | **X** | **X** | **X** |
| **2** | **$S_1$** | **Solid 1** | | **X** | **X** | | |
| **3** | **$S_2$** | **Solid 2** | | | **X** | | |
| **4** | **$S_3$** | **Solid 3** | | | **X** | | |
| **5** | **$C_2$** | **Chemical 2** | | | | | **X** |
| **6** | **$C_3$** | **Chemical 3** | | | | | **X** |

| Complexity Level | Explanation |
|---|---|
| **Solids 1** | **Descriptive Solids concentration field** |
| **Solids 2** | **Descriptive solids concentration field with specific solids transport rates** |
| **Solids 3** | **Simulated total solids** |
| **Solids 4** | **Three simulated solids types** |
| **Equil 1** | **Constant partition coefficient** |
| **Equil 2** | **Spatially-variable partition coefficients** |
| **Equil 3** | **Hydrophobic sorption** |
| **Equil 4** | **Solids-dependent partitioning** |
| **Equil 5** | **Sorption plus ionic speciation** |
| **Kinetic 1** | **Constant half lives or rate constants** |
| **Kinetic 2** | **Spatially-variable rate constants** |
| **Kinetic 3** | **Second order rates** |
| **Kinetic 4** | **Transformation products** |

As described in Chapter 7, the 6 systems for toxicant modeling are chemical 1, solids fraction 1, solids fraction 2, solids fraction 3, chemical 2, and chemical 3. Table 2 summarizes these systems and their use in several discrete levels

of complexity. These levels of complexity describe possible approaches to simulating solids, equilibrium reactions, and kinetic reactions. They are suggestive only. The user may choose to simulate any combination of these variables using any combination of the parameter functions and values described below.

# CHAPTER 2

## DATA GROUP A: MODEL IDENTIFICATION AND SIMULATION CONTROL

Basic simulation information is provided in Data Group A, beginning with titles and descriptions in Records 1 and 2. The number of systems (state variables) and segments are specified in Record 4. Calculational time steps are provided in Records 6 and 7, and print intervals in Records 8 and 9. System bypass options are set in Record 10.

### 2.1 RECORD FORMATS

Record 1--Title of Simulation (A5, A75)

| | | |
|---|---|---|
| SIMTYP | = | type of simulation; TOXI4 = toxics dataset; EUTRO = eutrophication dataset. (A5) |
| TITLE1 | = | descriptive title of simulation. (A75) |

Record 2--Description of Simulation (A80)

| | | |
|---|---|---|
| TITLE2 | = | description of simulation. (A80) |

Record 3--Record 4 Names (A80)

| | | |
|---|---|---|
| HEADER | = | names of Record 4 variables, positioned properly; for user convenience only. (A80) |

Record 4--Simulation Control Parameters (7I5, 2F5.0, F3.0, F2.0)

| | | |
|---|---|---|
| NOSEG | = | number of segments in model network. (I5) |
| NOSYS | = | number of model systems (state variables). (I5) |
| ICFL | = | flag controlling use of restart file; 0 = neither read from nor write to restart file (initial conditions located in input file); 1 = write final simulation results to restart file (initial conditions located in input file); 2 = read initial conditions from restart file created by earlier simulation, and write final simulation results to new restart file. (I5) |
| MFLAG | = | flag controlling messages printed on screen |

during simulation; 0 = all messages printed; 1 = simulation time only printed; 2 = all messages are suppressed. (I5)

JMASS = system number for which mass balance analysis will be performed; 0 = no mass balance table generated. (I5)

NEGSLN = negative solution option; 0 = prevents negative solutions; 1 = allows negative solutions. (I5)

INTYP = time step option; 0 = user inputs time step history; 1 = model calculates time step. (I5)

ADFAC = advection factor; 0 = backward difference; 0.5 = central difference; 0-0.4 recommended. (F5.0)

ZDAY = day at beginning of simulation; 1 is first day. (F5.0)

ZHR = hour at the beginning of simulation. (F3.0)

ZMIN = minute at the beginning of simulation. (F2.0)

TFLG = switch controlling generation of transport file; 0 = generate file; 1 = do not generate file. (I5)

Record 5--Runtime Print Segments (6I5)

ISEGOUT = up to six segment numbers to display at runtime; if there are six or more segments in the model network, the user should specify six print segment numbers. (I5)

Record 6--Number of Time Steps (I5)

NOBRK = number of different model time steps (I5)

Record 7--Time Steps (4(F10.0, F10.0))

DTS(I) = time step to be used until time T(I), days. (F10.0)

T(I) = time up to when time step DTS(I) will be

used, days. (F10.0)

Record 8--Number of Print Intervals (I5)

NPRINT = number of print intervals. (I5)

Record 9--Print Intervals (4(F10.0, F10.0))

PRINT(I) = print interval to be used until time TPRINT(I), days. (F10.0)

TPRINT(I) = time up to when print interval PRINT(I) will be used, days. (F10.0)

Record 10--System Bypass Options (16I5)

SYSBY(K) = bypass option for system K; 0 = system will be simulated; 1 = system will be bypassed. (I5)

## 2.2 THE EUTROPHICATION MODEL

When running EUTRO4, the number of systems, NOSYS, must be set to 8 in Record 4. The bypass options in Record 10, SYSBY(K), should be set to 0 for those variables checked in the relevant complexity level in Table 1; they should be set to 1 for those variables not checked in the relevant complexity level in Table 1.

## 2.3 THE TOXIC CHEMICAL MODEL

When running TOXI4, the number of systems, NOSYS, can be set from 1 to 6 in Record 4, depending upon the solids and kinetic complexity levels chosen for simulation. The bypass options in Record 10, SYSBY(K), should be set to 0 for those variables checked in the relevant complexity level in Table 2; they should be set to 1 for those variables not checked in the relevant complexity level in Table 2.

# CHAPTER 3

# DATA GROUP B: EXCHANGE COEFFICIENTS

Exchange coefficients for surface water and pore water are computed from input dispersion coefficients, cross-sectional areas, and characteristic lengths. Dispersion coefficients may vary in time according to piecewise-linear time functions, with groups of segment pairs having the same dispersion time function. Exchange data are read for each exchange field. Field one contains dispersion coefficients for water column exchanges. Field two contains exchange data for pore water exchange.

## 3.1 RECORD FORMATS

Record 1--Number of Exchange Fields (I5, 75X)

NRFLD = number of exchange fields. NRFLD will generally equal 2 for water column and pore water exchanges. (I5)

TITLE = name of data group. (75X)

If no exchange rates are to be read, set NRFLD to zero and continue with Data Group C. If only surface water exchanges are to be read, set NRFLD to 1 and input the proper values in records 2-6 and 12. If pore water exchanges are to be read, set NRFLD to 2 and input the proper values in records 2-12.

Record 2--Exchange Time Functions for Surface Water Field (I5, 2F10.0)

NTEX(1) = number of exchange time functions for field 1. (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 1 will be multiplied by this factor. (F10.0)

CONVR = conversion factor for exchanges in field 1. (F10.0)

To skip surface water exchange field, set NTEX(1) to zero and continue with the pore water exchange field (record 7) or the exchange bypass options (record 12).

*Records 3-6 are input as a group NTEX(1) times:*

Record 3--Exchange Data (I5)

NORS(1,NT) = number of exchanges for field 1, time function NT. (I5)

Record 4--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K) = area in square meters for exchange pair K. (F10.0)

EL(K) = characteristic length in meters for exchange pair K. (F10.0)

IR(K),JR(K) = segments between which exchange occurs. The order of the segments is unimportant. (2I5)

*Record 4 is repeated NORS(1,NT) times.*

Record 5--Number of Breaks in Time Function (I5)

NBRKR(1,NT) = number of values and times used to describe dispersion coefficient piecewise-linear time function. (I5)

Record 6--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K) = value of dispersion coefficient in $m^2$/sec at time TR(K). (F10.0)

TR(K) = time in days. (F10.0)

*Record 6 is repeated NBRKR(1,NT)/4 times.*

Record 7--Exchange Time Functions for Pore Water Field (I5, 2F10.0)

NTEX(2) = number of exchange time functions for field 2. (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 2 will be multiplied by this factor. (F10.0)

CONVR = conversion factor for exchanges in field 2.

(F10.0)

To skip pore water exchange field, set NTEX(2) to zero and continue with record 12.

*Records 8-11 are input as a group NTEX(2) times:*

Record 8--Exchange Data (I5)

NORS(2,NT) = number of exchanges for field 2, time function NT. (I5)

NT = 1, NTEX(2)

Record 9--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K) = area in square meters for exchange pair K. (F10.0)

EL(K) = characteristic length in meters for exchange pair K. (F10.0)

IR(K),JR(K) = segments between which exchange occurs. The order of the segments is unimportant. (2I5)

*Record 9 is repeated NORS(2,NT) times.*

Record 10--Number of Breaks in Time Function (I5)

NBRKR(2,NT) = number of values and times used to describe dispersion coefficient piecewise-linear time function. (I5)

Record 11--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K) = value of dispersion coefficient in $m^2$/sec at time TR(K). (F10.0)

TR(K) = time in days. (F10.0)

*Record 11 is repeated NBRKR(2,NT)/4 times.*

Record 12--Exchange Bypass Options (16I5)

RBY(K) = exchange bypass option for system K; 0 = exchange occurs in system K; 1 = bypass

exchange for system K. (I5)

*K = 1, NOSYS*

Record 1 is entered once for Data Group B. Records 2 through 6 are input for the surface water exchange field, with Records 3, 4, 5, and 6 being repeated for each time function in this exchange field. Record 4 uses as many lines as necessary to input NORS sets of A(K), EL(K), IR(K), and JR(K), with 1 set on each line. Record 6 uses as many lines as needed to input NBRKR pairs of RT(K) and TR(K), with 4 pairs occupying each line.

Records 7 through 11 are input for the pore water exchange field, with Records 8, 9, 10, and 11 being repeated for each time function in this exchange field. Record 9 uses as many lines as necessary to input NORS sets of A(K), EL(K), IR(K), and JR(K), with 1 set on each line. Record 11 uses as many lines as needed to input NBRKR pairs of RT(K) and TR(K), with 4 pairs occupying each line.

After data for all exchange fields are entered, Record 12 is input on the following line with NOSYS entries.

# CHAPTER 4

# DATA GROUP C: VOLUMES

Initial segment volumes are provided in Data Group C. In addition, segment type and underlying segment numbers are specified. Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow. These values are used in reaeration and volatilization calculations only (not in the basic transport calculations.)

## 4.1 RECORD FORMATS

Record 1--Preliminary Data (2I5, F10.0, 60X)

| | | |
|---|---|---|
| IVOPT | = | water column volume option -- 1 = constant water column volumes; 2, 3 = volumes adjusted to maintain flow continuity. (I5) |
| IBEDV | = | benthic volume option -- 0 = constant bed volumes; 1, bed volumes change in response to sediment transport. (I5) |
| TDINTS | = | benthic time step in days for recomputing porosity (if IBEDV = 0) or for sediment bed compaction (if IBEDV = 1). (F10.0) |
| TITLE | = | name of data group. (60X) |

Record 2--Scale Factors (2F10.0)

| | | |
|---|---|---|
| SCALV | = | scale factor for volumes. All volumes will be multiplied by this factor. (F10.0) |
| CONVV | = | conversion factor for volumes. (F10.0) |

*Record 3 is repeated NOSEG times:*

Record 3--Segment Types and Volumes (3I10, 5F10.0)

| | | |
|---|---|---|
| ISEG | = | segment number. |
| IBOTSG | = | segment immediately below ISEG. (I10) |
| ITYPE(ISEG) | = | segment types: 1 = surface water segment, 2 = subsurface water segment, 3 = upper bed |

segment, 4 = lower bed segment. (I10)

BVOL(ISEG) = volume of segment ISEG in cubic meters. (F10.0)

VMULT(ISEG) = hydraulic coefficient "a" for velocity in ISEG as a function of flow:

$$v = a Q^b$$

If b = 0, VMULT is a constant velocity in m/sec. (F10.0)

VEXP(ISEG) = hydraulic exponent "b" for velocity in ISEG as a function of flow (0-1). A value of 0.4 represents rectangular channels. (F10.0)

DMULT(ISEG) = hydraulic coefficient "c" for depth of ISEG as a function of flow:

$$d = c Q^d$$

If d = 0, DMULT is a constant depth in m. (F10.0)

DXP(ISEG) = hydraulic exponent "d" for depth of ISEG as a function of flow (0-1). A value of 0.6 represents rectangular channels. (F10.0)

Note that the four hydraulic geometry parameters are used to calculate segment velocity and depth, which are not used by WASP5 in transport calculations. These are used to calculate reaeration or volatilization from segments.

Records 1 and 2 are entered once for Data Group C. Record 3 is repeated NOSEG times. If ICFL = 2 in Data Group A, volumes are read from the restart file ( *.RST, where * is the input data set name), and Records 2 and 3 should not be included in the input data set.

# CHAPTER 5

# DATA GROUP D: FLOWS

## 5.1 RECORD FORMATS

Data Group D provides for the advective transport flows that are used in the model. Flows may be input for up to 6 transport fields. Field one consists of advective flows in the water column. Field two consists of pore water flows. Fields three, four, and five consist of sediment transport velocities and cross-sectional areas for solids. A separate sediment transport field is specified for each of up to 3 solids types. Field six is for evaporation and precipitation velocities and cross-sectional areas. All flows may vary in time according to piecewise linear time functions.

Record 1 is read first. If IQOPT = 1 or 2, Data Block D1 is read next; if IQOPT = 3, Data Block D1 is skipped. Data Blocks D2, D3, D4, D5, and D6 follow in order for NFIELD = 2, 3, 4, 5, and 6, respectively. Following all specified Data Blocks, Record 32 is read.

Record 1--Data Input Options: Number of Flow Fields (2I5, A12)

IQOPT = flow option:

1 = field one (advective) flows are specified directly by user. Individual flows at each segment interface are summed by the model, and the net flow is applied across the interface.

2 = field one flows are specified directly by the user. Individual flows at each segment interface are applied directly by the model.

3 = flows are read from a formatted file created by DYNHYD5 or other hydrodynamic model. (I5)

NFIELD = number of flow fields. The first two fields are surface water and pore water flows. An additional field (3, 4, or 5) is used for each type of solid modeled. Field 6 is used for evaporation and precipitation. If no

flows are used, set NFIELD to zero and continue with Data Group E. (I5)

HYDFIL = name of hydrodynamic file to be read by WASP5 during the simulation (for example, RIVER1.HYD). (A12)

DATA BLOCK D1: Direct Input of Field One Flows (IQOPT = 1,2)

Record 2--Number of Flow Time Functions (I5, 2F10.0)

NINQ(1) = number of time functions for Field One. If no flows are used in field one, set NINQ to zero and skip to next field. (I5)

SCALQ = scaling factor. All flows in Field one are multiplied by SCALQ. (F10.0)

CONVQ = units conversion factor. (F10.0)

*Records 3 - 6 are input as a group NINQ(1) times:*

Record 3--Number of Flows (I5)

NOQS(1,NI) = number of unit flow responses in field one, time function NI; each unit flow is defined for a single segment pair. (I5)

Record 4--Flow Routing for Field One (4(F10.0, 2I15))

BQ(1,NI,K) = portion of flow for field one, time function NI that flows between segment pair K. (F10.0)

JQ(1,NI,K) = upstream segment. (I5)

IQ(1,NI,K) = downstream segment. (I5)

*Record 4 is repeated NOQS(1,NI)/4 times.*

Record 5--Number of Breaks in Advective Time Functions (I5)

NBRKQ(1,NI) = the number of flows and times used to describe piecewise linear time function NI. (I5)

Record 6--Piecewise Linear Advective Time Function (4(2F10.0))

QT(1,NI,K) = advective flow in $m^3/s$. (F10.0)

TQ(1,NI,K) = time in days. (F10.0)

*Record 6 is repeated NBRKQ(1,NI) times.*

Record 2 is input once for Data Block D1. Records 3, 4, 5, and 6 are input once for each flow time function. Record 4 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets per line. Record 6 uses as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line.

DATA BLOCK D2: Field Two (Pore Water) Flows

Record 7--Number of Pore Water Time Functions (I5, 2F10.0)

NINQ(2) = number of pore water time functions. If no flows are used in Field Two, set NINQ to zero and skip to sediment transport fields. (I5)

SCALQ = scaling factor for pore water flows. (F10.0)

CONVQ = units conversion factor. (F10.0)

*Records 8 - 11 are input as a group NINQ(2) times:*

Record 8--Number of Flows (I5)

NOQS(2,NI) = number of segment pair flows in Field 2, time function NI. (I5)

Record 9--Flow Routing for Field Two (4(F10.0, 2I5))

BQ(2,NI,K) = portion of pore water flow for time function NI that flows between segment pair K. (F10.0)

JQ(2,NI,K) = upstream segment. (I5)

IQ(2,NI,K) = downstream segment. (I5)

*Record 9 is repeated NOQS(2,NI)/4 times.*

Record 10--Number of Breaks in Pore Water Time Function (I5)

NBRKQ(2,NI) = number of pore water flows and times used to describe piecewise linear time function NI. (I5)

Record 11--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(2,NI,K) = pore water flow in $m^3/s$. (F10.0)

TQ(2,NI,K) = time in days. (F10.0)

*Record 11 is repeated NBRKQ(2,NI)/4 times.*

Record 7 is input once for Data Group D2. Records 8, 9, 10 and 11 are input once for each pore water time function. Record 9 uses as many lines as necessary to input NOQS sets of BQ, JQ, and IQ, with four sets on each line. Record 11 uses as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line.

DATA BLOCK D3: Sediment 1 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids are modeled, skip directly to Record 32 (Flow Bypass Options).

Record 12--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(3) = number of velocity time functions for Field 3. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

*Records 13 - 16 are input as a group NINQ(3) times:*

Record 13--Number of Segment Pairs (I5)

NOQS(3,NI) = number of segment pairs involved in sediment 1 transport. (I5)

Record 14--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(3,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(3,NI,K) = segment sediment is transported from. (I5)

IQ(3,NI,K) = segment sediment is transported to. (I5)

*Record 14 is repeated NOQS(3,NI)/4 times.*

Record 15--Number of Breaks in Velocity Time Function (I5)

NBRKQ(3,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 16--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(3,NI,K) = sediment 1 transport velocity in m/s. (F10.0)

TQ(3,NI,K) = time in days. (F10.0)

*Record 16 is repeated NBRKQ(3,NI)/4 times.*

Record 12 is input once for Data Block D3. Records 13, 14, 15 and 16 are input for each velocity time function. Record 14 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 16 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D4: Sediment 2 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids 2 are modeled, enter 0 for NINQ(4), then skip directly to the next data block.

Record 17--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(4) = number of velocity time functions for Field 4. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

*Records 18 - 21 are input as a group NINQ(4) times:*

Record 18--Number of Segment Pairs (I5)

NOQS(4,NI) = number of segment pairs involved in sediment 2 transport. (I5)

Record 19--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(4,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(4,NI,K) = segment sediment is transported from. (I5)

IQ(4,NI,K) = segment sediment is transported to. (I5)

*Record 19 is repeated NOQS(4,NI)/4 times.*

Record 20--Number of Breaks in Velocity Time Function (I5)

NBRKQ(4,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 21--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(4,NI,K) = sediment 2 transport velocity in m/s. (F10.0)

TQ(4,NI,K) = time in days. (F10.0)

*Record 21 is repeated NBRKQ(4,NI)/4 times.*

Record 17 is input once for Data Block D4. Records 18, 19, 20 and 21 are input for each velocity time function. Record 19 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 21 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D.5: Sediment 3 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids 3 are modeled, enter 0 for NINQ(5), then skip directly to the next data block.

Record 22--Number of Velocity Time Functions (I5, 2F10.0)

| | | |
|---|---|---|
| NINQ(5) | = | number of velocity time functions for Field 5. (I5) |
| SCALQ | = | scaling factor for velocities. (F10.0) |
| CONVQ | = | units conversion factor. (F10.0) |

*Records 23 - 26 are input as a group NINQ(5) times:*

Record 23--Number of Segment Pairs (I5)

| | | |
|---|---|---|
| NOQS(5,NI) | = | number of segment pairs involved in sediment 3 transport. (I5) |

Record 24--Areas for Settling, Resuspension (4(F10.0, 2I5))

| | | |
|---|---|---|
| BQ(5,NI,K) | = | area in square meters between segment pair K. (F10.0) |
| JQ(5,NI,K) | = | segment sediment is transported from. (I5) |
| IQ(5,NI,K) | = | segment sediment is transported to. (I5) |

*Record 24 is repeated NOQS(5,NI)/4 times.*

Record 25--Number of Breaks in Velocity Time Function (I5)

| | | |
|---|---|---|
| NBRKQ(5,NI) | = | number of velocities and times used to describe piecewise linear time function NI. (I5) |

Record 26--Piecewise Linear Velocity Time Function (4(2F10.0))

| | | |
|---|---|---|
| QT(5,NI,K) | = | sediment 3 transport velocity in m/s. |

(F10.0)

TQ(5,NI,K) = time in days. (F10.0)

*Record 26 is repeated NBRKQ(5,NI)/4 times.*

Record 22 is input once for Data Block D5. Records 23, 24, 25 and 26 are input for each velocity time function. Record 24 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 26 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D6: Evaporation and Precipitation Field

Evaporation and precipitation flow data are input as velocities and areas. Velocities may vary in time to represent rainfall events or seasonal evaporation. No chemical is transported with evaporation, but volumes are adjusted to maintain continuity. If this field is not modeled, skip directly to Record 32 (Flow Bypass Options). After all transport field data are entered, Record 32 is input with NOSYS entries. If no evaporation or precipitation fields are specified, Record 32 follows Data Group D.5 (solids 3 transport).

Record 27--Number of Velocity Time Functions (I5, 2F10.0))

NINQ(6) = number of velocity time functions for Field 6. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

*Records 28 - 31 are input as a group NINQ(6) times:*

Record 28--Number of Segment Pairs (I5)

NOQS(6,NI) = number of segment pairs involved in evaporation or precipitation. (I5)

Record 29--Areas for Evaporation, Precipitation (4(F10.0, 2I5))

BQ(6,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(6,NI,K) = segment water is transported from; if = 0, this is precipitation. (I5)

IQ(6,NI,K) = segment water is transported to; if = 0, this is evaporation. (I5)

*Record 29 is repeated NOQS(6,NI)/4 times.*

Record 30--Number of Breaks in Velocity Time Function (I5)

NBRKQ(6,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 31--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(6,NI,K) = water transport velocity in m/s; if more traditional units of cm/day or cm/year are desired, then specify CONVQ = $1.1574E^{-7}$ or $3.169E^{-10}$, respectively. (F10.0)

TQ(6,NI,K) = time in days. (F10.0)

*Record 31 is repeated NBRKQ(6,NI)/4 times.*

**END OF DATA BLOCKS FOR D**

Record 32--Flow Bypass Options (16I5)

QBY(ISYS) = flow bypass option -- 0 = flow transport occurs in system ISYS; 1 = flow transport is bypassed for system ISYS. (I5)

*ISYS = 1, NOSYS*

The flow bypass option allows flow transport to be set to zero in one or more systems. The bypass option applies to all transport fields.

## 5.2 THE EXTERNAL HYDRODYNAMIC FILE

When IQOPT in Record 1 is set to 3, external flows and volumes will be read from a formatted ASCII file chosen by the user. This file begins with information on the WASP5

calculational time step, simulation start and end times, and flow connections. The body of the file is composed of sets of segment records and segment interface records that are repeated every time step for the entire simulation. The segment records specify instantaneous segment volumes, depths, and water velocities at the beginning of a time step. The segment interface records specify average interfacial flows during the time step.

WASP5 uses the interfacial flows to calculate mass transport, and the volumes to calculate constituent concentrations. Segment depths and velocities are used only to calculate reaeration or volatilization rates.

Five records comprise the external hydrodynamic file:

Record 1 -- Data Options (2I5, 3F20.0, I5)

| | | |
|---|---|---|
| NQSEG | = | Number of segments connected by flows from the hydrodynamic file. (I5) |
| NQINT | = | Number of interfacial flow pairs from the hydrodynamic file. (I5) |
| DELTQ | = | WASP5 time step; an even multiple of the hydrodynamic time step, seconds. (F20.0) |
| TBEGIN | = | Beginning time for the hydrodynamic file, in seconds. (F20.0) |
| TEND | = | Ending time for the hydrodynamic file, in seconds. (F20.0) |
| FILOPT | = | Switch controlling the contents of the hydrodynamic file; 0 = time variable segment depths and velocities are read; 1 = time variable segment depths and velocities are not read. (I5) |

Record 2 -- Segment Interface Pairs (2I5)

| | | |
|---|---|---|
| IQ(J) | = | First segment in interface "J", nominally where flow is *from*. (I5) |
| JQ(J) | = | Second segment in interface "J", nominally where flow is *to*. (I5) |

Note that positive values of flow go from IQ to JQ. Negative

values of flow go from JQ to IQ.

*Record 2 is repeated NQINT times, for J from 1 to NQINT.*

Record 3 -- Initial Segment Properties (4F20.0)

BVOL(I) = Volume of segment "I" at beginning of time step, $m^3$. (F20.0)

DUMMY = Dummy variable, not used by WASP5. (20.0)

DEPTH(I) = Average depth of segment "I", in meters. (F20.0)

VELOC = Average velocity of segment "I", m/sec. (F20.0)

*Record 3 is repeated NQSEG times, for I from 1 to NQSEG.*

*Records 4 and 5 are repeated as a unit for the number of time steps in the water quality simulation, or (TEND - TBEGIN)/DELTQ:*

Record 4 -- Segment Interfacial Flows (F20.0)

BQ(J) = Average flow in interfacial pair "J" during the time step, in $m^3$/sec. (F20.0)

*Record 4 is repeated NQINT times, for J from 1 to NQINT (in the same order as segment pairs are given in Record 2).*

Record 5 -- Segment Properties (4F20.0)

BVOL(I) = Volume of segment "I" at end of time step, $m^3$. (F20.0)

DUMMY = Dummy variable, not used by WASP5. (20.0)

DEPTH(I) = Average depth of segment "I", in meters. (F20.0)

VELOC = Average velocity of segment "I", m/sec. (F20.0)

*Record 5 is repeated NQSEG times, for I from 1 to NQSEG.*

Record 1 is input once. Record 2 is repeated NQINT times.

Record 3 is repeated NQSEG times. Records 4 and 5 are a set, and are repeated (as a set) (TEND - TBEGIN)/DELTQ times. Within each set, Record 4 is repeated NQINT times and Record 5 is repeated NQSEG times.

# CHAPTER 6

# DATA GROUP E: BOUNDARY CONCENTRATIONS

Data Group E supplies concentrations for each system at the model network boundaries. Model boundaries consist of those segments that import, export, or exchange water with locations outside the network, as specified in Data Groups B and D. All system concentrations from 1 to NOSEG must be supplied for each boundary. Boundary concentrations vary with time following a piecewise linear time function specified by the user in Records 3 and 4.

## 6.1 RECORD FORMATS

*Data Group E is repeated, in its entirety, NOSYS times.*

Record 1--Data Input Option--Number of Boundary Conditions (I10, 70X)

NOBC(K) = number of boundary conditions used for system K. (I10)

TITLE = name of data group. (70X)

If no boundary conditions are to be input for system K, set NOBC(K) equal to zero and either continue with the next system or go to Data Group F if K is the last system.

Record 2--Scale Factor for Boundary Conditions (2F10.0)

SCALB = scale factor for boundary conditions. All boundary conditions will be multiplied by this factor. (F10.0)

CONVB = unit conversion factor for boundary conditions. Boundary conditions are expected to be in mg/L (i.e. - $g/m^3$), in which case CONVB will be 1.0. (F10.0)

*Records 3-4 are input as a unit NOBC(K) times:*

Record 3--Boundary Location (2I5)

IBC(K) = boundary segment number. (I5)

NOBRK(K) = number of values and times used to describe the broken line approximation. The number of breaks must be equal for all boundary conditions within a system. (I5)

Record 4--Boundary Concentrations (4(2F10.0))

BCT(K) = value of the boundary concentration at time T(K) in mg/L. (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the broken line approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic, with period equation to T(NOBRK). All break times must agree for all segments, i.e., T(1) must be the same for all boundaries, T(2) must be the same for all boundaries, etc. (F10.0)

*Record 4 is repeated NOBRK(K)/4 times.*

Records 1 and 2 are entered once. Records 3 and 4 are a set and are repeated NOBC times. Within each NOBC set, Record 3 is entered once and Record 4 is repeated until NOBRK entries are input. Four entries (four BCT(K)-T(K) pairs) will fit on each 80-space line. The whole group (Records 1 - 4) is repeated NOSYS times, once for each model system.

## 6.2 THE EUTROPHICATION MODEL

When running EUTRO4, Data Group E is input 8 times, once for each system. For those systems being bypassed, the user may specify 0 for the number of boundary conditions, and skip to the next system.

The user should be careful to note that boundary concentrations for system 4, phytoplankton, are input as chlorophyll a, in µg/L. These are transformed internally to phytoplankton carbon using the carbon to chlorophyll ratio, which is specified in Data Group H as constant 46.

## 6.3 THE TOXIC CHEMICAL MODEL

When running TOXI4, Data Group E is input NOSYS times, once for each system simulated. NOSYS is specified in Data Group A, and has a maximum value of 6. For those systems being bypassed, the user may specify 0 for the number of boundary conditions, and skip to the next system.

The user should be careful to note that all boundary concentrations are input in the standard WASP units of mg/L (even though the output concentrations for chemical are in units of µg/L.)

# CHAPTER 7

# DATA GROUP F: WASTE LOADS

Data Group F is composed of two blocks of data. Data Block F1 contains the point source waste loads used in the model. These loads vary with time following a piecewise linear time function specified by the user in Records 3 and 4. Following complete specification of point source loads, nonpoint source loads are read from Data Block F2, which is composed of only one record in the input dataset. Nonpoint source loads vary with time in a daily step function read from an external loading file.

## 7.1 RECORD FORMATS

*Data Block F1 (records 1-4) is repeated in its entirety NOSYS times:*

Record 1--Number of Point Source Loadings (I10, 70X)

NOWK(ISYS) = number of point source loadings used for system ISYS. Loadings may also be considered as sources (loads) or sinks of a water quality constituent. If no loadings are to be input, set NOWK(ISYS) to zero, and continue with next system or go to next data group.(I10)

TITLE = name of data group. (70X)

If no point source loadings are to be input for system ISYS, set NOWK(ISYS) equal to zero and either continue with the next system or go to Data Group G if ISYS is the last system.

Record 2--Scale Factor for Point Source Loadings (2F10.0)

SCALW = scale factor for point source loadings. All loadings for system ISYS will be multiplied by this factor. (F10.0)

CONVW = unit conversion factor for point source loadings for system ISYS. Loadings are expected to be in kilograms per day. If loadings are given in English units (pounds per day), this factor will be 0.4535. (F10.0)

*Records 3-4 are input as a unit NOWK(ISYS) times:*

Record 3--Number of Point Sources (2I5)

IWK(K) = segment number that has point source loading BWK(K). (I5)

NOBRK(K) = number of breaks used to describe the loading function approximation. The number of breaks must be equal for all forcing functions within a system. (I5)

Record 4--Point Source Time Function (4(2F10.0))

WKT(K) = value of the point source loading at time T(K), in kg/day. (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic with period equal to T(NOBRK). All break times must agree for all segments; i.e., T(1) must be the same for all loads, T(2) must be the same for all loads, etc. (F10.0)

*Record 4 is repeated NOBRK(ISYS)/4 times.*

Records 1 and 2 are input once. Records 3 and 4 are a set and are repeated (as a set) NOWK times. Within each set, Record 3 is entered once and Record 4 is repeated until all NOBRK entries are entered. Four entries (WKT(K)-T(K) pairs) will fit on each 80-space line. The entire group (Records 1 - 4) is repeated NOSYS times, once for each system.

*Data Block F2, record 5, is input once:*

Record 5--Nonpoint Source Load Option (I10)

LOPT = nonpoint source load option; a value of 0 means that no nonpoint sources will be read from an external file; a value of 1 will cause the model to read a set of loads from an external file. The user will be prompted

by WASP5 to provide information on the external file. This file and its contents are described below. (I10)

## 7.2 THE EXTERNAL NONPOINT SOURCE FILE

When LOPT is set to 1, external nonpoint sources will be read from a formatted ASCII file chosen by the user. This file contains information on which WASP5 systems and segments receive nonpoint source loads, and a record of the nonzero loads by system, segment, and day.

Six records comprise the nonpoint source file.

Record 1--Data Options (A15, 3I5)

NPSMOD = Name or description of nonpoint source model or method of generation; this is echoed to the output file for the record. (A15)

NUMSEG = Number of segments receiving nonpoint source loads. (I5)

INTOPT = Interpolation option; 1 = step function (only one in code now). (I5)

NUMSYS = Number of WASP systems receiving nonpoint source loads. (I5)

Record 2--Loading Segments (I5)

LSEG(I) = segment number receiving loads. (I5)

*Record 2 is repeated NUMSEG times.*

Record 3--Loading Systems (20I5)

LSYS(I) = WASP system numbers receiving loads. (I5)

Record 4--System Descriptors (A15)

NAMESY(I) = Name or description of WASP systems receiving loads. (A15)

*Record 4 is repeated NUMSYS times.*

*Records 5 and 6 are repeated as a unit for the number of days that nonzero loads occur:*

Record 5--Loading Days (F10.0)

LDAY = Time in days for the following nonzero load. (F10.0)

Record 6--Nonpoint Source Loads (A15, 20F10.0)

NAMESY(I) = System name or description (not read in by WASP). (A15)

NPSWK(I,J) = Nonpoint source loads for WASP system "I" at all loading segments "J", in the order presented in Record 2. Loads are in kg/day. (20F10.0)

*Record 6 is repeated NUMSYS times.*

Record 1 is input once. Record 2 is repeated NUMSEG times. Record 3 is then input once. Record 4 is repeated NUMSYS times. Records 5 and 6 are a set and are repeated (as a set) NUMSYS times. Within each set, Record 5 is entered once and Record 6 is repeated NUMSYS times.

## 7.3 THE EUTROPHICATION MODEL

When running EUTRO4, Data Block F1 is input 8 times, once for each system. For those systems being bypassed, the user may specify 0 for the number of waste loads, and skip to the next system.

The user should note that waste loads for system 4, phytoplankton, are input as phytoplankton carbon, in kg/day.

## 7.4 THE TOXIC CHEMICAL MODEL

When running TOXI4, Data Block F1 is input NOSYS times, once for each system simulated. NOSYS is specified in Data Group A, and has a maximum value of 6. For those systems being bypassed, the user may specify 0 for the number of waste loads, and skip to the next system.

# CHAPTER 8

## DATA GROUP G: PARAMETERS

Parameters are spatially-variable characteristics of the water body. The definition of the parameters will vary, depending upon the structure and kinetics of the systems comprising each model. The input format, however, is constant. The number of parameters that is specified in Record 1 must be input for each segment.

### 8.1 RECORD FORMATS

Record 1--Number of Parameters (I10, 70X)

| | | |
|---|---|---|
| NOPAM | = | number of parameters required by the model. If no parameters are to be input, set NOPAM to zero and go to Data Group H. (I10) |
| TITLE | = | name of data group. (70X) |

Record 2--Scale Factors for Parameters (4(A5, I5, F10.0))

| | | |
|---|---|---|
| ANAME(ISC) | = | descriptive name for parameter ISC. (A5) |
| ISC | = | parameter number identifying parameter. (I5) |
| PSCAL(ISC) | = | scale factor for parameter ISC. (F10.0) |

*Record 2 is repeated NOPAM/4 times.*

*Records 3-4 are input as a unit NOSEG times:*

Record 3--Segment Number (I10)

| | | |
|---|---|---|
| ISG | = | segment number for the following parameter values. (I10) |

Record 4--Segment Parameters (4(A5, I5, F10.0))

| | | |
|---|---|---|
| PNAME(ISC) | = | an optional one to five alphanumeric character descriptive name for parameter PARAM(ISG,ISC). (A5) |
| ISC | = | parameter number identifying parameter. (I5) |

PARAM(ISEG,ISC)= the value of parameter ISC in segment ISG. (F10.0)

*Record 4 is repeated NOPAM/4 times.*

Record 1 is input once in Data Group G, occupying one line. Record 2 has NOPAM entries. Four entries will fit on one line; thus, Record 2 uses as many 80-space lines as needed to enter all NOPAM entries. Records 3 and 4 are repeated NOSEG times, once for each segment. For each segment, Record 4 uses as many lines as needed to enter all NOPAM entries.

## 8.2 THE EUTROPHICATION MODEL

Listed below are the 12 parameters available for EUTRO4 simulations. Six representative levels of analysis were outlined in Table 1. For Level 1 and 2 analyses, only TMPSG, TMPFN, SOD1D, and SODTA (3, 4, 9, and 11) need be specified. Spatially-variable reaeration rate constants may be directly specified using REARSG (14). For Level 3 analysis, VELFN, FNH4, and TOTLIM (1, 7, and 13) may be added (DEPTH, VELFN, and TOTLIM are used to compute reaeration; if rate constant K2 is specified (Constant 82), then VELFN, REARSG, and TOTLIM can be omitted; if parameter REARSG is specified, then VELFN and TOTLIM can be omitted). For analyses at Level 4 and above, all parameters should be considered.

| ISC | ANAME | Definition and Units |
|---|---|---|
| 1 | VELFN | Pointer to the time-variable velocity function to be used for ISEG. The four velocity functions are defined by the user in data group I. |
| 2 | SAL | Average salinity of ISEG, in g/L; used in calculation of DO saturation. |
| 3 | TMPSG | Segment temperature multiplier (CC). TMPSG varies overspace and can be either actual temperature or a normalized function, depending on the definition of TEMP. TMPSG(ISEG) * TEMP(TMPFN(ISEG)) = STP, the temperature of segment ISEG. |
| 4 | TMPFN | Flag designating the time-variable temperature function to be used for ISEG. The four |

| | | |
|---|---|---|
| | | temperature functions are defined by the user in data group I. |
| 5 | KESG | Segment extinction coefficient multiplier ($m^{-1}$). KESG varies over space and can be either an actual extinction coefficient or a normalized function, depending on the definition of KE. KESG(ISEG) * KE(KEFN(ISEG)) = Ke, the extinction coefficient for segment ISEG. |
| 6 | KEFN | Pointer designating the time variable extinction coefficient (KE) to be used for segment ISEG. The five extinction coefficients available are defined in data group I. |
| 7 | FNH4 | Average ammonium flux multiplier for segment ($mg/m^2$-day). |
| 8 | FPO4 | Average phosphate flux multiplier for segment ($mg/m^2$-day). |
| 9 | SOD1D | Sediment oxygen demand for segment ($g/m^2$-day). |
| 10-11 | RLGHTS | Used internally; not specified by the user. |
| 12 | SODTA | Segment specific temperature correction coefficient (theta) for sediment oxygen demand. |
| 13 | TOTLIM | Segment specific percent shading. |
| 14 | REARSG | Segment specific reaeration rate constant multiplier, used in combination with time function REAR. |

## 8.3 THE TOXIC CHEMICAL MODEL

Listed below are the 18 parameters that may be used by TOXI4. The user need input only those required to model the particular reactions being considered. For solids, equilibrium, and kinetics Level 1, no parameters are necessary.

| ISC | ANAME | Definition, Units, and Reactions Affected |
|---|---|---|
| 1 | VELFN | Pointer to water velocity time function (1-4); V. |
| 2 | TMPFN | Pointer to normalized temperature time function (1-4); ALL. |
| 3 | TEMP | Multiplier for water temperature time function (EC); ALL. |
| 4 | WVEL | Multiplier for wind velocity (10 meters above segment surface) time function (meters/sec); V. |
| 5 | REAR | Multiplier of time function 5, whose definition depends on volatilization option XV (constants 236,736,1336):<br>XV = 1 volatilization rate constant (m/day)<br>XV = 2,3 oxygen reaeration rate constant (m/day)<br>XV = 4,5 REAER not used; enter 0; V. |
| 6 | DOC | Dissolved organic carbon concentrations (mg/L); S, P. |
| 7 | FOC 1 | Fraction organic carbon of solids class 1; S. |
| 8 | FOC 2 | Fraction organic carbon of solids class 2; S. |
| 9 | FOC 3 | Fraction organic carbon of solids class 3; S. |
| 10 | CHPHL | Multiplier for phytoplankton chlorophyll concentration time function (mg/L); P. |
| 11 | PH | Multiplier for pH time function; H, I. |
| 12 | XKE2 | Light extinction coefficient for photochemically active light (1/meter); this value is used only for photolysis option XPHOTO = 2 (constants 286,886,1486). For photolysis option 1 or 2 when XKE2 = 0.0 the extinction coefficient is calculated from solids, DOC, and chlorophyll concentrations; P. |
| 13 | OXRAD | Concentration of oxidants, such as $O_3$ for $H_2O_2$ (moles/L); O. |
| 14 | BAC | Density of active bacteria (cells/100 cc) the units for bacterial density must be consistent with those used for the second order biodegradation rate constants KBIO20 (constants 146-160, 746-760, 1346-1360); the product of BAC and KBIO20 must be units of $day^{-1}$; B. |
| 15 | EXENV | Property of aquatic environment that affects the user-defined "extra reaction." The units for EXENV must be consistent with those used for second order rate constants KE20 (constant 576-590, 1176-1190, 1776-1790); the product of EXENV and KE20 must yield units of $day^{-1}$; E. |

| ISC | ANAME | Definition, Units, and Reactions Affected |
|---|---|---|
| 16 | TOTKG 1 | Total lumped first-order decay rate constant for chemical 1 in segment ($day^{-1}$). |
| 17 | TOTKG 2 | Total lumped first-order decay rate constant for chemical 2 in segment ($day^{-1}$). |
| 18 | TOTKG 3 | Total lumped first-order decay rate for chemical 3 in segment ($day^{-1}$). |

I = ionization, S = sorption, V = volatilization, B = biodegradation, H = hydrolysis, O = oxidation, P = photolysis, E = extra reaction

For equilibrium level 2, FOC 1 is used to enter partition coefficients. For equilibrium levels 3 and above, FOC 1 is fraction organic carbon of solids class 1. DOC may be entered. If two or three solids classes are being simulated (solids level 4), then FOC 2 and FOC 3 must be entered. For equilibrium level 5, PH values are necessary.

At kinetics level 2, TOTKG 1 is specified. If two or three chemicals are being simulated at this level, then TOTKG 2 and TOTKG 3 must be specified. Kinetics level 3 may require the remaining parameters, depending on the kinetic processes of importance. If water temperatures differ significantly from 20EC, then TEMP may be necessary for all processes (depending on the accuracy required of the simulation). Volatilization requires REAR for options 1, 2, and 3, but not for 4 and 5. If reaeration values are not available for volatilization options 2 and 3, then rates can be calculated internally if parameters DEPTH and VELOC are given. Volatilization options 4 and 5 require parameter WVEL.

Photolysis requires DEPTH values. In addition photolysis option 1 requires DOC and CHPHL. Photolysis option 2 may use either DOC and CHPHL values or XKE2 values. The remaining processes of hydrolysis, oxidation, biodegradation, and extra reaction require one parameter each: PH, OXRAD, BAC, and EXENV, respectively.

# CHAPTER 9

# DATA GROUP H: CONSTANTS

The definition of the constants will vary, depending upon the structure and kinetics of the systems comprising each model. This data group is subdivided into global constants and constants for each system (thus NOSYS+1 groups are read). Each of these groups can be subdivided into any number of fields containing similar kinds of data.

## 9.1 RECORD FORMATS

Record 1--Header (80X)

TITLE = name of data group. (80X)

*Records 2-4 are input as a group NOSYS+1 times:*

Record 2--Data Fields in Group ISYS (A10, I10)

CHNAME(ISYS) = a ten-character descriptive name for System (ISYS). (A10)

NFLD = number of fields of constants for this group; 0 = no constants for this group; the user may subdivide the constants into any number of arbitrary fields. (I10)

If no constants are to be input for this group, set NFLD equal to zero and continue with next group. Records 3 and 4 are repeated as a unit NFLD times.

Record 3--Number of Constants in Field (A10, I10)

FLDNAME = ten-character name identifying field of constants. (A10)

NCONS = number of constants to be entered in this field; 0 = no constants for this field (skip to next field). (I10)

Record 4--Constants (2(A10, I10, F10.0))

TNAME(ISC) = name identifying constant ISC. (A10)

ISC = number identifying constant; these numbers are set by model developer. (I10)

CONST(ISC) = value of constant ISC. (F10.0)

*Record 4 is repeated NCONS/2 times.*

Record 1 is entered once in Data Group H. Records 2 through 4 are entered as NOSYS + 1 groups. For each group, Records 3 and 4 are entered NFLD times. For each field, Record 4 uses as many lines as needed for NCONS entries (2 per line).

## 9.2 THE EUTROPHICATION MODEL

Listed below are the 42 constants available for a full eutrophication simulation. Chapters 4 and 5 discuss the constants required for each level of complexity in dissolved oxygen and eutrophication modeling. Default values for constants are 0 unless otherwise noted.

| ISC | ANAME | Definition and Units |
|---|---|---|
| 11 | K12C | Nitrification rate at 20EC, per day. |
| 12 | K12T | Temperature coefficient for K1320C. Default = 1.0. |
| 13 | KNIT | Half-saturation constant for nitrification-oxygen limitation, mg $O_2$/L. |
| 21 | K20C | Denitrification rate at 20EC, per day. |
| 22 | K20T | Temperature coefficient for K140C. Default = 1.0. |
| 23 | KNO3 | Half-saturation constant for denitrification oxygen limitation, mg$O_2$/L. |
| 41 | K1C | Saturated growth rate of phytoplankton ($day^{-1}$). |
| 42 | K1T | Temperature coefficient. Default = 1.0. |
| 43 | LGHTS | Light formulation switch: LGHTS = 1, use Di Toro et al. (1971) formulation; LGHTS = 2, use Dick Smith's (USGS) formulation. Default = 1. |

44 PHIMX Maximum quantum yield constant. Used only when LGHTS = 2, mg C/mole photons. Default = 720.

45 XKC Chlorophyll extinction coefficient. Used only when LGHTSW = 2, (mg chl**a**/$m^3$)$^{-1}$/m. Default = 0.017.

46 CCHL Carbon-to-chlorophyll ratio. Used only when LGHTSW = 1 (mg carbon/mg chl **a**). Default = 30.

47 IS1 Saturation light intensity for phytoplankton. Used only when LGHTSW = 1 (Ly/day). Default = 300.

48 KMNG1 Nitrogen half-saturation constant for nitrogen for phytoplankton growth, which also affects ammonia preference, mg-N/L. NOTE: This affects ammonia preference:

= 0, PNH3G1 = 1.0
= Large, PNH3G1 = $NH_3/(NH_3 + NO_3)$

NOTE: For standard model application, use a large KMNG1.

49 KMPG1 Phosphorous half-saturation constant for phytoplankton growth, mg $PO_4$-P/L.

50 K1RC Endogenous respiration rate of phytoplankton at 20EC, $day^{-1}$.

51 K1RT Temperature coefficient for phytoplankton respiration. Default = 1.0.

52 K1D Non-predatory phytoplankton death rate, $day^{-1}$.

53 K1G Grazing rate on phytoplankton per unit zooplankton population, L/cell-day.

54 NUTLIM Nutrient limitation option. 0 = minimum; 1 = multiplicative. Default = 0.

55 KPZDC Decomposition rate constant for phytoplankton in the sediment at 20EC, per day.

56 KPZDT Temperature coefficient for decomposition of phytoplankton in sediment. Default = 1.0.

| | | |
|---|---|---|
| 57 | PCRB | Phosphorus-to-carbon ratio in phytoplankton, mg P/mg C. Default = 0.025. |
| 58 | NCRB | Nitrogen-to-carbon ratio in phytoplankton, mg N/mg C. Default = 0.25. |
| 59 | KMPHY | Half-saturation constant for phytoplankton, mg carbon/L. NOTE: As phytoplankton concentrations increase, mineralization rates for organic nitrogen and organic phosphorus increase. If KMPHY is small, there is little phytoplankton effect on mineralization. If KMPHY is large, a large concentration of phytoplankton is needed to drive mineralization. For standard model application, use KMPHYT = 0. |
| 71 | KDC | CBOD deoxygenation rate at 20EC, per day. |
| 72 | KDT | Temperature coefficient for carbonaceous deoxygenation in water column. Default = 1.0. |
| 73 | KDSC | Decomposition rate of carbonaceous BOD in the sediment at 20EC, per day. |
| 74 | KDST | Temperature coefficient for carbonaceous deoxygenation in the sediment. Default = 1.0. |
| 75 | KBOD | Half saturation constant for carbonaceous deoxygenation oxygen limitation. |
| 81 | OCRB | Oxygen to carbon ratio in phytoplankton, mg $O_2$/mg C. Default = 32/12. |
| 82 | K2 | Reaeration rate constant at 20EC for entire water body, $day^{-1}$. NOTE: If K2 is not entered, the reaeration rate will be calculated as the product of parameter REARSG and time function REAR. If parameter REARSG is not entered, the reaeration rate will be calculated from water velocity, depth, and wind velocity. |
| 91 | K71C | Mineralization rate of dissolved organic nitrogen, per day. |
| 92 | K71T | Temperature coefficient for K1013C. Default = 1.0. |

| | | |
|---|---|---|
| 93 | KONDC | Decomposition rate constant for organic nitrogen in the sediment at 20EC, per day. |
| 94 | KONDT | Temperature coefficient for decomposition of organic nitrogen in the sediment. Default = 1.0. |
| 95 | FON | Fraction of dead and respired phytoplankton nitrogen recycled to organic nitrogen. Default = 1.0. |
| 100 | K83C | Mineralization rate of dissolved organic phosphorus, per day. |
| 101 | K83T | Temperature coefficient for K58C. Default = 1.0. |
| 102 | KOPDC | Decomposition rate of organic phosphorus in the sediment at 20EC, per day. |
| 103 | KOPDT | Temperature coefficient for decomposition of organic phosphorus in the sediment. Default = 1.0. |
| 104 | FOP | Fraction of dead and respired phytoplankton phosphorus recycled to organic phosphorus. Default = 1.0. |

## 9.3 THE TOXIC CHEMICAL MODEL

A large number of constants are available to characterize the various chemical reactions at different levels of complexity. Very few need be specified for any one simulation. Table 3 summarizes the constants that may be used for equilibrium and kinetics level 1. Only two of these need be specified--PIXC(1,1) and either a half life or a first order rate constant. For equilibrium and kinetics level 2, no constants need be specified--partition coefficients and rate constants are entered via parameters.

For kinetics level 3, some general chemical constants are usually available, as summarized in Table 4. MOLWT, SOLG, and VAPRG are sometimes used in volatilization computations, while LKOW can be used in sorption calculations.

If a chemical is ionic, then constants from Table 5 may be specified. For each ionic specie I, SPFLG(I) and PKA(I) must be specified. EPKA(I) may also be given. Ionic speciation is

considered to be equilibrium level 5. The presence of ionic species requires significantly more data specifications for the remaining processes.

Hydrophobic sorption at equilibrium levels may be simulated with constants from Table 6. If LKOC is unknown, then LKOW, AO, and A1 should be specified (if A0 and A1 are unknown, they default to log 0.6 and 1, respectively). NUX(1) and PIXC(I,1) should be left out. Solids-dependent partitioning constitutes equilibrium level 4. NUX(1) should be given a value of around 1. For equilibrium level 5, ionic sorption constants must also be specified. Their locations are given in Table 7.

For kinetics level 3, constants must be specified for each relevant process. Constants for volatilization, biodegradation, alkaline hydrolysis, neutral hydrolysis, acid hydrolysis, oxidation, and photolysis are given in Tables 8, 9, 11, 13, 15, 17, 19, and 20, respectively. Constants for a user-specified extra reaction are given in Table 22. If ionic speciation is being considered, then ionic rate constants must also be specified for each existing ionic specie. Locations of these constants are given in Tables 10, 12, 14, 16, 18, 21, and 23.

For kinetics level 4, reaction products are simulated. Four cases are illustrated in Figure 6.1 (in Part A of this manual). Yield coefficients for each relevant process must be specified. Yield coefficients for chemical 1, 2, and 3 reactions are listed in Tables 24, 25, and 26. The reactions themselves need not be second order to simulate reaction products.

**TABLE 3 CONSTANTS FOR SIMPLE TOXI4 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 111 | 711 | 1311 | PIXC(1,1) | Constant partition coefficient for sorption to solids (class 1), $l_w$/kgs |
| | | | $K_i$: | First order loss rate constants, $day^{-1}$ |
| 140 | 740 | 1340 | KV | Volatilization |
| 141 | 741 | 1341 | KBW | Water column biodegradation |
| 142 | 742 | 1342 | KBS | Benthic biodegradation |
| 181 | 781 | 1381 | KHOH | Alkaline hydrolysis |
| 182 | 782 | 1382 | KHN | Neutral hydrolysis |
| 183 | 783 | 1383 | KHH | Acid hydrolysis |
| 256 | 856 | 1456 | KO | Oxidation |
| 287 | 887 | 1487 | KF | Photolysis |
| 571 | 1171 | 1771 | KE | Extra reaction |
| | | | $TH_i$ | Half lives for reactions, day |
| 143 | 743 | 1343 | THBW | Water column biodegradation |
| 144 | 744 | 1344 | THBS | Benthic biodegradation |
| 252 | 852 | 1452 | THHOH | Alkaline hydrolysis |
| 253 | 853 | 1453 | THHN | Neutral hydrolysis |
| 254 | 854 | 1454 | THHH | Acid hydrolysis |
| 257 | 857 | 1457 | THO | Oxidation |
| 289 | 889 | 1489 | THF | Photolysis |
| 572 | 1172 | 1772 | THE | Extra reaction |

**TABLE 4 GENERAL CHEMICAL CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 9 | 609 | 1209 | TDINT | Time interval at which rate constants are recomputed, days |
| 81 | 681 | 1281 | MOLWT | Molecular weight, g/mole |
| 82 | 682 | 1282 | SOLG | Solubility, mg/L |
| 83 | 683 | 1283 | VAPRG | Vapor pressure, torr |
| 84 | 684 | 1284 | LKOW | Log octanol-water partition coefficient, $L_o/L_w$ |

**TABLE 5 IONIZATION CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 85 | 685 | 1285 | SFLG(1) | flags indicating existence of ionic species +, ++, -, --; if SPFLG(I) = 1, ionic species I exists |
| 86 | 686 | 1286 | SFLG(2) | |
| 87 | 687 | 1287 | SFLG(3) | |
| 88 | 688 | 1288 | SFLG(4) | |
| 91 | 691 | 1291 | PKA(1) | For ionic species I, the constant in the integrated Van't Hoff equation describing temperature dependence of the equilibrium dependence of the equilibrium constant for dissociation: log K(I) = -PKA(I) + (EPKA(I)/2.303 R) * $[T*T_R/(T-T_R)]$ |
| 92 | 692 | 1292 | PKA(2) | |
| 93 | 693 | 1293 | PKA(3) | |
| 94 | 694 | 1294 | PKA(4) | |
| 95 | 695 | 1295 | EPKA(1) | For ionic species I, the activation energy of the dissociation reaction, kcal/mole |
| 96 | 696 | 1296 | EPKA(2) | |
| 97 | 697 | 1297 | EPKA(3) | |
| 98 | 698 | 1298 | EPKA(4) | |
| 99 | 699 | 1299 | TREFI | Reference temperature at which dissociation reaction constants were measured, EC |

**TABLE 6 SORPTION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 84 | 684 | 1284 | LKOW | Log 10 of the octanol-water partition coefficient, log ($L_w/L_o$) |
| 101 | 701 | 1301 | LKOC | Log 10 of the organic carbon partition coefficient, log ($L_w/kg_{oc}$) |
| 102 | 702 | 1302 | A0 | Intercept in the $K_{ow}$ - $K_{oc}$ correlation: log $K_{oc}$ = A0 @ log $K_{ow}$; default = log 0.6 |
| 103 | 703 | 1303 | A1 | Slope in the $K_{ow}$ - $K_{oc}$ correlation; default = 1.0 |
| 106 | 706 | 1306 | NUX(1) | Solids-dependent partitioning parameter ($L_x$) of the chemical onto solids; default = $10^{12}$ makes $K_p$ independent of solids concentration |
| 111 | 711 | 1311 | PIXC(1,1) | Solids-independent (limiting) partition coefficient $K_{po}$ for sorption to solid 1, $L_w/kg_s$ |
| 116 | 716 | 1316 | PIXC(2,1) | Solids-independent (limiting) partition coefficient $K_{po}$ for sorption to solid 2, $L_w/kg_s$ |
| 121 | 721 | 1321 | PIXC(3,1) | Solids-independent (limiting) partition coefficient $K_{po}$ for sorption to solid 3, $L_w/kg_s$<br>If = 0, $K_{po}$ for neutral chemical will be calculated from LKOC and parameter FOC |
| -- | -- | -- | PIDOC | Partition coefficient for DOC; for neutral chemical, KOC is used; L/kg |

**TABLE 7 LOCATION OF IONIC SORPTION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 106 | 706 | 1306 | NUX(1) | 0 | S |
| 107 | 707 | 1307 | NUX(2) | + | S |
| 108 | 708 | 1308 | NUX(3) | ++ | S |
| 109 | 709 | 1309 | NUX(4) | - | S |
| 110 | 710 | 1310 | NUX(5) | -- | S |
| 111 | 711 | 1311 | PIXC(1,1) | 0 | S1 |
| 112 | 712 | 1312 | PIXC(1,2) | + | S1 |
| 113 | 713 | 1313 | PIXC(1,3) | ++ | S1 |
| 114 | 714 | 1314 | PIXC(1,4) | - | S1 |
| 115 | 715 | 1315 | PIXC(1,5) | -- | S1 |
| 116 | 716 | 1316 | PIXC(2,1) | 0 | S2 |
| 117 | 717 | 1317 | PIXC(2,2) | + | S2 |
| 118 | 718 | 1318 | PIXC(2,3) | ++ | S2 |
| 119 | 719 | 1319 | PIXC(2,4) | - | S2 |
| 120 | 720 | 1420 | PIXC(2,5) | -- | S2 |
| 121 | 721 | 1421 | PIXC(3,1) | 0 | S3 |
| 122 | 722 | 1422 | PIXC(3,2) | + | S3 |
| 123 | 723 | 1423 | PIXC(3,3) | ++ | S3 |
| 124 | 724 | 1424 | PIXC(3,4) | - | S3 |
| 125 | 725 | 1425 | PIXC(3,5) | -- | S3 |
| 126 | 726 | 1426 | PIDOC(1) | + | B |
| 127 | 727 | 1427 | PIDOC(2) | ++ | B |
| 128 | 728 | 1428 | PIDOC(3) | - | B |
| 129 | 729 | 1429 | PIDOC(4) | -- | B |

**TABLE 8 VOLATILIZATION CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 136 | 736 | 1336 | XV | Volatilization option:<br>0 = no volatilization<br>1 = measured volatilization<br>2 = measured reaeration + O'Conner for gas transfer<br>3 = measured reaeration + MacKay for gas transfer<br>4 = calculated using O'Conner<br>5 = calculated using MacKay |
| 137 | 737 | 1337 | HENRY | Henry's constant, atm-$m^3$/mole |
| 138 | 738 | 1338 | KLT | Volatilization temperature correction factor, dimensionless |
| 139 | 739 | 1339 | KVOG | Measured ratio of volatilization to reaeration rates |
| 2 | 2 | 2 | WTYPE | Water body type (0 = flowing stream, river, or estuary; 1 = stagnant pond or lake) |
| 5 | 5 | 5 | AIRTMP | Multiplier for air temperature time function |
| 8 | 608 | 1208 | ATMOS | Atmospheric concentration of chemical, Fg/L |

**TABLE 9 SECOND ORDER BIODEGRADATION CONSTANTS FOR TOTAL FOR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 146 | 746 | 1346 | KBIO20(1,1) | Second-order 20EC biodegradation rate constant for aqueous, DOC-sorbed, and sediment-sorped phases, mL/cells-day |
| 151 | 751 | 1351 | KBIO20(2,1) | |
| 156 | 756 | 1356 | KBIO20(3,1) | |
| 161 | 761 | 1361 | Q10DIS(1) | Temperature correction factor for biodegradation of aqueous, DOC-sorbed, and sediment-sorbed phases; multiplication factor for 10EC temperature increase |
| 166 | 766 | 1366 | Q10DOC(1) | |
| 171 | 771 | 1371 | Q10PAR(1) | |

**TABLE 10 LOCATION OF IONIC BIODEGRADATION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 146 | 746 | 1346 | KBIO20(1,1) | 0 | W |
| 147 | 747 | 1347 | KBIO20(1,2) | + | W |
| 148 | 748 | 1348 | KBIO20(1,3) | ++ | W |
| 149 | 749 | 1349 | KBIO20(1,4) | - | W |
| 150 | 750 | 1350 | KBIO20(1,5) | -- | W |
| 151 | 751 | 1351 | KBIO20(2,1) | 0 | B |
| 152 | 752 | 1352 | KBIO20(2,2) | + | B |
| 153 | 753 | 1353 | KBIO20(2,3) | ++ | B |
| 154 | 754 | 1354 | KBIO20(2,4) | - | B |
| 155 | 755 | 1355 | KBIO20(2,5) | -- | B |
| 156 | 756 | 1356 | KBIO20(3,1) | 0 | S |
| 157 | 757 | 1357 | KBIO20(3,2) | + | S |
| 158 | 758 | 1358 | KBIO20(3,3) | ++ | S |
| 159 | 759 | 1359 | KBIO20(3,4) | - | S |
| 150 | 760 | 1460 | KBIO20(3,5) | -- | S |
| 161 | 761 | 1461 | Q10DIS(1) | 0 | W |
| 162 | 762 | 1462 | Q10DIS(2) | + | W |
| 163 | 763 | 1463 | Q10DIS(3) | ++ | W |
| 164 | 764 | 1464 | Q10DIS(4) | - | W |
| 165 | 765 | 1465 | Q10DIS(5) | -- | W |
| 166 | 766 | 1466 | Q10DOC(1) | 0 | B |
| 167 | 767 | 1467 | Q10DOC(2) | + | B |
| 168 | 768 | 1468 | Q10DOC(3) | ++ | B |
| 169 | 769 | 1469 | Q10DOC(4) | - | B |
| 170 | 770 | 1470 | Q10DOC(5) | -- | B |
| 171 | 771 | 1471 | Q10PAR(1) | 0 | S |
| 172 | 772 | 1472 | Q10PAR(2) | + | S |
| 173 | 773 | 1473 | Q10PAR(3) | ++ | S |
| 174 | 774 | 1474 | Q10PAR(4) | - | S |
| 175 | 775 | 1475 | Q10PAR(5) | -- | S |

**TABLE 11 SECOND ORDER ALKALINE HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 184 | 784 | 1384 | TREFH | Reference temperature at which hydrolysis rates were measured, EC |
| 186 | 786 | 1386 | KH2O(1,1,1) | Second order, 20EC alkaline hydrolysis rate constants for aqueous, DOC-sorbed , and sediment-sorbed phases, L/mole-day |
| 191 | 791 | 1391 | KH2O(1,2,1) | |
| 196 | 796 | 1396 | KH2O(1,3,1) | |
| 231 | 831 | 1431 | EHOH(1) | Activation energy for alkaline hydrolysis, kcal/mole |

**TABLE 12 LOCATION OF IONIC ALKALINE HYDROLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 186 | 786 | 1386 | KH2O(1,1,1) | 0 | W |
| 187 | 787 | 1387 | KH2O(1,1,2) | + | W |
| 188 | 788 | 1388 | KH2O(1,1,3) | ++ | W |
| 189 | 789 | 1389 | KH2O(1,1,4) | - | W |
| 190 | 790 | 1390 | KH2O(1,1,5) | -- | W |
| 191 | 791 | 1391 | KH2O(1,2,1) | 0 | B |
| 192 | 792 | 1392 | KH2O(1,2,2) | + | B |
| 193 | 793 | 1393 | KH2O(1,2,3) | ++ | B |
| 194 | 794 | 1394 | KH2O(1,2,4) | - | B |
| 195 | 795 | 1395 | KH2O(1,2,5) | -- | B |
| 196 | 796 | 1396 | KH2O(1,3,1) | 0 | S |
| 197 | 797 | 1397 | HK2O(1,3,2) | + | S |
| 198 | 798 | 1398 | KH2O(1,3,3) | ++ | S |
| 199 | 799 | 1399 | KH2O(1,3,4) | - | S |
| 200 | 800 | 1400 | KH2O(1,3,5) | -- | S |
| 231 | 831 | 1431 | EHOH(1) | 0 | A |
| 232 | 832 | 1432 | EHOH(2) | + | A |
| 233 | 833 | 1433 | EHOH(3) | ++ | A |
| 234 | 834 | 1434 | EHOH(4) | - | A |
| 235 | 835 | 1435 | EHOH(5) | -- | A |

**TABLE 13 SECOND ORDER NEURAL HYDROLYSIS CONSTANTS FOR TOTAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 184 | 784 | 1384 | TREFH | Reference temperature at which hydrolysis rates were measured, EC |
| 201 | 801 | 1401 | KH2O(2,1,1) | 20EC neutral hydrolysis rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, $day^{-1}$ |
| 206 | 806 | 1406 | KH2O(2,2,1) | |
| 211 | 811 | 1411 | KH2O(2,3,1) | |
| 236 | 836 | 1436 | EHN(1) | Activation energy for neutral hydrolysis, kcal/mole |

**TABLE 14 LOCATION OF IONIC NEUTRAL HYDROLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 201 | 801 | 1401 | KH2O(1,1,2) | 0 | W |
| 202 | 802 | 1402 | KH2O(2,1,2) | + | W |
| 203 | 803 | 1403 | KH2O(3,1,2) | ++ | W |
| 204 | 804 | 1404 | KH2O(4,1,2) | - | W |
| 205 | 805 | 1405 | KH2O(5,1,2) | -- | W |
| 206 | 806 | 1406 | KH2O(1,2,2) | 0 | B |
| 207 | 807 | 1407 | KH2O(2,2,2) | + | B |
| 208 | 808 | 1408 | KH2O(3,2,2) | ++ | B |
| 209 | 809 | 1409 | KH2O(4,2,2) | - | B |
| 210 | 810 | 1010 | KH2O(5,2,2) | -- | B |
| 211 | 811 | 1411 | KH2O(1,3,2) | 0 | S |
| 212 | 812 | 1412 | KH2O(2,3,2) | + | S |
| 213 | 813 | 1413 | KH2O(3,3,2) | ++ | S |
| 214 | 814 | 1414 | KH2O(4,3,2) | - | S |
| 215 | 815 | 1415 | KH2O(5,3,2) | -- | S |
| 236 | 836 | 1436 | EHN(1) | 0 | A |
| 237 | 837 | 1437 | EHN(2) | + | A |
| 238 | 838 | 1438 | EHN(3) | ++ | A |
| 239 | 839 | 1439 | EHN(4) | - | A |
| 240 | 840 | 1440 | EHN(5) | -- | A |

**TABLE 15 SECOND ORDER ACID HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 184 | 784 | 1384 | TREFH | Reference temperature at which hydrolysis rates were measured, EC |
| 216 | 816 | 1416 | KH2O(3,1,1) | Second order, 20EC acid hydrolysis rate constant for aqueous, DOC-sorbed and sediment-sorbed phases, L/mole-day |
| 221 | 821 | 1421 | KH2O(3,2,1) | |
| 226 | 826 | 1426 | KH2O(3,3,1) | |
| 241 | 841 | 1441 | EHH(1) | Activation energy for aced hydrolysis, kcal/mole |

**TABLE 16 LOCATION OF IONIC ACID HYDROLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 216 | 816 | 1416 | KH2O(3,1,1) | 0 | W |
| 217 | 817 | 1417 | KH2O(3,1,2) | + | W |
| 218 | 818 | 1418 | KH2O(3,1,3) | ++ | W |
| 219 | 819 | 1418 | KH2O(3,1,4) | - | W |
| 220 | 820 | 1420 | KH2O(3,1,5) | -- | W |
| 221 | 821 | 1421 | KH2O(3,2,1) | 0 | B |
| 222 | 822 | 1422 | KH2O(3,2,2) | + | B |
| 223 | 823 | 1423 | KH2O(3,2,3) | ++ | B |
| 224 | 824 | 1424 | KH2O(3,2,4) | - | B |
| 225 | 825 | 1425 | KH2O(3,2,5) | -- | B |
| 226 | 826 | 1426 | KH2O(3,3,1) | 0 | S |
| 227 | 827 | 1427 | KH2O(3,3,2) | + | S |
| 228 | 828 | 1428 | KH2O(3,3,3) | ++ | S |
| 229 | 829 | 1429 | KH2O(3,3,4) | - | S |
| 230 | 830 | 1430 | KH2O(3,3,5) | -- | S |
| 241 | 841 | 1441 | EHH(1) | 0 | A |
| 242 | 842 | 1442 | EHH(2) | + | A |
| 243 | 843 | 1443 | EHH(3) | ++ | A |
| 244 | 844 | 1444 | EHH(4) | - | A |
| 245 | 845 | 1445 | EHH(5) | -- | A |

**TABLE 17 SECOND ORDER OXIDATION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 258 | 858 | 1458 | TREFO | Reference temperature at which oxidation rates were measured, EC |
| 261 | 861 | 1461 | KOX2O(1,1) | Second-order, 20EC oxidation rate constant for aqueous, DOC-sorbed, and sediment_sorbed phases, L/mole-day |
| 266 | 866 | 1466 | KOX2O(2,1) | |
| 271 | 871 | 1471 | KOX2O(3,1) | |
| 276 | 876 | 1476 | EOX(1) | Activation energy for oxidation, kcal/mole |

**TABLE 18 LOCATION OF IONIC OXIDATION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 261 | 861 | 1461 | KOX2O(1,1) | 0 | W |
| 262 | 862 | 1462 | KOX2O(2,1) | + | W |
| 263 | 863 | 1463 | KOX2O(3,1) | ++ | W |
| 264 | 864 | 1464 | KOX2O(4,1) | - | W |
| 265 | 865 | 1465 | KOX2O(5,1) | -- | W |
| 266 | 866 | 1466 | KOX2O(1,2) | 0 | B |
| 267 | 867 | 1467 | KOX2O(2,2) | + | B |
| 268 | 868 | 1468 | KOX2O(2,2) | ++ | B |
| 269 | 869 | 1469 | KOX2O(4,2) | - | B |
| 270 | 870 | 1470 | KOX2O(5,2) | -- | B |
| 271 | 871 | 1471 | KOX2O(1,3) | 0 | S |
| 272 | 872 | 1472 | KOX2O(2,3) | + | S |
| 273 | 873 | 1473 | KOX2O(3,3) | ++ | S |
| 274 | 874 | 1474 | KOX2O(4,3) | - | S |
| 275 | 875 | 1475 | KOX2O(5,3) | -- | S |
| 276 | 876 | 1476 | EOX(1) | 0 | All |
| 277 | 877 | 1477 | EOX(2) | + | All |
| 278 | 878 | 1478 | EOX(3) | ++ | All |
| 279 | 879 | 1479 | EOX(4) | - | All |
| 280 | 880 | 1480 | EOX(5) | -- | All |

**TABLE 19 TOXI4 PHOTOLYSIS CONSTANTS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 286 | 886 | 1486 | XPHOTO | Photolysis option: 0 = no photolysis; 1 = computed from absorptivity; 2 = measured surface rate |
| 288 | 888 | 1488 | RFLATG | Latitude at which surface photolysis rate was measured, degree and tenths (option 2) |
| 291 | 891 | 1491 | KDPG(1) | Measured surface photolysis rate for neutral specie, $day^{-1}$ (option 2) |
| 296 | 896 | 1496 | LAMAXG(1) | Wavelength of maximum light absorption for neutral specie, nm (option 2) |
| 301-346 | 901-946 | 1501-1546 | ABS(K,1,L) | Molar absorptivity of neutral specie of chemical K at wavelength number L, L/mole-cm-ln10 (option 1) |
| 551 | 1151 | 1751 | QUANTG(1,1) | Quantum yield of dissolved neutral chemical |
| 556 | 1156 | 1756 | QUANTG(1,2) | Quantum yield of dissolved neutral chemical |
| 561 | 1161 | 1761 | QUANTG(3,1) | Quantum yield of dissolved neutral chemical |

L = Wavelength 1-46 (see Tables 7.12 and 7.13 in Part A of this document).

**TABLE 20 GLOBAL CONSTANTS FOR TOXI4 PHOTOLYSIS OPTION 1**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 1 | 601 | 1201 | TO | Julian date at beginning of run |
| 3 | 603 | 1203 | ELEVG | Average ground surface elevation, m |
| 4 | 604 | 1204 | LATG | Latitude of water body, degrees |
| 6 | 606 | 1206 | XLITE | Water surface light intensity option; 0 = do not compute light; 1 = annual average; 2 = average for month indicated by TO; 3 = monthly step function |
| 7 | 607 | 1207 | DFACG | Ratio of optical path length to vertical depth; 1.17 |
| 11-23 | 611-623 | 1211-1223 | CLOUDG(1) | Mean monthly cloudiness, in tenths of full sky coverage (0-10) |
| 24-36 | 624-636 | 1224-1236 | AIRTYG(1) | Mean monthly air mass type; 1 = rural, 2 = urban, 3 = maritime, 4 = tropospheric |
| 37-49 | 637-649 | 1237-1249 | RHUMG(1) | Mean monthly daylight relative humidity, percent |
| 50-62 | 650-662 | 1250-1262 | ATURBG(1) | Mean monthly atmospheric turbidity, in equivalent aerosol layer thickness km |
| 63-75 | 663-675 | 1263-1275 | OZONEG(1) | Mean monthly ozone content of atmosphere, in cm NTP (0.2 - 0.3) |

**TABLE 21 LOCATION OF IONIC PHOTOLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 291 | 891 | 1491 | KDPG(1) | 0 | A |
| 292 | 892 | 1492 | KDPG(2) | + | A |
| 293 | 893 | 1493 | KDPG(3) | ++ | A |
| 294 | 894 | 1494 | KDPG(4) | - | A |
| 295 | 895 | 1495 | KDPG(5) | -- | A |
| 296 | 896 | 1496 | LAMAXG(1) | 0 | A |
| 297 | 897 | 1497 | LAMAXG(2) | + | A |
| 298 | 898 | 1498 | LAMAXG(3) | ++ | A |
| 299 | 899 | 1499 | LAMAXG(4) | - | A |
| 300 | 900 | 1500 | LAMAXG(5) | -- | A |
| 301-346 | 901-946 | 1501-1546 | ABS(K,1,L) | 0 | A |
| 351-396 | 951-996 | 1551-1596 | ABS(K,2,L) | + | A |
| 401-446 | 1001-1046 | 1601-1646 | ABS(K,3,L) | ++ | A |
| 451-496 | 1051-1096 | 1561-1696 | ABS(K,4,L) | - | A |
| 501-546 | 1101-1146 | 1701-1746 | ABS(K,5,L) | -- | A |
| 551 | 1151 | 1751 | QUANTG(1,1) | 0 | W |
| 552 | 1152 | 1752 | QUANTG(1,2) | ++ | W |
| 553 | 1153 | 1753 | QUANTG(1,3) | + | W |
| 554 | 1154 | 1754 | QUANTG(1,4) | - | W |
| 555 | 1155 | 1755 | QUANTG(1,5) | -- | W |
| 556 | 1156 | 1756 | QUANTG(2,1) | 0 | B |
| 557 | 1157 | 1757 | QUANTG(2,2) | + | B |
| 558 | 11458 | 1758 | QUANTG(2,3) | ++ | B |

**TABLE 21 LOCATION OF IONIC PHOTOLYSIS CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 559 | 1159 | 1759 | QUANTG(2,4) | - | B |
| 560 | 1160 | 1760 | QUANTG(2,5) | -- | B |
| 561 | 1161 | 1761 | QUANTG(3,1) | 0 | S |
| 562 | 1162 | 1762 | QUANTG(3,2) | ++ | S |
| 563 | 1163 | 1763 | QUANTG(3,3) | + | S |
| 564 | 1164 | 1764 | QUANTG(3,4) | - | S |
| 565 | 1165 | 1765 | QUANTG(3,5) | -- | S |

**TABLE 22 EXTRA SECOND ORDER REACTIONS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 573 | 1173 | 1773 | TREFE | Reference temperature at which extra reaction rates were measured, EC |
| 576 | 1176 | 1776 | KE2O(1,1) | Second-order, 20EC extra reaction rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, 1/[E]-day |
| 581 | 1181 | 1781 | KE2O(2,1) | |
| 586 | 1186 | 1786 | KE2O(3,1) | |
| 591 | 1191 | 1791 | EEX(1) | Activation energy for extra reaction, kcal/mole |

**TABLE 2.5.23 LOCATION OF IONIC EXTRA REACTION CONSTANTS**

| Constant Number | | | | | |
|---|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Ionic Specie | Sorptive Phase |
| 576 | 1176 | 1776 | KE2O(1,1) | 0 | W |
| 577 | 1177 | 1777 | KE2O(1,2) | + | W |
| 578 | 1178 | 1778 | KE2O(1,3) | ++ | W |
| 579 | 1179 | 1779 | KE2O(1,4) | - | W |
| 580 | 1180 | 1780 | KE2O(1,5) | -- | W |
| 581 | 1181 | 1781 | KE2O(2,1) | 0 | B |
| 582 | 1182 | 1782 | KE2O(2,2) | + | B |
| 583 | 1183 | 1783 | KE2O(2,3) | ++ | B |
| 584 | 1184 | 1784 | KE2O(2,4) | - | B |
| 585 | 1185 | 1785 | KE2O(2,5) | -- | B |
| 586 | 1186 | 1786 | KE2O(3,1) | 0 | S |
| 587 | 1187 | 1787 | KE20(3,2) | + | S |
| 588 | 1188 | 1788 | KE2O(3,3) | ++ | S |
| 589 | 1189 | 1789 | KE2O(3,4) | - | S |
| 590 | 1190 | 1790 | KE2O(3,5) | -- | S |
| 591 | 1191 | 1791 | EEX(1) | 0 | All |
| 592 | 1192 | 1792 | EEX(2) | + | All |
| 593 | 1193 | 1793 | EEX(3) | ++ | All |
| 594 | 1194 | 1794 | EEX(4) | - | All |
| 595 | 1195 | 1795 | EEX(5) | -- | All |

**TABLE 24 YIELD CONSTANTS FOR CHEMICAL 1 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| | | | Y( )12: | Yield coefficient for production of $C_2$ from $C_1$, $mgC_2/mgC_1$ |
| 176 | | | YBW12 | Water column biodegradation |
| 178 | | | YBS12 | Benthic biodegradation |
| 246 | | | YHOH12 | Alkaline hydrolysis |
| 248 | | | YHN12 | Neutral hydrolysis |
| 250 | | | YHH12 | Acid hydrolysis |
| 281 | | | YOX12 | Oxidation |
| 566 | | | YF12 | Photolysis |
| 596 | | | YE12 | Extra reaction |
| | | | Y( )13: | Yield coefficient for production of $C_3$ from $C_1$, $mgC_2/mgC_1$ |
| 177 | | | YBW13 | Water column biodegradation |
| 179 | | | YBS13 | Benthic biodegradation |
| 247 | | | YHOH13 | Alkaline hydrolysis |
| 249 | | | YHN13 | Neutral hydrolysis |
| 251 | | | YHH13 | Acid hydrolysis |
| 282 | | | YOX13 | Oxidation |
| 567 | | | YF13 | Photolysis |
| 597 | | | YE13 | Extra reaction |

**TABLE 25 YIELD CONSTANTS FOR CHEMICAL 2 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| | | | Y( )21: | Yield coefficient for production of $C_1$ from $C_2$, $mgC_2/mgC_1$ |
| | 776 | | YBW21 | Water column biodegradation |
| | 778 | | YBS21 | Benthic biodegradation |
| | 846 | | YHOH21 | Alkaline hydrolysis |
| | 848 | | YHN21 | Neutral hydrolysis |
| | 850 | | YHH21 | Acid hydrolysis |
| | 881 | | YOX21 | Oxidation |
| | 1166 | | YF21 | Photolysis |
| | 1196 | | YE21 | Extra reaction |
| | | | Y( )23: | Yield coefficient for production of $C_3$ from $C_2$, $mgC_3/mgC_2$ |
| | 777 | | YBW23 | Water column biodegradation |
| | 779 | | YBS23 | Benthic biodegradation |
| | 847 | | YHOH23 | Alkaline hydrolysis |
| | 849 | | YHN23 | Neutral hydrolysis |
| | 851 | | YHH23 | Acid hydrolysis |
| | 882 | | YOX23 | Oxidation |
| | 1167 | | YF23 | Photolysis |
| | 1197 | | YE23 | Extra reaction |

**TABLE 26 YIELD CONSTANTS FOR CHEMICAL 3 REACTIONS**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| | | | Y( )31: | Yield coefficient for production of $C_1$ from $C_3$, $mgC_1/mgC_2$ |
| | | 1376 | YBW31 | Water column biodegradation |
| | | 1378 | YBS31 | Benthic biodegradation |
| | | 1446 | YHOH31 | Alkaline hydrolysis |
| | | 1448 | YHN31 | Neutral hydrolysis |
| | | 1450 | YHH31 | Acid hydrolysis |
| | | 1481 | YOX31 | Oxidation |
| | | 1766 | YF31 | Photolysis |
| | | 1796 | YE31 | Extra reaction |
| | | | Y( )32: | Yield coefficient for production of $C_2$ from $C_3$, $mgC_2/mgC_3$ |
| | | 1377 | YBW32 | Water column biodegradation |
| | | 1379 | YBS32 | Benthic biodegradation |
| | | 1447 | YHOH32 | Alkaline hydrolysis |
| | | 1449 | YHN32 | Neutral hydrolysis |
| | | 1451 | YHH32 | Acid hydrolysis |
| | | 1482 | YOX32 | Oxidation |
| | | 1767 | YF32 | Photolysis |
| | | 1797 | YE32 | Extra reaction |

# CHAPTER 10

## DATA GROUP I: KINETIC TIME FUNCTIONS

The definition of the kinetic time functions will vary depending upon the structure and the kinetics of the systems comprising each model. The input format, however, is constant. Time functions are input as piecewise linear functions.

### 10.1 RECORD FORMATS

Record 1--Number of Time Functions (I10, 70X)

NFUNC = number of time functions required by the model. If no time functions are to be input, set NFUNC equal to zero and go to Data Group J. (I10)

TITLE = name of data group. (70X)

*Records 2-3 are input as a group NFUNC times:*

Record 2--Time Function Descriptions (A5, 2I5)

ANAME(ISC) = an optional one to five alphanumeric character descriptive name for the time function I. (A5)

NOBRK(ISC) = number of breaks used to describe the time function I. (I5)

ISC = number identifying the time function; these numbers are set by the model developer. (I5)

Record 3--Time Functions (4(2F10.0))

VALT(K) = value of time function ISC at time T(K). (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK). (F10.0)

*Record 3 is repeated NOBRK(ISC)/4 times.*

Record 1 in entered once in Data Group I. Records 2 and 3, as a set, are repeated NFUNC times. Within each NFUNC set, Record 2 is input once and Record 3 uses as many 80-space lines as needed to input NOBRK entries. Four entries (four VALK(K)-T(K) pairs) will fit on each 80-space line.

## 10.2 THE EUTROPHICATION MODEL

Listed below are the 22 time functions available for eutrophication. Only TEMP(1) is required for Level 1 and 2 analyses. For Level 3 analyses, TFNH4, VELN(1), and WIND may be added (WIND is needed only for calculating reaeration in non-flowing water bodies such as lakes). For analyses at Level 4 and above, ITOT, F, KE, and TFPO4 should be used. For resolution of spatial variability in temperature, light extinction, and water velocity the four TEMP functions, the five KE functions, and the four VELN functions may be used.

Many of the time functions operate in conjuction with a parameter "pointer" in Data Group G. The parameter value specifies which of several time functions for temperature, light extinction, or water velocity are to be associated with each segment. Time functions 1-4 are the four temperature functions available for parameter TMPFN. Time functions 8-12 are the five extinction coefficient functions for parameter KEFN. Functions 15-18 are the four water velocity options for VELFN.

| ISC | ANAME | Defininion and Units |
|---|---|---|
| 1 | TEMP(1) | Time-variable temperature function 1. TEMP(K) can be either a normalized function or an actual temperature in EC, depending upon the definition of the parameter multiplier TMPSG(ISEG). |
| 2 | TEMP(2) | Time-variable temperature function 2, unitless or EC. |
| 3 | TEMP(3) | Time-variable temperature function 3, unitless or EC. |
| 4 | TEMP(4) | Time-variable temperature function 4, unitless or EC. |
| 5 | ITOT | Total daily solar radiation, langleys. |

| | | |
|---|---|---|
| 6 | F | Fraction of day with sufficient light for growth, days. |
| 7 | WIND | Wind velocity, m/sec. |
| 8 | KE(1) | Time-variable extinction coefficient function 1. This can be either a normalized function or an actual extinction coefficient in $m^{-1}$, depending upon the definition of the parameter multiplier KESG(ISEG). |
| 9 | KE(2) | Time-variable extinction coefficient function 2, unitless or $m^{-1}$. |
| 10 | KE(3) | Time-variable extinction coefficient function 3, unitless or $m^{-1}$. |
| 11 | KE(4) | Time-variable extinction coefficient function 4, unitless or $m^{-1}$. |
| 12 | KE(5) | Time-variable extinction coefficient function 5, unitless or $m^{-1}$. |
| 13 | TFNH4 | Normalized ammonium flux from bed, unitless. |
| 14 | TFPO4 | Normalized phosphate flux from bed, unitless. |
| 15 | VELN(1) | Time variable velocity function 1, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C. |
| 16 | VELN(2) | Time variable velocity function 2, m/sec. |
| 17 | VELN(3) | Time variable velocity function 3, m/sec. |
| 18 | VELN(4) | Time variable velocity function 4, m/sec. |
| 19 | ZOO | Herbivorous zooplankton population, mgC/L. |
| 20 | SALFN | Time variable salinity function, mg/l. This function gets multiplied by the segment specific salinity multiplier entered in the parameter sector. |
| 21 | AIRTMP | Time variable ambient air temperature, EC. This provides air temperature data for the wind driven |

reaeration algorithms and is required.

22 XICEVR This is the time variable ice cover function, %. This provides the percentage of water surface area available for reaeration. Note that 100% (entered as 1.0) indicates all surface area is available for reaeration.

## 10.3 THE TOXIC CHEMICAL MODEL

Listed below are the 17 time functions available in TOXI4. The parameters and time functions interact in such away to allow the user segment specific control of environmental data. For more details see the parameter input section.

Two of the time functions operate in conjuction with a parameter "pointer" in Data Group G. The parameter value specifies which of four time functions for temperature or water velocity are to be associated with each segment. Time functions 1-4 are the four temperature functions available for parameter TMPFN. Time functions 5-8 are the four water velocity options for VELFN.

| ISC | ANAME | VALT(ISC) |
|---|---|---|
| 1 | TEMPN(1) | Time-variable temperature function 1. TEMPN(K) can be either a normalized function or an actual temperature in EC, depending upon the definition of the parameter multiplier TEMP(ISEG). |
| 2 | TEMPN(2) | Time variable temperature function 2, unitless or EC. |
| 3 | TEMPN(3) | Time variable temperature 3, unitless or EC. |
| 4 | TEMPN(4) | Time variable temperature 4, unitless or EC. |
| 5 | VELN(1) | Time variable velocity function 1, m/sec. This velocity is added to the net velocity VELOCG(ISEG) parameters read in Data Group C. |
| 6 | VELN(2) | Time variable velocity function 2, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C. |

| | | |
|---|---|---|
| 7 | VELN(3) | Time variable velocity function 3, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C. |
| 8 | VELN(4) | Time variable velocity function 4, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C. |
| 9 | WINDN | Time variable wind function, m/sec. This time function is multiplied by the segment specific wind multiplier WVEL entered in the parameter section. |
| 10 | PHNW | Time variable ph function. This time function is multiplied by the segment specific ph multiplier ph enter in the parameter section. |
| 11 | PHNS | Normalized benthic pH function, dimensionless. This is multiplied by the segment pH multiplier PH(ISEG) for benthic segments. |
| 12 | REARN | Time variable reaeration coefficient, per day. This variable is multiplied by the segment specific variable REAR. entered in the parameter section. |
| 13 | AIRTMPN | Air temperature, C. Used for calculating reaeration rate. |
| 14 | CHLN | Phytoplankton chlorophyll concentration, mg/l. This variable is multiplied by the segment specific variable CHPHL entered in the parameter section |
| 15 | PHTON | Normalized light intensity, dimensionless. This is used for photolysis option 2 to adjust the measured rate constant under controlled light intensity to a predicted rate constant under ambient light intensity. |
| 16 | BACNW | Time variable bacteria concentration in the water column, mg/l. This is multiplied by the segment specific multiplier BAC entered in the parameter section. |

| | | |
|---|---|---|
| 17 | BACNS | Normalized benthic bacteria function, dimensionless. This is multiplied by the segment bacteria multiplier BAC(ISEG) for benthic segments. |

For kinetics levels 1 and 2, no time functions need be specified. For kinetics level 3, time functions for each relevant process may be specified. TEMPN can affect all reactions. Volatilization option 1 uses REARN. Volatilization options 4 and 5 use WINDN and AIRTMPN. Volatilization options 2 and 3 use either VELN or REARN. Photolysis option 1 uses CHLN; photolysis option 2 requires PHTON. Hydrolysis and ionization use PHNW and PHNS. Biodegradation uses BACNW and BACNS. Functions not specified default to 1.0.

# CHAPTER 11

# DATA GROUP J: INITIAL CONDITIONS

## 11.1 RECORD FORMATS

The initial conditions are the segment concentrations and densities for the state variables at time zero (the start of the simulation).

*Records 1-2 are input as a group NOSYS times:*

Record 1--System Information (A40, I5, F5.0, F10.0, 20X)

| | | |
|---|---|---|
| CHEML | = | chemical or system name (A40). |
| IFIELD | = | solids field (3, 4, or 5) that transports this system in its pure or sorbed form (I5). |
| DSED | = | density of system; 0.0 for chemical, 0.5-2.5 for solids, kg/L. (F5.0). |
| CMAX | = | maximum concentration allowed, mg/L. (F10.0) |
| TITLE | = | name of data group. (20X) |

Record 2--Initial Conditions (3(A5, 2F10.0))

| | | |
|---|---|---|
| ANAME(K) | = | an optional one to five alphanumeric character descriptive name or number identifying segment K. (A5) |
| C(ISYS,K) | = | initial concentration in segment K of system ISYS in the appropriate units, mg/L. (F10.0) |
| DISSF | = | dissolved fraction of chemical in segment K. (F10.0) |

*Record 2 is repeated NOSEG/3 times.*

Records 1 and 2 are a set and will be repeated NOSYS times. Within each NOSYS set, Record 2 will use as many 80-space lines as needed to input NOSEG entries. Three entries (ANAME-C-DISSF) will fit on one line. After NOSEG entries have been entered in a NOSYS set, begin the next NOSYS set on the following line. If

ICFL = 2 in Data Group A, initial conditions are read from the restart file (*.RST, where * is the input data set name), and Data Group J should not be included in the input data set.

## 11.2 THE EUTROPHICATION MODEL

Data Group J is input as a unit 8 times, once for each system. In record 1, solids transport fields must be specified for the particulate fraction of each system. In EUTRO4, solids field 3 is equated to particulate organic matter, solids field 4 is phytoplankton, and solids field 5 is inorganic sediment. The following specifications, then, are recommended for systems 1 through 8:

IFIELD(1) = 3 (solids field 1)

IFIELD(2) = 5 (solids field 3)

IFIELD(3) = 5 (solids field 3)

IFIELD(4) = 4 (solids field 2)

IFIELD(5) = 3 (solids field 1)

IFIELD(6) = 5 (solids field 3)

IFIELD(7) = 3 (solids field 1)

IFIELD(8) = 3 (solids field 1)

The density of each solid field must also be specified in record 1. This property is not used in EUTRO4. The user may enter 1.0 for the density of each system.

The dissolved fraction of each system in each segment must be specified in record 2. The user should take care to specify the dissolved fractions for dissolved oxygen (system 6) of 1.0 and the dissolved fractions for phytoplankton (system 4) of 0.0.

## 11.3 THE TOXIC CHEMICAL MODEL

Data Group J is input as a unit NOSYS times, once for each system. In record 1, solids transport fields must be specified for each solid (i.e.- variables 2, 3, and 4). While solids transport fields are also specified for each chemical (variables

1, 5, and 6), the values are nominal. TOXI4 will calculate the actual transport of the sorbed chemical fractions using internal partitioning relationships.

In Record 2, the dissolved fraction of each system in each segment must be specified. These values should be 1.0 for each solid variable (2, 3, and 4). Dissolved fraction values for each chemical are nominal. TOXI4 will calculate the actual dissolved fractions using internal partitioning relationships.

# CHAPTER 12

# WASP5 OUTPUT

## 12.1 GENERAL CONSIDERATIONS

WASP5 simulations produce several files that may be examined by the user. These files use the file name of the input data set with a unique extension. The most important of these are the simulation result files -- *.TDF for TOXI5 and *.EDF for EUTRO5 (i.e.- a TOXI5 input dataset named POND.INP produces an output file named POND.TDF). These formatted files contain all kinetic display variables for each segment at each print interval throughout the simulation. These display variables include state variable concentrations along with a selection of calculated variables and rates. Available display variables for EUTRO5 and TOXI5 are summarized in the eutrophication and toxics sections below.

The simulation results files can be processed with the post processing programs available with the WISP package or the W4DSPLY program which is provided with the mainframe version. The program will prompt the user for information.

Other files created by a WASP simulation include *.OUT, *.TRN, *.MSB, and *.RST (where * is the name of the input data set). The OUT file contains a record of the input data plus any simulation error messages that may have been generated. It may be examined from WISP by selecting the OUT file (alt-F, curser to OUT, return, escape) and using the BROWSE command from the menu.

The TRN file contains a set of transport-associated variables for each segment at each print interval throughout the simulation. These variables include the time step (day), calculated maximum time steps (day), segment volumes ($m^3$), segment flows ($m^3$/sec), flow changes ($m^3$/sec), time constants for segment flow ($day^{-1}$), segment exchange flows ($m^3$/sec), the time constant for segment exchanges ($day^{-1}$), the segment dispersion coefficient ($m^3$/sec), and the numerical dispersion coefficient ($m^2$/sec).

The MSB file contains a mass balance record for one designated system in the model network as a whole (in kg). For each print interval, this file records the accumulated mass in from advection, dispersion, and loading; the accumulated mass out

through advection, dispersion, burial (or volatilization, and kinetic transformation; the total resident mass; and the residual (unaccounted for) mass.

The RST file contains a snapshot of volumes and concentrations of each system in each segment at the conclusion of the simulation. This file can be read by WASP5 to continue a series of simulations.

## 12.2 THE EUTROPHICATION MODEL

The standard WASP5 output files were summarized above. EUTRO5 stores in the EDF file 42 display variables. These variables are listed below. To examine these variables, the user may run WASP5 postprocessor.

**EUTRO4 DISPLAY VARIABLES**

| Number | Variable | Definition |
|---|---|---|
| 1 | DEPTHG(I) | Segment Depth, m |
| 2 | STP | Water Temperature, EC |
| 3 | WIND | Wind Speed, m/sec |
| 4 | VEL | Water Velocity, m/sec |
| 5 | DO | Dissolved Oxygen, mg/L |
| 6 | DOMIN | DO Minimum, mg/L |
| 7 | DOMAX | DO Maximum, mg/L |
| 8 | CS | DO Saturation, mg/L |
| 9 | PERSAT | Percent DO Saturation, % |
| 10 | KA | Effect Reaeration Rate, $day^{-1}$ |
| 11 | K2WSAVE | Wind Driven Reaeration, $day^{-1}$ |
| 12 | K2HSAVE | Current Driven Reaeration, $day^{-1}$ |
| 13 | SOD1D(I) | Sediment Oxygen Demand, g/m2/day |
| 14 | CBOD | CBOD, mg/L |
| 15 | BOD5 | BOD5, mg/L |
| 16 | UBOD | Ultimate BOD, mg/L |
| 17 | TEMPBOD | BOD decay rate constant, $day^{-1}$ |

**EUTRO4 DISPLAY VARIABLES**

| Number | Variable | Definition |
|---|---|---|
| 18 | PHYT | Phytoplankton Carbon Biomass, mg/L |
| 19 | TCHLAX | Phytoplankton Chlorophyll **a**, Fg/L |
| 20 | GP1 | Phytoplankton Growth Rate, $day^{-1}$ |
| 21 | DP1 | Phytoplankton Death Rate, $day^{-1}$ |
| 22 | SR19P | Phytoplankton DO Production, mg/L/day |
| 23 | SK19P | Phytoplankton DO Consumption, mg/L/day |
| 24 | CCHL1 | Phyt. Carbon to Chl. **a** Ratio, mg/mg |
| 25 | RLGHTS(I,1) | Light Limit for Phyt. Growth |
| 26 | RNUTR | Nutrient Limit for Phyt. Growth |
| 27 | XEMP1 | Phosphorus Limit for Phyt. Growth |
| 28 | XEMP2 | Nitrogen Limit for Phyt. Growth |
| 29 | ITOTMP | Light at Segment Surface, langleys/day |
| 30 | IS1 | Saturating Light Intensity, langleys/day |
| 31 | IAV | Light at Top of Segment, langleys/day |
| 32 | IAVBOT | Light at Bottom of Segment, langleys/day |
| 33 | NH3 | Ammonia Nitrogen, mg/L |
| 34 | NO3 | Nitrate Nitrogen, mg/L |
| 35 | CN | Available Inorganic Nitrogen, mg/L |
| 36 | TON | Total Organic Nitrogen, mg/L |
| 37 | TIN | Total Inorganic Nitrogen, mg/L |
| 38 | TN | Total Nitrogen, mg/L |
| 39 | OPO4 | Available Inorganic Phosphorus, mg/L |
| 40 | TIP | Total Inorganic Phosphorus, mg/L |
| 41 | TOP | Total Organic Phosphorus, mg/L |
| 42 | OP | Nonliving Organic Phosphorus, mg/L |

## 12.3 THE TOXIC CHEMICAL MODEL

The standard WASP5 output files were summarized in Section 2.3. TOXI5 stores in the TDF file 18, 30, or 42 kinetic display variables, depending on whether 1, 2, or 3 chemicals were simulated. These variables are defined below. To examine these variables in tabular form, the user may run the WASP5 postprocessor as explained above.

**TOXI4 DISPLAY VARIABLES**

| Constant Number | | | | |
|---|---|---|---|---|
| $C_1$ | $C_2$ | $C_3$ | Variable | Definition |
| 1 | | | TOTSOSL | Total solids concentration, mg/L |
| 2 | | | SOLID 1 | Solids type 1 concentration, mg/L |
| 3 | | | SOLID 2 | Solids type 2 concentration, mg/L |
| 4 | | | SOLID 3 | Solids type 3 concentration, mg/L |
| 5 | | | STEMP | Segment temperature, EC |
| 6 | | | ITYPE | Segment type (1, 2, 3, or 4) |
| 7 | 19 | 31 | TOTCHEM | Total chemical concentration (1, 2, or 3), Fg/L |
| 8 | 20 | 32 | TOTDIS | Dissolved chemical concentration, Fg/L |
| 9 | 21 | 33 | TOTDOC | DOC-sorbed chemical concentration, Fg/L |
| 10 | 22 | 34 | TOTPAR | Total sorbed chemical concentration, Fg/L |
| 11 | 23 | 35 | TOTPAR1 | Total sorbed chemical concentration, Fg/kg |
| 12 | 24 | 36 | TOTION | Total ionic chemical concentration, Fg/L |
| 13 | 25 | 37 | KBIO | Biodegradation rate constant, $day^{-1}$ |
| 14 | 26 | 38 | KHYD | Total hydrolysis rate constant, $day^{-1}$ |
| 15 | 27 | 39 | KFOT | Photolysis rate constant, $day^{-1}$ |
| 16 | 28 | 40 | KVOL | Volatilization rate constant, $day^{-1}$ |
| 17 | 29 | 41 | KOX | Oxidation rate constant, $day^{-1}$ |
| 18 | 30 | 42 | KEXT | Extra rate constant, $day^{-1}$ |